Galactic Chemical Evolution and Radioactivities in the Early Solar System

Michael Joseph Bojazi
Clemson University, mbojazi@yahoo.com

Follow this and additional works at: https://tigerprints.clemson.edu/all_dissertations

Recommended Citation
https://tigerprints.clemson.edu/all_dissertations/2240

This Dissertation is brought to you for free and open access by the Dissertations at TigerPrints. It has been accepted for inclusion in All Dissertations by an authorized administrator of TigerPrints. For more information, please contact kokeefe@clemson.edu.
GALACTIC CHEMICAL EVOLUTION AND RADIOACTIVITIES IN THE EARLY SOLAR SYSTEM

A Dissertation
Presented to
the Graduate School of
Clemson University

In Partial Fulfillment
of the Requirements for the Degree
Doctor of Philosophy
Physics

by
Michael J. Bojazi, Jr.
December 2018

Accepted by:
Dr. Bradley S. Meyer, Committee Chair
Dr. Sean D. Brittain
Dr. Dieter H. Hartmann
Dr. Jeremy R. King
Dr. Chad E. Sosolik
Abstract

A proper accounting for the inferred abundances of the roughly 10 short-lived radioactivities in the early Solar System requires a comparison to their expectations from an appropriate model of Galactic chemical evolution (GCE) (e.g., [115]). Because the timescale for mixing between phases in the interstellar medium (ISM) is comparable to the lifetime of many of the short-lived radioactivities, the GCE model should follow different ISM phases and the mixing between them. The model must also account for the long temporal distance between the rare astrophysical events that produce many of the short-lived species, such as mass transfer from a low-mass star to its white-dwarf companion leading to a thermonuclear supernova or a binary neutron-star collision that may lead to production of r-process isotopes. In this work, we present expectations for the abundances of short-lived radioactivities in the early Solar System with a detailed GCE model inclusive of these effects.

Our model, as discussed in chapter 6 with a star-formation rate consistent with the current Galactic-disk gas fraction and mixing time for ejecta into star-forming regions of $\sim 10^7$ yr, provides abundances of $^{53}$Mn and $^{60}$Fe in Solar-mass stars forming at the time of the Sun’s birth that are in reasonable agreement with the inferred values [115][245]. Corroborated by many studies, the $^{26}$Al/$^{27}$Al ratio is too low and requires special injection (e.g., [84]). In our model, as the $^{41}$Ca abundance varies widely, the observed value [151] cannot be accommodated, although this species may be injected along with $^{26}$Al [27]. The model has difficulty accounting for the abundance of $^{36}$Cl, which may be produced by irradiation in the early Solar System [270]. We can account for the abundances of the r-process radioactivities, $^{107}$Pd and $^{129}$I, as products of binary neutron-star mergers and interpret the abundance of $^{182}$Hf via production in the shells of massive stars, which also contribute to the abundances of $^{107}$Pd and $^{129}$I.
Dedication

I dedicate this thesis to my parents, brothers John and Frank, and sister Dee. Beginning as teenagers, our parents raised 3 boys solely on our father’s salary of an electrician while our mother attended law school. Even in the face of divorce, for which I did not take well, I graduated high school at the top of my class and was awarded a generous scholarship and multiple grants to attend college. I always knew I wanted to study science. As I near the completion of my time here at Clemson, I dedicate this work to them.

Since graduating college, I always found myself far from home of Philadelphia, PA, where my family still resides. No matter how far the distance separating us, I could always count on my siblings to be there for me regardless. Their support without actually physically being present meant that much more. I dedicate this work to them as well.
Acknowledgments

First and foremost, I would like to thank my advisor, Dr. Bradley S. Meyer, for his guidance and support as I set out to accomplish all objectives during my time here at Clemson University. From coursework and the Ph.D. qualifying exam, my first publication after earning my Master’s degree and the subsequent collaborations following multiple travel excursions across the country, and finally to my Ph.D. project as I prepare to defend, never have I found him to be frustrated or annoyed whether I stopped by his office for a quick question or sought clarification on a complicated topic. It is this demeanor of his that has made working with him a true pleasure and my time in the physics graduate program a delight.

Secondly, I would like to thank the Department of Physics and Astronomy for their support over the years. In particular, I would have been lost without Celeste Hackett, Amanda Ellenburg, and Lori Rholetter sharing the role as my “South Carolina Mom” and advising me about the department and life in general. Thank you, ladies. A few years into the program, Dr. Jason Brown generously offered me a cup of coffee. Since then, he has graciously kept me caffeinated free of charge. As a graduate student getting by on a stipend, his kind gesture made a huge difference to my budget and for that, I will always be grateful. And since that first cup of coffee years ago, we have developed a friendship I feel will continue well beyond my time at Clemson. Thank you, Dr. Brown. I would like to thank Dr. Dieter Hartmann for his patience with my struggles in his first-year Classical Mechanics course. I would like to thank Dr. Chad Sosolik for engaging in friendly banter with me whenever our paths crossed in the PandA Cafe. And thank you to Dr. Jeremy King for always welcoming me in his home to watch the latest WWE pay-per-view event, as the cost of such broadcasts was far outside my budget. My interactions with the faculty and staff of the department have reflected positively on my character by inspiring me to achieve my goals while selflessly helping others to do the same.

Finally, I would like to thank Clemson University for the opportunity to pursue my degrees in a wonderfully-accommodating environment. To ensure success in the program, and, life in general, one must find a balance between work and extracurricular activities. Clemson University has always hosted a plethora of events for graduate students to attend and meet other students. I am grateful for all the people I became friends with through such events. Knowing them has been a joy and absolutely made graduate school much more fun.
# Table of Contents

Title Page .................................................................................. i
Abstract .................................................................................. ii
Dedication .................................................................................. iii
Acknowledgments ....................................................................... iv
List of Tables ............................................................................ viii
List of Figures ............................................................................ ix

1 Introduction ................................................................. 1
   1.1 The Fundamental Problem of the Short-Lived Radioactivities ............. 1
   1.2 Aluminum-Magnesium Isochron .................................................. 2
   1.3 Outline of this Work ................................................................. 10

2 Nucleosynthesis of the Galactic Radioactivities .................. 11
   2.1 AGB Evolution ........................................................................ 11
   2.2 Aluminum-26 ......................................................................... 12
   2.3 Chlorine-36 and Calcium-41 ...................................................... 15
   2.4 Manganese-53 ........................................................................ 17
   2.5 Iron-60 .................................................................................. 19
   2.6 Iodine-129 and Hafnium-182 .................................................... 21
   2.7 Palladium-107 ....................................................................... 22
   2.8 Samarium-146 ...................................................................... 23
   2.9 Plutonium-244 ..................................................................... 24

3 Yields .................................................................................. 25

4 An Introduction to Galactic Chemical Evolution .................. 27
   4.1 Evolution of Gas Mass ............................................................. 28
   4.2 Evolution of Primary Mass Fraction ......................................... 29
   4.3 Evolution of Secondary Mass Fraction ....................................... 32

5 Comparison of Simple GCE Models with ICE .................... 36
   5.1 IRA: Contradiction between Analytic and Numerical Models ............ 37
   5.2 The Fix .................................................................................. 39
   5.3 From Extreme (Instantaneous/Infinite) to Realistic (Finite) Lifetimes .... 46

6 Inhomogeneous GCE ......................................................... 50
7 Analysis of the Galactic Chemical Evolution of the Short-Lived Radioactivities 59
7.1 Halo + Single ISM Zone ................................................................. 59
7.2 Solar-Mass Stellar Composition: 1 ISM Zone vs. 32 ISM Zones .................. 67

8 Analysis of the Galactic Chemical Evolution of the Long-Lived Radioactivities . 84
8.1 Potassium-40 ................................................................. 84
8.2 Uranium-235 and Uranium-238 ...................................................... 85
8.3 Thorium-232 ................................................................. 87
8.4 Future Analysis ................................................................. 88

9 Conclusions ................................................................. 89

Appendices ................................................................. 91
A Nuclear and Atomic Masses and Binding Energies ................................. 92
A.1 Definition of Mass Defect and Binding Energy ....................................... 92
A.2 Binding Energy as Applied Work .......................................................... 93
A.3 Determination of Binding Energies and Nuclear Masses ...................... 94
A.4 Binding Energy per Nucleon and Causes of Observable Patterns ............ 96
A.5 Historical Formulation of Binding Energy and Nuclear Mass Equations .... 99

B Nuclear Decay ................................................................. 104
B.1 Origins of the Radioactive Decay Law ................................................ 104
B.2 Numerics of the Radioactive Decay Law ............................................... 107
B.3 Types and Energetics of Radioactive Decay .......................................... 114

C Sampling a Probability Distribution .................................................. 134
C.1 From Discrete to Continuous Random Variables ................................... 134
C.2 Steps for Sampling ................................................................. 136

D The Poisson Distribution ................................................................. 139
D.1 The Poisson Process and Examples ................................................... 139
D.2 Derivation Methods for the Poisson Distribution ................................... 140
D.3 Spontaneous Radioactive Decay ........................................................ 142
D.4 Application to Star Formation .......................................................... 144

E The Initial Mass Function ................................................................. 147
E.1 Definition and Normalization .............................................................. 147
E.2 The Alpha-Plot ................................................................. 149
E.3 Possible Causes for Alpha Scatter ....................................................... 150
E.4 The Present-Day Initial Mass Function .............................................. 152
E.5 Final Thoughts on Kroupa (2001) Study ............................................ 152
E.6 The IMF Plot ................................................................. 153
E.7 Normalizing the Kroupa (2001) IMF .................................................. 157
E.8 Cumulative Distribution Functions of the IMF .................................... 159
E.9 Sampling from the IMF ................................................................. 160

F The Inhomogeneous Chemical Evolution Tool ........................................ 162

G Fictitious Species ................................................................. 166
G.1 Definition and Naming ................................................................. 166
G.2 Ejection of Stable Masses and Resultant Contributions ......................... 167
G.3 Ejection of Radioactive Masses and Resultant Contributions .................... 169
List of Tables

1.1 ................................................................. 10
9.1 ................................................................. 89
E.1 Number and mass percents for stellar objects of the IMF. ........................................ 150
E.2 Number and mass percents for stellar objects of the PDMF. ........................................ 152
List of Figures

1.1 Measured magnesium and aluminum-magnesium isotopic abundance ratios in multiple minerals of a CAI from a fragment of the Allende meteorite. Excesses in the $^{26}\text{Mg}$ abundance correlate with the $^{27}\text{Al}/^{24}\text{Mg}$ abundance ratio, consequently substantiating the existence of $^{26}\text{Al}$ in the early Solar System. ........................................ 5

1.2 Snapshots of aluminum-magnesium isochron for observed early Solar System $^{26}\text{Al}/^{27}\text{Al}$ isotopic abundance ratio of $5 \times 10^{-5}$ inferred from CAIs. ................................. 6

1.3 X-ray elemental map of the CR carbonaceous chondrite, PCA 91082. This sample contains both CAIs and chondrules, the arrows pointing out the locations of each. The abundances of magnesium (red), calcium (green), and aluminum (blue) are featured. ............................ 7

1.4 X-ray elemental map of a CAI from the CV3 carbonaceous chondrite, Efremovka. The regions of various minerals are identified. As before, the abundances of magnesium (red), calcium (green), and aluminum (blue) are featured. ................................. 8

1.5 Snapshots of aluminum-magnesium isochron for observed early Solar System $^{26}\text{Al}/^{27}\text{Al}$ isotopic abundance ratio of $1 \times 10^{-5}$ inferred from chondrules. ......................... 9

2.1 Energy-level diagram for decay of $^{26}\text{Al}$ [278]. ............................................. 13

2.2 Energy-level diagram for decay of $^{36}\text{Cl}$ [37]. .............................................. 15

2.3 Energy-level diagram for decay of $^{41}\text{Ca}$ [190]. ......................................... 16

2.4 Energy-level diagram for decay of $^{53}\text{Mn}$ [7]. ........................................... 18

2.5 Energy-level diagram for decay of $^{60}\text{Fe}$ [52]. .......................................... 19

2.6 Energy-level diagram for decay of $^{129}\text{I}$ [58]. .......................................... 21

2.7 Energy-level diagram for decay of $^{182}\text{Hf}$ [234]. .................................. 22

2.8 Energy-level diagram for decay of $^{107}\text{Pd}$ [9]. ......................................... 23

2.9 Energy-level diagram for decay of $^{146}\text{Sm}$ [197]. .................................. 23

2.10 Energy-level diagram for decay of $^{244}\text{Pu}$ [233]. .................................. 24

4.1 Mass-fraction yield of $^{17}\text{O}$ for stars of varying initial masses and metallicities. .... 33

5.1 Mass fraction of $^{16}\text{O}$ in the gas for a single-zone IRA calculation (red) and the exact solution of Eq. (4.9) (blue). ......................................................... 37

5.2 Mass-fraction yield of $^{16}\text{O}$ for stars of varying initial masses and metallicities. .... 40

5.3 Mass fraction of $^{16}\text{O}$ in the gas for a single-zone IRA calculation (solid red curve) and the exact solution of Eq. (4.9) (blue circles). ............................................. 41

5.4 Mass fraction of $^{17}\text{O}$ in the gas for a single-zone IRA calculation (solid red curve) and the exact solution of Eq. (4.14) (blue circles) for 5 mass-metallicity-yield points. .... 43

5.5 Mass fraction of $^{17}\text{O}$ in the gas for a single-zone IRA calculation (solid red curve) and the exact solution of Eq. (4.14) (blue circles) for 8 mass-metallicity-yield points. .... 43

5.6 Mass fraction of $^{17}\text{O}$ in the gas for a single-zone IRA calculation (solid red curve) and the exact solution of Eq. (4.14) (blue circles) for 14 mass-metallicity-yield points. .... 44

5.7 Mass fraction of $^{17}\text{O}$ in the gas for a single-zone IRA calculation (solid red) and the exact solution of Eq. (4.14) (blue circles) for 27 mass-metallicity-yield points. .... 44
5.8 Disk gas mass for a single-zone IRA calculation (solid red) and the exact solution of Eq. (4.14) (blue circles). ........................................... 45
5.9 Disk gas mass for a single-zone IRA (red) and non-IRA (blue) calculation. .... 46
5.10 Mass fraction of $^{16}$O in the gas for a single-zone IRA (red) and non-IRA (blue) calculation. ......................................................... 47
5.11 Mass fraction of $^{17}$O in the gas for a single-zone IRA (red) and non-IRA (blue) calculation. ......................................................... 48
5.12 Disk gas mass for a single-zone IRA (red) and non-IRA (blue) calculation, zoomed in for $0 < t < 1$ Gyr. ................................. 48
5.13 Disk gas mass for a single-zone IRA (red) and non-IRA (blue) calculation, zoomed in for $0 < t < 200$ Myr. ................................. 49
6.1 Schematic of our Galactic structure consisting of 32 annular zones enclosing the halo zone and the ongoing mixing between them. .................. 51
6.2 Snapshot of 3 spiral mass-density arms propagating across the Solar annulus. ... 52
6.3 Galactic-disk gas fraction at 13.5 Gyr as a function of star-formation timescale for $10^4 M_\odot$ of total mass. ........................................ 53
6.4 Galactic-disk gas fraction at 13.5 Gyr as a function of star-formation timescale for $10^5 M_\odot$ of total mass. ........................................ 54
6.5 Galactic-disk gas fraction at 13.5 Gyr as a function of star-formation timescale for $10^6 M_\odot$ of total mass. ........................................ 54
6.6 Galactic-disk gas fraction at 13.5 Gyr as a function of star-formation timescale for $32 \times 10^6 M_\odot$ of total mass. ........................................ 55
6.7 Galactic-disk gas fraction at 13.5 Gyr as a function of star-formation timescale for $10^7 M_\odot$ of total mass. ........................................ 55
7.1 Mass fractions of $^{26}$Al and $^{27}$Al in the gas for a single-zone, full-yield, non-IRA calculation with hot zones. ...................................... 60
7.2 Ratio of mass fractions of $^{26}$Al and $^{27}$Al in the gas for a single-zone, full-yield, non-IRA calculation with hot zones. ...................................... 61
7.3 Zoomed-in mass fraction of $^{27}$Al in the gas for a single-zone, full-yield, non-IRA calculation with hot zones. ...................................... 61
7.4 Mass fractions of $^{56}$Fe and $^{56}$Fe in the gas for a single-zone, full-yield, non-IRA calculation with hot zones. ...................................... 61
7.5 Mass fractions of $^{129}$I and $^{127}$I in the gas for a single-zone, full-yield, non-IRA calculation with hot zones. ...................................... 62
7.6 Zoomed-in mass fraction of $^{127}$I in the gas for a single-zone, full-yield, non-IRA calculation with hot zones. ...................................... 63
7.7 Mass-fraction yield of multiple isotopes for Solar-metallicity stars of varying initial masses. ................................................................. 64
7.8 Mass fractions of $^{182}$Hf and $^{180}$Hf in the gas for a single-zone, full-yield, non-IRA calculation with hot zones. ...................................... 64
7.9 Zoomed-in mass fraction of $^{180}$Hf in the gas for a single-zone, full-yield, non-IRA calculation with hot zones. ...................................... 65
7.10 Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for 3 single-zone, full-yield, non-IRA calculations with hot zones and 1 without. The dashed lines represent the meteoritic values. ................................. 67
7.11 Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values. ................................. 68
7.12 Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the single-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values. .......................................................... 69
7.13 Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values. .......................................................... 70
7.14 Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the single-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values. .......................................................... 71
7.15 Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values. .......................................................... 71
7.16 Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the single-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values. .......................................................... 72
7.17 Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values. .......................................................... 73
7.18 Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the single-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values. .......................................................... 74
7.19 Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values. .......................................................... 74
7.20 Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the single-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values. .......................................................... 76
7.21 Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values. .......................................................... 76
7.22 Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values. .......................................................... 77
7.23 Mass-fraction ratios from simple diffusion calculation for a mixing timescale of $10^6$ yr. .......................................................... 78
7.24 Mass-fraction ratios from simple diffusion calculation for a mixing timescale of $10^7$ yr. .......................................................... 78
7.25 Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values. .......................................................... 81
7.26 Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values. .......................................................... 82
7.27 Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values. .......................................................... 82
7.28 Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values. .......................................................... 83
7.29 Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values. .......................................................... 83
E.7 Number of stars born per area or volume as sampled from the IMF for 10,000 stars for reduced number-density range. ................................................................. 156
E.8 Number of stars born per area or volume as sampled from the IMF for 10,000 stars for reduced number-density and mass ranges. .............................................. 157
G.1 Fractional contribution to late-forming Solar-mass stars as a function of merger time. ................................................................. 168
G.2 Fractional contribution to late-forming Solar-mass stars as a function of merger time. ................................................................. 168
G.3 Fractional contribution to late-forming Solar-mass stars as a function of merger time for radioactive $^{129}$I. ................................................................. 171
G.4 Fractional contribution to late-forming Solar-mass stars as a function of merger time for radioactive $^{238}$U. ................................................................. 172
G.5 Zooming in on Fig. (G.4). ................................................................. 172
G.6 Mean isotope age for a stable species inside newly-created Solar-mass stars. ................................................................. 175
G.7 Zooming in on Fig. (G.6). ................................................................. 176
G.8 Mean isotope age for $^{129}$I inside newly-created Solar-mass stars. ................................................................. 176
G.9 Zooming in on Fig. (G.8). ................................................................. 177
G.10 Mean isotope age for $^{238}$U inside newly-created Solar-mass stars. ................................................................. 178
G.11 Zooming in on Fig. (G.10). ................................................................. 178
H.1 Abundance determinations in five r-process-rich halo stars, based on new atomic lab data, compared with two Solar-System r-process-only predictions. ............... 185
H.2 Abundance comparisons between 10 r-process-rich halo stars and Solar-System r-process values. ................................................................. 185
H.3 r-Process abundance comparisons between ultra-metal-poor halo star, CS 22892–052, and Sun. ................................................................. 186
H.4 Logarithmic abundances in r-process-rich halo stars. Filled squares indicate detections while curves represent Solar-System s-, r-, and s- + r-process abundance distributions. 186
H.5 Logarithmic abundances and abundance differences in r-process-rich halo stars. Filled squares indicate detections while curves represent Solar-System s-, r-, and s- + r-process abundance distributions. ................................................................. 187
H.6 Abundances relative to iron for various isotopes of metal-poor Bond giants. ................................................................. 187
H.7 Early Galactic enrichment history of the r-process element, europium, in chemical evolution models identifying binary neutron-star mergers as the sole birthplace of r-process isotopes. ................................................................. 191
H.8 Nuclear abundance pattern for the 1.35-1.35 M$_\odot$ (left) and 1.2-1.5 M$_\odot$ (right) mergers with 3 equations of state as compared to the Solar r-process abundance distribution. ................................................................. 192
H.9 Nuclear abundance pattern for the 1.35-1.35 M$_\odot$ mergers with two other equations of state as compared to the Solar r-process abundance distribution. ................................................................. 192
H.10 Nuclear abundance patterns for selected trajectories (top) and comparison of the corresponding weighted average to the Solar r-process abundance distribution (bottom). 193
H.11 Time-frequency representations of data for GW170817 as observed by the LIGO-Hanford (top), LIGO-Livingston (middle), and Virgo (bottom) detectors. Times are shown relative to August 17, 2017 12:41:04 UTC. ................................................................. 194
H.12 Combined time-frequency representation of data for GW170817 as observed by the LIGO-Hanford and LIGO-Livingston detectors. ................................................................. 195
H.13 Pseudo-color images of SSS17a in the host galaxy, NGC 4993. (A) Images taken 0.5 days and (B) 4.5 days post merger, the blue arrow marking the transient. ................................................................. 196
H.14 Near-infrared spectral sequence of GW170817 from the Gemini-South telescope, with each epoch’s age in days after the GW trigger emphasized to the left. ................................................................. 197
H.15 Sketch of the various mass-loss mechanisms from the remnant of a binary NS or NSBH (neutron-star-black-hole) merger. ................................................................. 198
H.16 Best fit of the red kilonova model to the spectrum at 4.5 days post merger for the listed parameters. 199

I.1 Windblown Bubble Around a Wolf-Rayet Star 201
I.2 $^{26}$Al Ejected from Massive Stars 203
I.3 Schematic of Solar-System Formation 208

J.1 Final $^{41}$Ca mass fraction as a function of interior mass coordinate 1 year after the 1.0 B explosion of s25a28 for the indicated reaction networks. Also shown for comparison is the pre-supernova value from Ref. [212]. 210
J.2 Pre-supernova mass fractions of relevant species as a function of interior mass coordinate for stellar model s25a28 of Ref. [212]. 211
J.3 Time evolution of the mass fractions of relevant species in zone 284 during the E = 1.0 B explosion of s25a28. 213
J.4 Time evolution of the proton and neutron mass fractions in zone 284 during the E = 1.0 B explosion of s25a28. 213
J.5 Time evolution of the $^{41}$Ca mass fraction in zones 268, 284, and 308 during the E = 1.0 B explosion of s25a28. 218
J.6 Time evolution of the $^{41}$Ca mass fraction in zone 284 during the E = 1.0 B explosion of s25a28 for the indicated reaction networks. 219
J.7 Net integrated currents of interest for the rates of this work in zone 284 for the 1-year interval after the 1.0 B explosion of s25a28. 220
J.8 Net integrated currents of interest for the rates of Ref. [229] in zone 284 for the 1-year interval after the 1.0 B explosion of s25a28. 221
J.9 Difference in the net integrated currents of interest for the rates of this work and those of Ref. [229] in zone 284 for the 1-year interval after the 1.0 B explosion of s25a28. 222
J.10 Difference in the net integrated currents of interest for the updated $^{41}$K($p$,α)$^{38}$Ar rate of this work and that of Ref. [229] in zone 284 for the 1-year interval after the 1.0 B explosion of s25a28. 223
J.11 Time evolution of the $^{41}$Ca mass fraction in zone 284 during the E = 1.0 B explosion of s25a28 for the indicated reaction networks. 224
J.12 Time evolution of the $^{41}$K mass fraction in zone 284 during the E = 1.0 B explosion of s25a28 for the indicated reaction networks. 225
J.13 Difference in the net integrated currents of interest for the updated $^{41}$Ca($n$,α)$^{38}$Ar rate of this work and that of Ref. [229] in zone 284 for the 1-year interval after the 1.0 B explosion of s25a28. 226
Chapter 1

Introduction

1.1 The Fundamental Problem of the Short-Lived Radioactivities

Short-lived radioactivities are radioactive isotopes with mean lifetimes of no more than 150 million years that were alive in the early Solar nebula but have since decayed across the duration of the Solar System and are now extinct. The complement of short-lived radioactivities (SLRs) we will study include $^{26}$Al, $^{36}$Cl, $^{41}$Ca, $^{53}$Mn, $^{60}$Fe, $^{107}$Pd, $^{129}$I, $^{146}$Sm, $^{182}$Hf, and $^{244}$Pu, with mean lifetimes as low as 100 thousand years. The presence of these radioactivities in the early Solar nebula has been inferred from excesses of their daughter isotopes embedded within primitive meteorites found and analyzed via various physical and chemical means over the last 50 years.

Throughout the history of the Milky Way Galaxy, generations of stars have come into existence via the gravitational collapse of matter, evolved as multiple stages of core and shell nucleosynthesis imposed structural and cosmetic changes, and subsequently died amid violent supernova explosions or pulsations and stellar winds that drove off the outer layers of each star to reveal an inert core. The ejecta from these final whispers of life expanded into the surrounding interstellar medium (ISM) and eventually mixed with the matter there. Short-lived radioactive nuclei of the ejecta underwent spontaneous decay during this period of transport and mixing. Following a sufficient passage of time, we expect the rate of stellar production and ejection of these nuclei and their consequent injection into the ISM to become balanced by their rate of decay, as formulated
in models of Galactic Chemical Evolution (GCE). The ISM thus likely acquired steady-state abundances of the radioactive nuclei that are now representative of a component of its current chemical composition. We also expect the abundances of stable nuclei of the ejecta, however, to experience a net increase in the ISM across many generations. That cloud of material out of which condensed the Solar System inherited the background steady-state and stable abundances. Models of GCE can be used to predict, as a function of time, the ratio of the abundance of a radioactive isotope to that of its corresponding stable reference isotope.

The great conundrum encompassing the now-extinct SLRs of the early Solar System is the discrepancy between their abundances as inferred from meteorites and those as predicted from GCE. There continues to be much difficulty in reconciling the meteoritic abundances to a plausible setting for the Solar System’s birth. Perhaps the Giant Molecular Cloud containing the proto-Solar nebula experienced a recent burst of star formation. Did one or more supernovae from this burst occur near the proto-Solar nebula before or as it was condensing and thereby inject freshly-synthesized radioactivities into it? Or, in the absence of any recent star formation, did an adjacent supernova suddenly transpire contemporaneously with the condensing proto-Solar nebula and contribute some fraction of its ejecta to the emerging Solar System? Before we can attempt to seek answers to such questions, a review of how the abundances of SLRs are measured is in order. I take the famous SLR, $^{26}\text{Al}$, as an example [115][81].

### 1.2 Aluminum-Magnesium Isochron

Of particular importance is the short-lived radionuclide, $^{26}\text{Al}$, as excesses in its daughter isotope, $^{26}\text{Mg}$, embedded within meteorite samples, combined with its brief (relative to the age of the Solar System) mean lifetime of roughly 1 million years, provide direct evidence for its existence at the time of formation of the meteorites’ parent rocky bodies early in the Solar System’s history. Before discussing said evidence, consider a sample with a parent radioactive isotope, $P$, that undergoes spontaneous decay to its daughter isotope, $D$, according to the universal decay equation (see appendix B),

$$\frac{dN_P}{dt} = -\lambda N_P,$$

in which $N_P$ denotes the number of $P$ nuclei at time, $t$, and the rate of change of that number is proportional to the probability of decay per unit time, or, $\lambda$. Solving Eq. (1.1) yields the number
of $P$ nuclei remaining at time, $t$:

$$N_P = N_{P0}e^{-\lambda(t-t_0)},$$

where $t_0$ is the time of formation of the sample and $N_{P0}$ is the number of $P$ nuclei in the sample at that time. The number of daughter nuclei created after time, $t$, then, is given by the following difference:

$$N_D = N_{P0} - N_P = N_{P0} - N_{P0}e^{-\lambda(t-t_0)} = N_{P0}(1 - e^{-\lambda(t-t_0)}).$$

If, however, enough time has passed, all of the parent nuclei will have decayed into the daughter nuclei and $N_D$ in Eq. (1.2) becomes $N_{P0}$ for $t \gg t_0$. The meteorites having formed out of the cloud of material of the Solar nebula some 4.5 billion years ago, such is the reason for the absence of $^{26}$Al and excess in $^{26}$Mg in minerals extracted and analyzed over the last 50 years.

To obtain the total number of daughter nuclei in the sample, we must also account for the daughter nuclei that were already present and not the result of parental decay. Hence,

$$N_D = N_{P0} + N_{D0},$$

$N_{D0}$ representing that initial amount. Now, consider the number ratio of isotopes of a given nuclear species in dividing both sides of Eq. (1.3) by the number of nuclei of a stable isotope of the daughter species:

$$\frac{N_D}{N_{D'}} = \frac{N_{P0}}{N_{P'}} + \frac{N_{D0}}{N_{D'}},$$

$N_{D'}$ denoting the number of nuclei of that stable isotope. If we rewrite Eq. (1.4) by isolating the number of nuclei of another stable isotope, this time of the parent species, from the first term on the right side, we arrive at a useful chronometer:

$$\frac{N_D}{N_{D'}} = \frac{N_{P0}}{N_{P'}} \frac{N_{P'}}{N_{D'}} + \frac{N_{D0}}{N_{D'}},$$

the number of nuclei of this stable isotope similarly denoted as $N_{P'}$ [94].
As the number of nuclei of a given nuclear species is the product of its abundance, \( Y \), and the total number of nucleons, \( N_n \), we can rewrite Eq. (1.5) accordingly:

\[
\frac{Y_D N_n}{Y_{D'} N_n} = \frac{Y_{P0} N_n}{Y_{P'} N_n} \frac{Y_{D0} N_n}{Y_{D'} N_n} + \frac{Y_{D0} N_n}{Y_{D'} N_n}
\]

\[
\Rightarrow \frac{Y_D}{Y_{D'}} = \frac{Y_{P0} Y_{P'}}{Y_{P'} Y_{D'}} + \frac{Y_{D0}}{Y_{D'}}.
\] (1.6)

For the Al-Mg system, in which \(^{26}\text{Al}\) decays into \(^{26}\text{Mg}\), the corresponding stable isotopes are \(^{27}\text{Al}\) and \(^{24}\text{Mg}\) and Eq. (1.6) takes the particular form of

\[
\frac{Y(^{26}\text{Mg})}{Y(^{24}\text{Mg})} = \frac{Y((^{26}\text{Al})_0)}{Y(^{27}\text{Al})} \frac{Y(^{27}\text{Al})}{Y(^{24}\text{Mg})} + \frac{Y((^{26}\text{Mg})_0)}{Y(^{24}\text{Mg})}.
\]

In implying the abundances of the above equation, we can remove its clunkiness:

\[
\frac{^{26}\text{Mg}}{^{24}\text{Mg}} = \frac{^{26}\text{Al}}{^{27}\text{Al}} \frac{^{27}\text{Al}}{^{24}\text{Mg}} + \frac{^{26}\text{Mg}}{^{24}\text{Mg}}.
\]

Assuming an isolated system (sample not subject to exterior effects that might otherwise alter the meteorite’s surface), the abundances of the stable \(^{24}\text{Mg}\) and \(^{27}\text{Al}\) isotopes remain unchanged throughout the 4.5 billion years of Solar-System evolution. We can therefore denote their abundances interchangeably by the initial and current amounts since both values are identical:

\[
\frac{^{26}\text{Mg}}{^{24}\text{Mg}} = \frac{^{26}\text{Al}}{^{27}\text{Al}} \frac{^{27}\text{Al}}{^{24}\text{Mg}} + \frac{^{26}\text{Mg}}{^{24}\text{Mg}}.
\] (1.7)

Equation (1.7) is in the form of a line (i.e., \( y = mx + b \)), the slope given by the initial isotopic abundance ratio of \(^{26}\text{Al}/^{27}\text{Al}\) present in the early Solar System and the y-intercept expressed as that initial ratio of \(^{26}\text{Mg}/^{24}\text{Mg}\).

Figure (1.1) [281] highlights the significance of Eq. (1.7). The \(^{26}\text{Mg}/^{24}\text{Mg}\) and \(^{27}\text{Al}/^{24}\text{Mg}\) abundance ratios were measured in different minerals of a Calcium-Aluminum-rich Inclusion (CAI) from a fragment of the Allende meteorite, the values for the magnesium ratio plotted on the y-axis and those for the aluminum-magnesium ratio on the x-axis. The remarkable result is a line
Zinner (2002)

Figure 1.1: Measured magnesium and aluminum-magnesium isotopic abundance ratios in multiple minerals of a CAI from a fragment of the Allende meteorite. Excesses in the $^{26}$Mg abundance correlate with the $^{27}$Al/$^{24}$Mg abundance ratio, consequently substantiating the existence of $^{26}$Al in the early Solar System.

reminiscent of Eq. (1.7), emphasizing the correlation between these ratios. The slope of $\sim 5 \times 10^{-5}$ gauges the $^{26}$Al/$^{27}$Al abundance ratio at the time of Solar-System formation and thus confirms the existence of $^{26}$Al in the early Solar nebula. However, abundances measured in chondrules infer initial aluminum ratios ranging from $\sim 3 \times 10^{-6}$ to $\sim 1.6 \times 10^{-5}$ [263] while analysis of FUN (Fractionation and Unidentified Nuclear effects) CAIs indicates little aluminum to be present 4.5 billion years ago ($^{26}$Al/$^{27}$Al $\leq 5 \times 10^{-6}$ [146][147][65][154][269]).

There are two explanations for these differences. First, the material of the Solar nebula was uniform in composition and the CAIs, FUN CAIs, and chondrules all formed at different times. For instance, the FUN CAIs could have formed earlier than both the CAIs and chondrules and before possible stellar injection of $^{26}$Al from a nearby supernova. The FUN CAIs would have locked up a lower initial $^{26}$Al abundance for the same constant $^{27}$Al, $^{24}$Mg, and $^{26}$Mg abundances in CAIs,
FUN CAIs, and chondrules. Less $^{26}\text{Mg}$ abundance would thereby result from the decay of $^{26}\text{Al}$ in FUN CAIs. Similarly, the FUN CAIs could have formed later than both the CAIs and chondrules. By the time of formation of the FUN CAIs, much of the initial $^{26}\text{Al}$ abundance would have decayed and the FUN CAIs acquired this low amount. Again, the decay of this small abundance produces the correspondingly-small $^{26}\text{Mg}/^{24}\text{Mg}$ abundance ratio measured in these minerals. Second, the material of the Solar nebula was not uniform in composition. The creation of CAIs, FUN CAIs, and chondrules contemporaneously and at different locations within an inhomogeneous distribution of $^{26}\text{Al}$ eventually bore the isotopic signatures seen in today’s meteorite samples.

To fully grasp and, in turn, appreciate the monumental breakthrough that might otherwise appear understated in Fig. (1.1), ruminate on the snapshots of Fig. (1.2). Starting with the top-left
Krot (2002)

Figure 1.3: X-ray elemental map of the CR carbonaceous chondrite, PCA 91082. This sample contains both CAIs and chondrules, the arrows pointing out the locations of each. The abundances of magnesium (red), calcium (green), and aluminum (blue) are featured.

snapshot, time increases in millions of years from (a) to (d). Each red diamond on the red line symbolizes one of the minerals in Fig. (1.1). At the beginning of the Solar System (i.e., $t = 0$), assuming a homogeneous nebular composition, all of the minerals formed with the same $^{26}\text{Mg}$, $^{24}\text{Mg}$, $^{26}\text{Al}$, and $^{27}\text{Al}$ isotopic abundances. The minerals, though, exhibit dissimilar chemistry. Figure (1.3) [134] displays an X-ray elemental map of a cross-section from the CR carbonaceous chondrite, PCA 91082 [225], discovered in Antarctica in 1991, with CAIs and chondrules clearly marked. Another X-ray elemental map from a fragment of the Efremovka meteorite [5], discovered in Russia (formerly USSR) in 1962, peeks inside of a CAI to uncover its constituent minerals, including spinel (MgAl$_2$O$_4$), hibonite (CaAl$_{12}$O$_{19}$), melilite (Ca$_2$Al$_2$SiO$_7$-Ca$_2$MgSi$_2$O$_7$ solid solution), and pyroxene (silicon-aluminum oxide), all discernable in Fig. (1.4) [247]. How the minerals formed is beyond the scope of this project. Suffice it to say, each mineral formed with aluminum isotopes bonded to magnesium isotopes in varying proportions, hence the spread in initial $^{27}\text{Al}/^{24}\text{Mg}$ abundance ratios in Fig. (1.2). As such bonding is governed by the number of electrons and, thus, atomic number, each mineral also formed with a constant proportion of magnesium isotopes, hence the identical initial $^{26}\text{Mg}/^{24}\text{Mg}$ abundance ratios in Fig. (1.2) [135] [70].
Figure 1.4: X-ray elemental map of a CAI from the CV3 carbonaceous chondrite, Efremovka. The regions of various minerals are identified. As before, the abundances of magnesium (red), calcium (green), and aluminum (blue) are featured.

Owing to similar chemical properties, comparable quantities of $^{26}\text{Al}$ and $^{27}\text{Al}$ reacted with $^{24}\text{Mg}$ upon formation of the minerals. A high initial $^{27}\text{Al}$ to $^{24}\text{Mg}$ abundance ratio in a given mineral thereby equates to a high initial $^{26}\text{Al}$ to $^{24}\text{Mg}$ abundance ratio. Likewise, low initial $^{27}\text{Al}$ to $^{24}\text{Mg}$ and $^{26}\text{Al}$ to $^{24}\text{Mg}$ abundance ratios are mutually inclusive. Because $^{26}\text{Al}$ decays to $^{26}\text{Mg}$ with a half-life of 717,000 years, the larger the initial aluminum content in a given mineral, the larger the $^{26}\text{Mg}$ abundance produced across a particular duration. In traversing the snapshots of Fig. (1.2), the mineral with an initial $^{27}\text{Al}/^{24}\text{Mg}$ abundance ratio of 245 yields the maximum growth in $^{26}\text{Mg}$ abundance, and, therefore, $^{26}\text{Mg}/^{24}\text{Mg}$ abundance ratio, after 8.45 million years, by which point all of the $^{26}\text{Al}$ abundance has decayed. Conversely, the minerals with initial $^{27}\text{Al}/^{24}\text{Mg}$ abundance ratios of 2.5 and 9.1 undergo minimal growth of the $^{26}\text{Mg}/^{24}\text{Mg}$ abundance ratio. This mix of initial $^{27}\text{Al}/^{24}\text{Mg}$ abundance ratios gives rise to a series of points connected by a line with positively-increasing slope, the value post-$^{26}\text{Al}$-decay disclosing the $^{26}\text{Al}/^{27}\text{Al}$ abundance ratio at the time of Solar-System formation, as derived above.

For the snapshots of Fig. (1.2), the final slope of $5 \times 10^{-5}$ corresponds to the early Solar $^{26}\text{Al}/^{27}\text{Al}$ abundance ratio inferred from CAIs. The snapshots of Fig. (1.5) show a similar trajectory...
Figure 1.5: Snapshots of aluminum-magnesium isochron for observed early Solar System $^{26}\text{Al}/^{27}\text{Al}$ isotopic abundance ratio of $1 \times 10^{-5}$ inferred from chondrules.

of the slope with a final value of $1 \times 10^{-5}$ corresponding to the early Solar $^{26}\text{Al}/^{27}\text{Al}$ abundance ratio inferred from chondrules. These previously-discussed discrepancies in initial aluminum abundance ratios inferred from Al-Mg systematics of different mineral types imply spatial discontinuities in their formation across an inhomogeneous Solar nebula, or temporal discontinuities across hundreds of millions of years within a uniform Solar nebula. Chondrules and FUN CAIs may have formed in a region of the Solar nebula deplete in aluminum content or during a time after which much of the initial $^{26}\text{Al}$ abundance had decayed. We will consider all possibilities in the analysis of our results.
The table below consolidates much of the current information on the SLRs present in the early Solar System, including their effective mean lifetimes, reference isotopes and relative abundance ratios, and sites of nucleosynthesis as established from the available evidence. The goal of this thesis is to reconcile the abundances in the context of a plausible model for Galactic nucleosynthesis and chemical evolution. To do this, I first review the nucleosynthesis of these species in chapter 2. I then discuss stellar yields for nucleosynthesis in chapter 3. I introduce Galactic chemical evolution (GCE) in chapter 4 through simple analytic GCE models and compare their results to the output of computational models in chapter 5. I present my inhomogeneous chemical evolution (ICE) model in chapter 6 and calculation of the abundances of SLRs in chapter 7. Since the data are available in my runs, I also add some comments on long-lived radioactivities in chapter 8. In chapter 9, I conclude with a discussion of our results.

As this work spans a number of topics in nuclear astrophysics, computational techniques, and Galactic astronomy, I have written several appendices to provide additional details on various topics. They are included in this thesis for reference. The appendices also include summaries of two papers I published with groups at the University of Chicago and Argonne National Laboratory. We will follow-up this work in the coming weeks with the submission of a manuscript for publication of our results.

### Table 1.1

<table>
<thead>
<tr>
<th>Radiouclide</th>
<th>Mean Lifetime (Myr)</th>
<th>Stable Nuclide</th>
<th>Reference</th>
<th>Inferred ESS Ratio</th>
<th>Source(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{26}\text{Al}$</td>
<td>1.034</td>
<td>$^{27}\text{Al}$</td>
<td></td>
<td>$5.23 \times 10^{-3}$</td>
<td>super-AGB and massive stars, CCSN, SNIa</td>
</tr>
<tr>
<td>$^{36}\text{Cl}$</td>
<td>0.435</td>
<td>$^{35}\text{Cl}$</td>
<td></td>
<td>$2.44 \times 10^{-5}$</td>
<td>super-AGB and massive stars, irradiation, CCSN, SNIa</td>
</tr>
<tr>
<td>$^{41}\text{Ca}$</td>
<td>0.134</td>
<td>$^{40}\text{Ca}$</td>
<td></td>
<td>$4.60 \times 10^{-9}$</td>
<td>super-AGB and massive stars, irradiation, CCSN, SNIa</td>
</tr>
<tr>
<td>$^{53}\text{Mn}$</td>
<td>5.396</td>
<td>$^{55}\text{Mn}$</td>
<td></td>
<td>$7.00 \times 10^{-6}$</td>
<td>massive stars, CCSN, SNIa</td>
</tr>
<tr>
<td>$^{60}\text{Fe}$</td>
<td>3.780</td>
<td>$^{56}\text{Fe}$</td>
<td></td>
<td>$1.16 \times 10^{-8}$</td>
<td>super-AGB and massive stars, CCSN, SNIa, ECSN</td>
</tr>
<tr>
<td>$^{107}\text{Pd}$</td>
<td>9.378</td>
<td>$^{108}\text{Pd}$</td>
<td></td>
<td>$6.60 \times 10^{-5}$</td>
<td>massive stars, CCSN, NS-NS mergers</td>
</tr>
<tr>
<td>$^{129}\text{I}$</td>
<td>22.650</td>
<td>$^{127}\text{I}$</td>
<td></td>
<td>$1.28 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td>$^{146}\text{Sm}$</td>
<td>98.103</td>
<td>$^{144}\text{Sm}$</td>
<td></td>
<td>$8.28 \times 10^{-3}$</td>
<td>massive stars, CCNS, SNIa</td>
</tr>
<tr>
<td>$^{182}\text{Hf}$</td>
<td>12.840</td>
<td>$^{180}\text{Hf}$</td>
<td></td>
<td>$1.02 \times 10^{-4}$</td>
<td>massive stars, CCSN, NS-NS mergers</td>
</tr>
<tr>
<td>$^{244}\text{Pu}$</td>
<td>115.416</td>
<td>$^{238}\text{U}$</td>
<td></td>
<td>$7.00 \times 10^{-3}$</td>
<td>CCSN, NS-NS mergers</td>
</tr>
</tbody>
</table>

1.3 Outline of this Work

Table (1.1) consolidates much of the current information on the SLRs present in the early Solar System, including their effective mean lifetimes, reference isotopes and relative abundance ratios, and sites of nucleosynthesis as established from the available evidence. The goal of this thesis is to reconcile the abundances in the context of a plausible model for Galactic nucleosynthesis and chemical evolution. To do this, I first review the nucleosynthesis of these species in chapter 2. I then discuss stellar yields for nucleosynthesis in chapter 3. I introduce Galactic chemical evolution (GCE) in chapter 4 through simple analytic GCE models and compare their results to the output of computational models in chapter 5. I present my inhomogeneous chemical evolution (ICE) model in chapter 6 and calculation of the abundances of SLRs in chapter 7. Since the data are available in my runs, I also add some comments on long-lived radioactivities in chapter 8. In chapter 9, I conclude with a discussion of our results.

As this work spans a number of topics in nuclear astrophysics, computational techniques, and Galactic astronomy, I have written several appendices to provide additional details on various topics. They are included in this thesis for reference. The appendices also include summaries of two papers I published with groups at the University of Chicago and Argonne National Laboratory. We will follow-up this work in the coming weeks with the submission of a manuscript for publication of our results.
Chapter 2

Nucleosynthesis of the Galactic Radioactivities

2.1 AGB Evolution

As a massive star evolves, successive flashes of shell burning following the various phases of core burning and fuel exhaustion result in additional production of those isotopes previously synthesized in the core. Multiple dredge-up episodes interspersed between these flash burnings are responsible for the convective mixing that transports the ashes, or freshly-synthesized isotopes, to the surface of the star. Such freshly-synthesized isotopes include the products of s-process nucleosynthesis, the origin of the neutrons feeding this process as described below.

Preceding the arrival of the third dredge-up during the AGB stage of stellar evolution, a helium-burning shell and hydrogen-burning shell remain separated in mass coordinate by a thin, radiative, helium intershell. The helium-burning shell surrounds the inert carbon-oxygen core while the hydrogen-burning shell is just inside of the convective hydrogen envelope. The mass of the intershell increases as the ashes of hydrogen-shell burning accumulate near the bottom (in mass coordinate) of this region. The pressure and temperature subsequently rise and thereby facilitate the onset of an unstable phase of helium burning once the intershell mass reaches a critical value. These helium-shell flashes, or thermal pulses, generate luminosities on the order of $10^8 \, L_\odot$ that drive convection throughout the intershell and uniformly mix the products of helium burning, including
$^{12}\text{C}$, $^{16}\text{O}$, and $^{22}\text{Ne}$ (produced via $^{14}\text{N}(\alpha,\gamma)^{18}\text{F}(\beta^+\nu)^{18}\text{O}(\alpha,\gamma)^{22}\text{Ne}$). A short burst of neutrons via $^{22}\text{Ne}(\alpha,n)^{25}\text{Mg}$, accompanying the thermal pulses for temperatures greater than $\approx 3 \times 10^8$ K, contributes to the production of s-process nuclei up to $A = 88$. The sudden surge of energy from the thermal pulses also causes the helium-burning shell and intershell to expand and cool, the cessation of hydrogen-shell burning serving as a consequence of such structural changes. In turn, the convective envelope penetrates beyond the hydrogen-burning shell and into the $\alpha$- and $^{12}\text{C}$-rich intershell, whereby abundant $^{12}\text{C}$ reacts with protons of the envelope to produce $^{13}\text{C}$ via $^{12}\text{C}(p,\gamma)^{13}\text{N}(\beta^+\nu)^{13}\text{C}$ in a thin layer designated as the ”$^{13}\text{C}$ pocket”. The details of the mechanism by which protons diffuse from the hydrogen envelope to the helium intershell remain shrouded in mystery to this day. During the interval between thermal pulses, convection transports the $^{13}\text{C}$ inwards where temperatures are high enough for the activation of $(\alpha,n)$ reactions on it and other species. The s-process nuclei synthesized in this manner have $A$ ranging from 88 to 208.

Upon extinguishment of a helium-shell flash, the penetration of the convective envelope, in addition to importing protons to the intershell, results in the transport of helium-burning products and other freshly-synthesized isotopes to the surface of the star in a process called the third dredge-up. With a pause in energy generation, the star suffers envelope contraction and eventual reignition of hydrogen-shell burning. The cycle repeats as the helium intershell grows in mass once more with the ashes of hydrogen-shell burning.

Stars of initial mass between $\approx 1 \text{M}_\odot$ and $\approx 9-10 \text{M}_\odot$ end their lives as stellar winds disperse much of the outer convective envelope to create a planetary nebula that inevitably mixes with the material of the ISM, leaving behind an inert and degenerate carbon-oxygen core called a white dwarf. More massive stars evolve beyond the AGB stage and explode as supernovas upon death, leaving behind a neutron star or black hole. These winds or explosions eject nuclei into, and thereby enrich, the surrounding ISM.

### 2.2 Aluminum-26

$^{26}\text{Al}$ has an effective mean lifetime of $\approx 1,034,000$ years, the disintegration occurring by competition between electron capture and beta-plus decay (see appendix B) to the excited states of $^{26}\text{Mg}$ highlighted in the energy-level diagram of Fig. (2.1) [278]. It is produced in hydrostatic hydrogen-shell burning via the CNO cycle during the AGB stage of stellar evolution and in hydro-
static hydrogen-core burning for stars initially more massive than 11 M_☉, also via the CNO cycle. For temperatures exceeding ≈30 million K, the Mg-Al chains of the CNO cycle activate and initiate the production of 26Al via \(^{25}\text{Mg}(p,\gamma)^{26}\text{Al}\). For more massive stars or those with initial metallicity less than solar, or for later thermal pulses during the AGB stage, temperatures exceeding ≈55 million K facilitate the destruction of \(^{24}\text{Mg}\) by \(^{24}\text{Mg}(p,\gamma)^{25}\text{Al} \beta^+ \gamma^{25}\text{Mg}\), thus replenishing the links of the Mg-Al chain and further increasing the abundance of 26Al. However, for these high temperatures, the production of 26Al is compensated by its main destruction via \(^{26}\text{Al}(p,\gamma)^{27}\text{Si} \beta^+ \gamma^{27}\text{Al}\), the net abundance of 26Al thereby remaining nearly independent of temperature.

For hydrogen-shell production, some fraction of 26Al may be destroyed upon penetration of the convective envelope into the helium intershell as neutrons from \(^{22}\text{Ne}(\alpha,n)^{25}\text{Mg}\) and \(^{13}\text{C}(\alpha,n)^{16}\text{O}\) capture onto the freshly-synthesized nuclei. The 26Al not destroyed in these deep layers is then transported to the surface of the star on a timescale of every 10^3-10^5 years, much less than the mean lifetime of 26Al and thereby ensuring a steady supply of this radioactive isotope at the surface. For hydrogen-core production, a significant fraction of 26Al may decay or be destroyed in subsequent helium-core burning. The 26Al not destroyed in the core is transported via convection to the outer layers. For Wolf-Rayet stars or the Wolf-Rayet stage of stellar evolution, the 26Al produced in the
core and not yet transported to the surface is exposed upon removal of the envelope by stellar winds. Such stellar winds also carry $^{26}$Al already present at the surface to the ISM. For stars massive enough to explode as supernovas upon death, whatever $^{26}$Al remains in the core and outer layers is ejected into the ISM as well.

For stars of initial mass $\geq 4 \, M_\odot$, temperatures at the base of the hydrogen envelope reach $\approx 50$ million K and hydrogen-burning reactions ignite across the duration between thermal pulses in a process called hot-bottom burning. The Mg-Al chains, as before, result in the production of $^{26}$Al and efficient mixing via convection carries it to the surface. The third dredge-up is hence not needed to transport the products of this burning.

Hydrostatic carbon-core and hydrostatic and explosive carbon-shell burning also contribute to the production of $^{26}$Al via a secondary $(p,\gamma)$ reaction on $^{25}$Mg. For hydrostatic burning, the abundance of $^{25}$Mg originates from the CNO cycle. For explosive burning, a significant fraction of $^{25}$Mg is synthesized as neutron-capture reactions on $^{24}$Mg. Protons for the $(p,\gamma)$ reaction are released via $^{12}$C($^{12}$C,p)$^{23}$Na, one of the primary reactions of carbon burning, and $^{23}$Na(α,p)$^{26}$Mg, another secondary reaction. Other secondary reactions on various nuclei, including the helium-burning ashes, $^{12}$C and $^{16}$O, and the heavy products of carbon burning, $^{23}$Na and $^{20}$Ne, operate during these stages of burning as well. Such secondary reactions involve the capture of protons, neutrons, and α-particles released by $^{12}$C($^{12}$C,p)$^{23}$Na, $^{12}$C($^{12}$C,α)$^{20}$Ne, and $^{12}$C($^{12}$C,n)$^{23}$Mg and encompass the following: $^{23}$Na(p,α)$^{20}$Ne, $^{23}$Na(α,γ)$^{20}$Ne, $^{20}$Ne(α,γ)$^{24}$Mg, $^{22}$Na(n,p)$^{22}$Ne, the $(p,\gamma)$ reactions on $^{21}$Ne, $^{22}$Ne, $^{25}$Mg, and $^{26}$Mg, and the (α,n) reactions on $^{13}$C, $^{21}$Ne, and $^{22}$Ne.

Hydrostatic neon-core and hydrostatic and explosive neon-shell burning produce additional amounts of $^{26}$Al, again via a secondary $(p,\gamma)$ reaction on $^{25}$Mg. For hydrostatic burning, much of the abundance of $^{25}$Mg remains intact near the completion of carbon burning. As above, for explosive burning, a significant fraction of $^{25}$Mg is synthesized as neutron-capture reactions on $^{24}$Mg. However, only $^{23}$Na(α,p)$^{26}$Mg provides the main source of protons for the $(p,\gamma)$ reaction, $^{23}$Na being one of the products of carbon burning. The primary reaction operating during these stages of burning is $^{20}$Ne(γ,α)$^{16}$O, $^{16}$O leftover from carbon burning and the temperatures now high enough for photons to break down nuclei via photo-disintegrations and, in turn, release the α-particles for the aforementioned capture by $^{23}$Na. Other secondary reactions include $^{20}$Ne(α,γ)$^{24}$Mg(α,γ)$^{28}$Si, $^{23}$Na(α,p)$^{26}$Mg(α,n)$^{29}$Si, $^{24}$Mg(α,p)$^{27}$Al(α,p)$^{30}$Si, $^{23}$Na(α,p)$^{26}$Mg, $^{21}$Ne(α,n)$^{24}$Mg, $^{25}$Mg(α,n)$^{28}$Si, and $^{26}$Mg(α,n)$^{29}$Si. The released protons then capture onto various nuclei, including $^{26}$Mg and $^{23}$Na,
in (p,\(\gamma\)) reactions while the released neutrons undergo (n,\(\gamma\)) reactions on such nuclei as \(^{20}\text{Ne}\), \(^{24}\text{Mg}\), and \(^{28}\text{Si}\) [125][118][202][276].

### 2.3 Chlorine-36 and Calcium-41

\(^{36}\text{Cl}\) has an effective mean lifetime of \(\approx 434,000\) years, the disintegration occurring 98.1\% of the time by beta-minus decay to the ground state of \(^{36}\text{Ar}\) and 1.9\% and 0.0015\% of the time by electron capture and beta-plus decay (see appendix B), respectively, each to the ground state of \(^{36}\text{S}\). \(^{41}\text{Ca}\) has a mean lifetime of \(\approx 149,000\) years, the disintegration occurring by electron capture to the ground state of \(^{41}\text{K}\). Figures (2.2) and (2.3) feature the corresponding energy-level diagrams [37][190]. Both radioactive isotopes are produced in AGB stars or the AGB stage of stellar evolution during helium-intershell burning, as well as in massive stars during hydrostatic helium-core and -shell burning via the s-process and hydrostatic oxygen-core and -shell burning and explosive oxygen-shell burning via neutron-capture reactions from neutrons released in the breakdown of heavy nuclei.

![Energy-level diagram for decay of \(^{36}\text{Cl}\) [37].](attachment:image)

The s-process of helium-core burning occurs near helium exhaustion as temperatures in the core rise above \(2.5 \times 10^8\) K and, in turn, allow efficient release of neutrons by \(^{22}\text{Ne}(\alpha,n)^{26}\text{Mg}\). The
substantial abundance of $^{22}\text{Ne}$ is attributable to the earlier destruction of $^{14}\text{N}$, produced in CNO-cycle processing during hydrogen-core burning, via $^{14}\text{N}(\alpha,\gamma)^{18}\text{F} (\beta^{+}\nu)^{18}\text{O} (\alpha,\gamma)^{22}\text{Ne}$. Winds from Wolf-Rayet stars or the Wolf-Rayet stage of stellar evolution aid in the dispersal of the freshly-synthesized yields of $^{36}\text{Cl}$ and $^{41}\text{Ca}$ into the ISM once convection transports the nuclei to the outer layers of the star.

Production of $^{36}\text{Cl}$ and $^{41}\text{Ca}$ via the s-process of helium-intershell burning occurs as thermal pulses activate the $^{22}\text{Ne}$ neutron source during the AGB stage of stellar evolution, the transient yet high neutron density necessary because the neutrons released via $^{13}\text{C}(\alpha,n)^{16}\text{O}$ span only the thin layer of the $^{13}\text{C}$ pocket while those of the $^{22}\text{Ne}$ source span the entire intershell together with the $^{35}\text{Cl}$ and $^{40}\text{Ca}$ seed nuclei. The $^{35}\text{Cl}(n,\gamma)^{36}\text{Cl}$ and $^{40}\text{Ca}(n,\gamma)^{41}\text{Ca}$ neutron-capture reactions can proceed at a much faster rate with the copious abundances of neutrons and $^{35}\text{Cl}$ and $^{40}\text{Ca}$ seed nuclei available across the intershell versus the meager abundances present in the $^{13}\text{C}$ pocket.

For massive stars undergoing oxygen-core and -shell burning, the neutrons released via $^{16}\text{O}(^{16}\text{O},n)^{31}\text{S}$ become available for capture by $^{35}\text{Cl}$ and $^{40}\text{Ca}$, thereby increasing the abundances of the radioactive isotopes, $^{36}\text{Cl}$ and $^{41}\text{Ca}$, within these regions of the star. The production of neutrons via $^{12}\text{C}(^{12}\text{C},n)^{23}\text{Mg}$ during carbon-core and -shell burning, as well as the neutrons released
in secondary reactions, such as $^{25}\text{Mg}(\alpha,n)^{28}\text{Si}$, $^{26}\text{Mg}(\alpha,n)^{29}\text{Si}$, and $^{26}\text{Mg}(p,n)^{28}\text{Si}$, during neon-core and -shell burning, also contribute to the synthesis of $^{36}\text{Cl}$ and $^{41}\text{Ca}$.

Explosive oxygen-shell burning yields similar products to that of hydrostatic oxygen-core and -shell burning. Explosive carbon- and neon-shell burning also exhibit a similar spectrum of products to that of the corresponding hydrostatic core- and shell-burning phases, with additional production of neutron-rich isotopes from $A = 36$-$88$ attributable to capture of neutrons liberated in $(\alpha,n)$ reactions [125][118][202][276].

### 2.4 Manganese-53

$^{53}\text{Mn}$ has a mean lifetime of $\approx 5,396,000$ years, the disintegration occurring by electron capture (see appendix B) to the ground state of $^{53}\text{Cr}$, the energy-level diagram visible in Fig. (2.4) [271][7]. It is produced in massive stars during hydrostatic oxygen- and silicon-core and -shell burning, and during explosive oxygen- and silicon-shell burning. The following reactions encompass the fusion of two $^{16}\text{O}$ nuclei in oxygen burning: $^{16}\text{O}(^{16}\text{O},^{31}\text{S})n$, $^{16}\text{O}(^{16}\text{O},^{31}\text{P})p$, $^{16}\text{O}(^{16}\text{O},^{30}\text{Si})2p$, $^{16}\text{O}(^{16}\text{O},^{30}\text{P})d$, and $^{16}\text{O}(^{16}\text{O},^{28}\text{Si})\alpha$. These unbound protons, neutrons, and $\alpha$-particles then interact with other nuclei not yet disassociated to form intermediate-mass isotopes of Si, S, Cl, Ar, K, Ca, Ti, and Cr, including $^{28}\text{Si}$, $^{32,33,34}\text{S}$, $^{35,37}\text{Cl}$, $^{36,38}\text{Ar}$, $^{39,41}\text{K}$, $^{40,42}\text{Ca}$, $^{46}\text{Ti}$, and $^{50}\text{Cr}$. Concurrently, photo-disintegration reactions provide another source of light particles, as the temperature has reached a value ($\approx 1.5$-$3 \times 10^9$ K) to incite such destruction of weakly-bound nuclei. Heavy nuclei synthesized via the $s$-process in earlier phases of helium, carbon, and neon burning are now destroyed by energetic photons as these high shell temperatures result in significant probability of decay via $(\gamma,p)$, $(\gamma,n)$, and $(\gamma,\alpha)$ reactions. The light particles also aid in the creation of the aforementioned heavier and more tightly-bound nuclei via $p$-, $n$-, and $\alpha$-capture reactions.

During oxygen burning, the forward and reverse reactions among pairs of nuclei begin to advance at the same rate. As the temperature of the system rises throughout the evolution, additional forward and reverse reaction pairs soon operate at those rates and various equilibrium clusters of nuclei take form. Such reactions that achieve balance include $^{28}\text{Si}(n,\gamma)^{29}\text{Si}$ and $^{29}\text{Si}(\gamma,n)^{28}\text{Si}$, and $^{29}\text{Si}(p,\gamma)^{30}\text{P}$ and $^{30}\text{Si}(\gamma,p)^{29}\text{Si}$, with the rates of all three reactions in mutual equilibrium. Near the completion of oxygen burning, two large clusters remain in balance, one with nuclei in the mass range $24 \leq A \leq 46$ and the other with iron-peak nuclei. $^{53}\text{Mn}$ is produced in the decay of $^{53}\text{Fe}$,
one of the iron-peak nuclei created in the build-up of heavy isotopes during these quasi-statistical equilibrium processes.

The most abundant products of oxygen burning, $^{28}\text{Si}$ and $^{31}\text{S}$, suffer destruction via photodisintegration reactions during silicon burning, breaking down to protons, neutrons, and $\alpha$-particles before reassembling into $^{28}\text{Si}$ and heavier S, Ar, Ca, Ti, Cr, Fe, and Ni isotopes as the light particles capture onto $^{28}\text{Si}$, $^{31}\text{S}$, and other nuclei. As before during oxygen burning, the synthesis of $^{53}\text{Fe}$ in this build-up of heavy nuclei and its subsequent decay results in the production of $^{53}\text{Mn}$. For even higher temperatures possibly reached during hydrostatic silicon-shell burning and within the inner layers undergoing hydrostatic oxygen-core and -shell burning, and absolutely acquired during explosive silicon-shell burning, the subset of reactions connecting the previously-established equilibrium clusters begin to come into balance with the cluster reactions. Soon after the onset of silicon burning, the two clusters merge into a single cluster in which all reactions propagate at the same rate and the system has, in turn, achieved full nuclear statistical equilibrium. Such an equilibrium dissipates as the matter expands and the temperature cools in response to the passing shock wave. Due to the inactivity of reactions from decreasing temperature and density and to the large abundance of $\alpha$-particles that remain unbound after shock passage, this process is called $\alpha$-rich freeze-out [125][118][202][276].
2.5 Iron-60

$^{60}\text{Fe}$ has a mean lifetime of $\approx 3,780,000$ years, the disintegration occurring by beta-minus decay (see appendix B) to an excited metastable state of $^{60}\text{Co}$ in the energy-level diagram of Fig. (2.5) [52][198]. It is produced in AGB stars or the AGB stage of stellar evolution during helium-intershell burning, as well as in massive stars (initial mass $\geq 20 \, M_\odot$) during hydrostatic and explosive helium-shell and carbon-shell burning, via neutron captures on unstable $^{59}\text{Fe}$ nuclei in the s-process and n-process. Minimal production also occurs via the s-process during hydrostatic helium-core burning, the freshly-synthesized nuclei expelled to the ISM in the winds of Wolf-Rayet stars or the Wolf-Rayet stage of stellar evolution. For temperatures greater than $2 \times 10^9$ K, significant destruction of $^{60}\text{Fe}$ occurs via photo-disintegrations and proton-capture reactions. Below this upper limit, though, $^{60}\text{Fe}$ is destroyed as $^{60}\text{Fe}(n,\gamma)^{61}\text{Fe}$ at a rate always prevalent over that of its $\beta^-$ decay.

![Energy-level diagram for decay of $^{60}\text{Fe}$](image)

Figure 2.5: Energy-level diagram for decay of $^{60}\text{Fe}$ [52].

Competition between the neutron-capture rate of $^{59}\text{Fe}$ and its $\beta^-$-decay rate determines the production rate of $^{60}\text{Fe}$ during these burning phases. Equating the two rates provides an order-of-magnitude estimate of the neutron densities and corresponding temperatures necessary for crossing
the $^{59}\text{Fe}$ bottleneck. The neutron density, and thus temperature, must be high enough for the rate of neutron capture of $^{59}\text{Fe}$ to exceed that of its $\beta^-$ decay and hence result in a net abundance increase of $^{60}\text{Fe}$. But if the neutron density and corresponding temperature is too high, much of the freshly-synthesized $^{60}\text{Fe}$ will be subsequently consumed via photo-disintegrations and proton captures.

The neutron densities achieved via $^{13}\text{C}(\alpha,n)^{16}\text{O}$ during helium burning of the interpulse periods in the $\alpha$- and $^{12}\text{C}$-rich radiative intershell in low-mass AGB stars are not high enough for the neutron-capture rate of unstable $^{59}\text{Fe}$ to compete with its corresponding decay rate. Production of $^{60}\text{Fe}$ is thus inhibited because much of the neutron-capture flow across the iron isotopes terminates with the decay of $^{59}\text{Fe}$. However, for AGB stars of initial mass greater than $\approx 3.5\ M_\odot$, the peak temperatures reached in the intershell cause the activation of the $^{22}\text{Ne}(\alpha,n)^{25}\text{Mg}$ neutron source. Such a source yields neutron densities several orders of magnitude larger than the $^{13}\text{C}$ neutron source, thereby resulting in significant production of $^{60}\text{Fe}$ since the decay of $^{59}\text{Fe}$ can no longer compete.

Helium and carbon core-burning temperatures in massive stars ($20\ M_\odot \leq M \leq M_\odot 120$) are too low ($\leq 3 \times 10^8\ K$) for the subsequent neutron densities to result in significant production of $^{60}\text{Fe}$. Shell-burning temperatures, on the other hand, are above that minimum value of $\approx 4 \times 10^8\ K$ such that neutron densities via $^{22}\text{Ne}(\alpha,n)^{25}\text{Mg}$ aid in the creation of much $^{60}\text{Fe}$. While abundant during helium burning, $\alpha$-particles for the $^{22}\text{Ne}$ neutron source during carbon burning arise by $^{12}\text{C}^{(12}\text{C,}\alpha)$ at temperatures in excess of $\approx 10^9\ K$. Neon-shell burning also produces a large amount of neutrons. However, the transitory nature of this convective shell prevents the transportation and build-up of ample $^{60}\text{Fe}$ in the outer layers of the star.

Because of the ephemeral timescales ($\approx 1\ s$) involved in explosive burning, it is only during explosive carbon burning that the peak temperatures reached contribute to appreciable neutron densities and corresponding $^{60}\text{Fe}$ production. For lower peak temperatures, not enough neutrons are released during the explosion to result in a sizeable synthesis of $^{60}\text{Fe}$. And too much $^{60}\text{Fe}$ is destroyed for higher peak temperatures. The temperatures and neutron densities achieved during explosive burning fall between those values representative of the s- and r-processes, and such a neutron-burst process has been designated as the n-process [125][118][202][276].
2.6 Iodine-129 and Hafnium-182

$^{129}$I has a mean lifetime of $\approx 22,650,000$ years while $^{182}$Hf has a mean lifetime of $\approx 12,980,000$ years, the disintegrations occurring by beta-minus decay (see appendix B) to an excited state of $^{129}$Xe and an excited state of $^{182}$Ta, respectively. Figure (2.6) depicts the energy-level diagram for the decay of $^{129}$I [58][274] and Fig. (2.7) depicts the corresponding $^{182}$Hf diagram [234]. Both are produced in bulk via the r-process at a site that remains inconclusive as the source of this nucleosynthesis (see appendix H).

![Energy-level diagram for decay of $^{129}$I](image)

Figure 2.6: Energy-level diagram for decay of $^{129}$I [58].

Negligible amounts of $^{129}$I and $^{182}$Hf are also made via the s-process in AGB stars or the AGB stage of stellar evolution during helium-intershell / burning. $^{129}$I is produced by neutron captures on Te isotopes followed by the $\beta$-decay of $^{129}$Te, expressed as $^{126}$Te(n,\(\gamma\))$^{127}$Te (n,\(\gamma\))$^{128}$Te (n,\(\gamma\))$^{129}$Te ($\beta\(-\)$)$^{129}$I. Production of $^{129}$I can also occur as neutron captures on $^{127}$I and $^{128}$I via $^{127}$I(n,\(\gamma\))$^{128}$I(n,\(\gamma\))$^{129}$I. However, the short mean lifetimes of $^{127}$Te ($\approx 13.5$ hours) and $^{128}$I ($\approx 36$ minutes) inhibit the build-up of $^{129}$Te and $^{129}$I, as the rate of decay of the branching isotopes exceeds their corresponding neutron-capture rates. Similarly, $^{182}$Hf is produced as neutron captures across the following chain of Hf isotopes: $^{176}$Hf(n,\(\gamma\))$^{177}$Hf (n,\(\gamma\))$^{178}$Hf (n,\(\gamma\))$^{179}$Hf (n,\(\gamma\))$^{180}$Hf (n,\(\gamma\))$^{181}$Hf (n,\(\gamma\))$^{182}$Hf.
But the short mean lifetime of $^{181}$Hf ($\approx 61$ days and decreased by a factor of 30 for helium-burning conditions) results in much of the flow proceeding through the $\beta^-$-decay of $^{181}$Hf to $^{181}$Ta.

Finally, substantial contributions to the abundances of $^{129}$I and $^{182}$Hf come also from the n-process during explosive helium burning of massive stars. As mentioned previously for $^{60}$Fe nucleosynthesis, the temperatures and densities achieved during explosive burning reside between those values representative of the s- and r-processes. Such burning parameters are sufficient for significant branching across the unstable $^{128}$I and $^{181}$Hf isotopes to occur via $^{128}$I(n,γ)$^{129}$I and $^{181}$Hf(n,γ)$^{182}$Hf, thereby increasing the $^{129}$I and $^{182}$Hf yields relative to their corresponding s-process yields [125][118][202][276].

### 2.7 Palladium-107

$^{107}$Pd has a mean lifetime of $\approx 9,380,000$ years, the disintegration occurring by beta-minus decay (see appendix B) to the ground state of $^{107}$Ag emphasized in the energy-level diagram of Fig. (2.8) [1][9]. It is produced in both the s-process and r-process (see appendix H), the former via helium-intershell burning in AGB stars or during the AGB stage of stellar evolution [153][276].
2.8 Samarium-146

\(^{146}\text{Sm}\), produced solely in the p-process [118][153][178], has a mean lifetime of \(\approx 148,600,000\) years and disintegrates by alpha decay (see appendix B) to the ground state of \(^{246}\text{U}\) (Fig. (2.9) [197]).

Figure 2.8: Energy-level diagram for decay of \(^{107}\text{Pd}\) [9].

\[ \begin{align*}
\text{\(^{107}\text{Pd}\) (6.5E+6 y)} & \quad 5/2^+ \quad 0^+ \\
\beta^- & \quad \text{decay} \quad 100.00\% \\
Q_{\beta^-} & \quad 0.0330 \\
& \quad \beta^- \quad 0.0 \quad 1/2^- \\
& \quad \text{\(^{107}\text{Ag}\) (stable)}
\end{align*} \]

Figure 2.9: Energy-level diagram for decay of \(^{146}\text{Sm}\) [197].
2.9 Plutonium-244

$^{244}\text{Pu}$ has an effective mean lifetime of $\approx 117,000,000$ years, the disintegration occurring predominantly by alpha decay (see appendix B) to the ground and first-excited states of $^{240}\text{U}$. The decay scheme of Fig. (2.10) illustrates both transitions [233][39]. Small ($\approx 0.121\%$) and negligible ($7.3 \times 10^{-9} \%$) fractions disintegrate via spontaneous fission and the rare, neutrinoless, double-beta-minus decay, respectively [29][162][207][144][98][251]. $^{244}\text{Pu}$ is produced solely in the r-process (see appendix H) [252][73][153].

![Energy-level diagram for decay of $^{244}\text{Pu}$](image)

Figure 2.10: Energy-level diagram for decay of $^{244}\text{Pu}$ [233].
Chapter 3

Yields

In the evolution of the Galaxy, a forming star is a sink for interstellar gas and dust. Once the star dies, however, it returns some of the mass it borrowed from the interstellar medium. That returned mass has been modified from its initial composition by stellar nucleosynthesis in typically becoming more enriched in heavier nuclear species. To follow how the abundances of species grow in the interstellar medium, GCE calculations thus need the enriched composition in the returned mass from stars of all initial masses from each stellar generation. This collection of data one terms the “stellar yields”. The current set of stellar yields for our GCE calculations include the following:

- **Massive Stars**: The yields for stars in the initial-mass range, $12 \leq M/M_\odot \leq 40$, are extracted from Ref. [276]. To accommodate species absent from this file, I have written XML stylesheets to add their yields. This allows us to include species like $^{127}$I, $^{129}$I, $^{180}$Hf, and $^{182}$Hf throughout the Galaxy’s evolution (see Refs. [179] and [180] for their relevance to our GCE calculations). As most of these species are secondary in nature, we scale their yields to the input stellar metallicity with the values at Solar metallicity inferred from those in Rauscher et al. (2002) [212].

- **Low-Mass Stars**: For now, low-mass stars simply return the composition they started with. This means I am not including the nucleosynthesis from these stars (i.e., the s-process in AGB stars [125][152]).

- **Type Ia Supernovae**: Thermonuclear supernovae are explosions of white-dwarf remnants left behind by dying low-mass stars. The mechanism for such supernovae is either single
degenerate, in which a single white dwarf accretes enough mass from a companion to ignite, or double degenerate, in which two white dwarfs merge violently and explode. For now, I am considering only single-degenerate thermonuclear supernovae and currently employing the W7 yields [196][249].

• **r Process:** In view of the current understanding, the r-process of nucleosynthesis occurs either in core-collapse supernovae or the merger of two neutron stars. For the yields from both, I do not use output from a particular model but rather data from the Solar-System r-process abundances. One of the great discoveries of stellar astronomy over the last few decades is the finding that extremely-low-metallicity stars, having formed early in the Galaxy from matter enriched by one or a few r-process events, comprise r-process elemental abundances in good agreement with the Solar r-process abundance pattern. The implication is that all r-process events produce similar isotopic yields (see appendix H for further review). I take this implication seriously and therefore use the Solar r-process abundances as my r-process yields. To simulate r-process nucleosynthesis from core-collapse supernovae, we include r-process material as part of that ejected mass (the amount a free parameter).

I consider radioactivities such as $^{129}$I to be the progenitors of the ultimate daughter species. Thus, for example, I place all of the r-process abundances of $^{129}$Xe into $^{129}$I. For the actinides such as $^{235}$U, $^{238}$U, and $^{232}$Th, I estimate yields by assuming equal progenitor abundances in the trans-uranium decay chains [122], the level chosen such that $^{232}$Th and $^{127}$I abundances in stars forming near the time of the Sun’s birth match the inferred Solar values.
Chapter 4

An Introduction to Galactic Chemical Evolution

To account for the abundances of short-lived radioactivities in the early Solar System, I have found it necessary to account for a non-homogeneous interstellar medium (ISM) and finite timescales for stellar lifetimes and events. Nevertheless, it is convenient to consider simple models of Galactic Chemical Evolution (GCE) that assume 1) the “instantaneous mixing approximation” (IMA) such that stellar ejecta instantaneously mix within the Galaxy (or region of the Galaxy under consideration) and 2) the “instantaneous recycling approximation” (IRA) such that stars that do return mass to the ISM do so instantaneously. In effect, the IRA divides stellar populations into two classes of stars. The first class is low-mass stars that live longer than the age of the Galaxy and simply lock up gas and dust over Galactic history. The second class is high-mass stars that have short lifetimes compared to the age of the Galaxy and are treated as forming and dying instantaneously. In the course of their (assumed instantaneous) lifetimes, they increment the mass fractions of heavy species and return a fraction $R$ of their mass to the ISM. The remaining mass $1 - R$ stays behind in a stellar remnant (a white dwarf, neutron star, or black hole). With the IMA and IRA, a set of analytic models can be developed that provide insight into GCE. In the next chapter, I will evaluate the validity of such analytic models in the light of more detailed numerical models.
4.1 Evolution of Gas Mass

I follow Tinsley (1980) [250] and Clayton (1985) [63] to develop analytic models of GCE. These authors express the evolution of the mass of gas in the disk of the Galaxy as

$$\frac{dM_G}{dt} = -\Psi (1 - R) + f(t).$$

Here, $M_G$ is the Galactic gas mass, $\Psi$ is the star-formation rate (mass of gas going into stars per unit time), and $f(t)$ is the infall rate (mass of Galactic halo material falling onto the disk to build it up per unit time). The IRA appears in this equation through the $(1 - R)$ term because of any mass going into stars, a fraction $R$ is returned instantaneously. This means a fraction $(1 - R)$ of the mass going into stars is lost from the gas forever as it is locked up into (infinitely) long-lived stars or stellar remnants. I follow Clayton and assume that the star-formation rate is linearly dependent on the gas mass; thus,

$$\Psi (1 - R) = \omega M_G,$$

where $\omega$ is the (assumed constant) gas-consumption rate with units of inverse time. For the time evolution of the gas mass, this yields

$$\frac{dM_G}{dt} = -\omega M_G + f(t). \quad (4.1)$$

In the absence of infall (the so-called “closed-box model”), the solution to Eq. (4.1) is an exponential decline of gas mass with time. In what follows, I instead assume an infall of metal-poor material from the halo onto the Galactic disk with the rate of transfer exponentially decaying on a timescale of 1 billion years. This choice of the infall function is motivated by the use of similar exponential infall in previous GCE models to account for various observational constraints of the Milky Way. For example, by incorporating an exponential infall with a radially-dependent timescale into their simple model of Galaxy evolution, Boissier & Prantzos (1999) [43] were able to accurately reproduce (to within error) the current gas surface density, final stellar surface density, current star-formation rate, current type-II supernova rate, G-dwarf differential metallicity distribution, and present-day mass function of the Solar neighborhood, and the total gas and star masses, current star-formation rate, current type-Ia and type-II supernova rates, and current gas, stellar, star-
formation-rate, and metallicity profiles of the Galactic disk as a whole. Thereby replacing \(f(t)\) of Eq. (4.1) with \(\frac{M_0}{\tau} e^{-\frac{t}{\tau}}\) leads to

\[
M_G(t) = \frac{M_0}{\tau} \frac{1}{\omega - \frac{1}{\tau}} \left( e^{-\frac{t}{\tau}} - e^{-\omega t} \right),
\]  

(4.2)

for the gas mass as a function of time via the use of an integrating factor in solving the linear first-order differential equation. If \(\frac{1}{\tau} < \omega\), Eq. (4.2) makes sense as written. However, if \(\frac{1}{\tau} > \omega\), ease of reading dictates we rewrite the equation as

\[
M_G(t) = \frac{M_0}{\tau} \frac{1}{\frac{1}{\tau} - \omega} \left( e^{-\omega t} - e^{-\frac{t}{\tau}} \right).
\]  

(4.3)

This form will ensure proper interpretation of the resulting mass fractions of primary and secondary species in the gas.

### 4.2 Evolution of Primary Mass Fraction

#### 4.2.1 Case 1: \(\frac{1}{\tau} < \omega\)

From Tinsley (1980) [250] and Clayton (1985) [63], the mass fraction of a stable primary species in the gas of the Galactic disk evolves as

\[
\frac{dZ_p}{dt} = y_z \omega - Z_p \frac{f(t)}{M_G(t)},
\]  

(4.4)

where \(y_z\) is the stellar yield of the primary species. What does that mean exactly? It is the increment in the mass of the primary species per increment in the mass of stars and remnants averaged over the initial mass function (IMF) for a stellar generation. It can be negative if, in fact, the species is destroyed by nuclear processing, positive if the species is newly-created, and zero if no change occurs inside a given star. Also a linear first-order differential equation, we may again utilize an integrating factor to solve for \(Z_p\) of Eq. (4.4) upon replacing \(f(t)\) and \(M_G(t)\) with their corresponding expressions. For the case in which \(\frac{1}{\tau} < \omega\) and the gas mass takes the form of Eq. (4.2), we find

\[
Z_p(t) = \frac{y_z \omega}{\beta} - \frac{y_z \omega t}{e^{\omega t} - 1},
\]  

(4.5)
where \( \beta \equiv \omega - \frac{1}{\tau} \).

In the long-time limit, for \( \beta t \gg 1 \), the second term vanishes as the exponential in the denominator blows up:

\[
Z_p(t \to \infty) \to \frac{y_z \omega}{\beta},
\]

(4.6)

the primary mass fraction approaching an asymptotic value at late times. To understand this behavior, we return to Eq. (4.4) and note, in particular, that

\[
\frac{f(t)}{M_G(t)} = \frac{\beta}{1 - e^{-\beta t}}
\]

(4.7)

from Eq. (4.2) and our expression for the exponential infall. At late times, \( \frac{f}{M_G} \to \beta \) and

\[
\frac{dZ_p}{dt} \to y_z \omega - \beta Z_p.
\]

In solving this equation for \( Z_p \) as a function of time, the long-time dependence of the primary mass fraction is then to reach the steady-state value given by Eq. (4.6). Because the gas-consumption timescale (inverse of \( \omega \)) is longer than the infall timescale, there is time for the infall rate to catch up to and come into balance with the star-formation rate (proportional to \( M_G(t) \)). The rate of enrichment of the primary mass fraction by instantaneously-dying stars then equals its rate of dilution by metal-poor infall; hence, a constant value for \( Z_p \) is attained.

In the short-time limit, for \( \beta t \ll 1 \), we may expand the exponential in the denominator of the second term to second-order in \( t \) (neglecting all negligible higher-order \( t \) terms) to simplify Eq. (4.5) accordingly:

\[
Z_p(t \to 0) \to \frac{y_z \omega}{\beta} - \frac{y_z \omega t}{\beta t (1 + \frac{1}{2} \beta t)}
\]

\[
= \frac{y_z \omega}{\beta} - \frac{y_z \omega}{\beta} \left( \frac{1}{1 + \frac{1}{2} \beta t} \right).
\]
Likewise, we may expand the second factor of the second term:

\[ Z_p(t \to 0) \to \frac{y_z\omega}{\beta} - \frac{y_z\omega}{\beta} \left( 1 - \frac{1}{2} \beta t \right) \]

\[ \approx \frac{1}{2} y_z\omega t. \quad (4.8) \]

Early in the Galaxy, the halo has not yet had enough time to appreciably dilute the ISM. The star-formation rate grows linearly in time with the gas mass as it builds up from the halo. Correspondingly, the rate at which stars instantaneously die and inject their matter into the ISM grows linearly in time with the rising gas mass. Hence, the growing reservoir of the Galactic disk is continually enriched by successively larger amounts of the ejected primary species. The result, then, is the linear enrichment of the primary mass fraction of Eq. (4.8).

4.2.2 Case 2: \( \frac{1}{\tau} > \omega \)

For the case in which \( \frac{1}{\tau} > \omega \) and the gas mass takes the form of Eq. (4.3), we find

\[ Z_p(t) = \frac{y_z\omega t}{1 - e^{-\beta t}} - \frac{y_z\omega}{\beta}, \quad (4.9) \]

where, now, \( \beta \equiv \frac{1}{\tau} - \omega \). In the long-time limit, for \( \beta t \gg 1 \), the exponential in the denominator of the first term vanishes:

\[ Z_p(t \to \infty) \to y_z\omega t - \frac{y_z\omega}{\beta}. \quad (4.10) \]

To understand this behavior, now note that

\[ \frac{f(t)}{M_G(t)} = \frac{\beta}{e^{\beta t} - 1} \]

and, therefore, at late times, \( \frac{1}{M_G} \to 0 \) and the solution to Eq. (4.4) for the primary mass fraction, in turn, approaches a linear dependence in time. Because the star-formation timescale exceeds the infall timescale, the infall eventually shuts off and the Galaxy simply enriches its primary mass fraction in time with the ejecta from the instantaneously-dying stars. By a similar expansion to that in the case for \( \omega - \frac{1}{\tau} \), the short-time behavior here proves identical to the former case. Whereas, in the short-time limit, the dying stars continually add primary abundances to a growing reservoir, in
the long-time limit, they add to a dwindling reservoir (see Fig. ) since the halo no longer contributes mass. Although the stellar death and injection rate decreases linearly in time with the falling gas mass, fresh primary abundances still cumulatively add to the reservoir, albeit in smaller amounts. The net effect is a linear growth in the primary mass fraction at late times as governed by Eq. (4.10). Finally, a quick inspection of Eqs. (4.5) and (4.9) reveals the symmetry of the two solutions, as one may be extracted from the other by changing the sign of $\beta$.

4.3 Evolution of Secondary Mass Fraction

From Clayton & Pantelaki (1986) [64], the yield of a stable secondary species varies in time in direct proportion to the primary mass fraction of the gas because the stellar nucleosynthesis of such species requires the presence of pre-existing primary metals. If stars form without the intake of primary isotopes (early in the Galaxy), then those stars will not produce and eject secondary isotopes. If, on the other hand, stars form from a gaseous reservoir abundant in primary isotopes, the amount of secondary isotopes produced and ejected will depend on the primary intake. The larger the primary mass fraction taken up by the star as it forms, the greater the number of seed nuclei to spawn secondary species and thus contribute to the eventual ejected secondary mass fraction. Figure (4.1) exposes the strong dependence of the secondary $^{17}$O yields on initial metallicity of a star of given initial mass, a pattern in stark contrast to the primary $^{16}$O yields of Fig. (5.2). Denoting the yield, $y_s$, as $\alpha Z_p(t)$ for some constant, $\alpha$, allows us to express the corresponding time evolution of the secondary mass fraction as

$$\frac{dZ_s}{dt} = y_s \omega - Z_s \frac{f(t)}{M_G(t)}$$

$$= \alpha \omega Z_p(t) - Z_s \frac{f(t)}{M_G(t)}. \quad (4.11)$$

4.3.1 Case 1: $\frac{1}{\tau} < \omega$

Somewhat more complicated, the time rate of change of the secondary mass fraction remains linear and first-order after replacing $Z_p(t)$ and $\frac{f(t)}{M_G(t)}$ in Eq. (4.11) with Eqs. (4.5) and (4.7),
respectively, for the case in which $\frac{1}{\tau} < \omega$. The solution becomes

$$Z_s(t) = \alpha y z \omega^2 \left[ -\frac{t^2}{2(e^{\beta t} - 1)} - \frac{t}{\beta(e^{\beta t} - 1)} + \frac{1}{\beta^2} \right].$$ \hspace{1cm} (4.12)

In the long-time limit, for $\beta t \gg 1$, the first and second terms inside the brackets vanish as the exponential in each denominator blows up:

$$Z_s(t \to \infty) \to \frac{\alpha y z \omega^2}{\beta^2},$$ \hspace{1cm} (4.13)

the secondary mass fraction approaching an asymptotic value at late times. By recalling the balance of the enrichment (stellar birth and instantaneous death) and dilution (infall from Galactic halo) rates at late times that led to a constant primary mass fraction, we may modify Eq. (4.11) to
understand the long-time limit for the evolution of the secondary mass fraction:

\[
\frac{dZ_s}{dt} = \frac{\alpha \omega^2 y_z}{\beta} - \beta Z_s,
\]

the asymptotic values for the primary mass fraction and \( \frac{f(t)}{M(t)} \) in place of their time dependencies. The solution to this equation in the long-time limit is that steady-state value of Eq. (4.13). The yield from the instantaneously-dying stars directly proportional to the gaseous primary mass fraction, the latter held constant implies the former will also be held constant across each stellar generation. The aforementioned balance of this continuous enrichment by the infall guarantees the constancy of the gaseous secondary mass fraction.

In the short-time limit, for \( \beta t \ll 1 \), we may double-expand (as above for the primary mass fraction) the exponential in the denominator of the first and second terms of Eq. (4.12) to acquire a quadratic growth of the secondary mass fraction:

\[
Z_s(t \to 0) \to \alpha y_z \omega^2 \left( \frac{1}{2} t^2 + \frac{1}{2\beta} t \right).
\]

In the absence of significant infall early in the Galaxy, stellar yields dominate the contamination of the ISM by primary and secondary isotopes. We previously deduced the linear enrichment of the primary mass fraction. The rate at which instantaneously-dying stars inject secondary isotopes will thereby grow with time, \( t \), a faster growth in the gaseous secondary mass fraction (quadratic as opposed to linear) the result.

### 4.3.2 Case 2: \( \frac{1}{\tau} > \omega \)

For the case in which \( \frac{1}{\tau} > \omega \), the secondary mass fraction varies as

\[
Z_s(t) = \alpha y_z \omega^2 \left[ \frac{t^2}{2(1 - e(1 - \beta t))} - \frac{t}{\beta(1 - e(1 - \beta t))} + \frac{1}{\beta^2} \right], \quad (4.14)
\]

the symmetry with the prior case enabling extraction via \( \beta \to -\beta \) in Eq. (4.12). In the long-time limit, for \( \beta \) (now \( \frac{1}{\tau} - \omega t \) \( \gg 1 \)), the quadratic nature of the secondary mass fraction is immediately apparent in the vanishing of the exponential in the denominator of the first and second terms:

\[
Z_s(t \to \infty) \to \alpha y_z \omega^2 \left[ \frac{1}{2} t^2 - \frac{1}{\beta} t + \frac{1}{\beta^2} \right].
\]
As we saw with the primary mass fraction, the cessation of infall at late times facilitates its linear time evolution. And the last discussion illuminated the ensuing faster rise in the gaseous secondary mass fraction, though at early times. Just as the infall had yet to appreciably kick in early in the Galaxy, so, too, does it lack a strong kick late in the Galaxy when the halo has mostly depleted. Analogous quadratic growths of the gaseous secondary mass fraction thereby emerge. Regarding the short-time limit, for $\beta t \ll 1$, it is identical to that for the case in which $\frac{1}{\tau} < \omega$. 
Chapter 5

Comparison of Simple GCE Models with ICE

In chapter 4, I examined the governing equations of GCE in the context of the instantaneous mixing and recycling approximations. I presented solutions to these equations under the assumption of metal-poor infall that declined exponentially in time. In this chapter, I compare these results to calculations with ICE, the numerical GCE model I have developed with Dr. Bradley Meyer of Clemson University. The comparisons necessarily and constantly refer back to the equations of chapter 4. Some of the computational details of ICE (an Inhomogeneous Chemical Evolution code suite) are provided in Appendix F. In summary, ICE models a heterogeneous ISM, follows the formation of stars and their finite lifetimes, computes the enrichment of the mass fractions of species in the ISM from stellar activity, and records the abundances with which new stars form. To compare with the analytic model presented in chapter 4, I use ICE to model the evolution of a single ISM zone (with exponentially declining infall in time). I first assume stars with mass $M \geq 1 \, M_\odot$ have short ($\approx 1$ day) lifetimes and stars with mass $M < 1 \, M_\odot$ have infinite lifetimes to allow the numerical model to mimic the IRA. I then restore the finite stellar lifetimes to see their effect on simple GCE models. I explore, in particular, the evolution of the ISM gas mass and abundances of a primary (taken to be $^{16}\text{O}$) and secondary (taken to be $^{17}\text{O}$) species. Through this study, I confirm ICE’s capabilities and gain insight into details of GCE.
5.1 IRA: Contradiction between Analytic and Numerical Models

For a chosen set of free parameters (star-formation timescale, total mass, schmidt exponent, halo-mix timescale, etc.), the evolution of the primary $^{16}$O mass fraction as a function of time in our numerical model is highlighted by the red curve of Fig. (5.1). The blue curve follows the corresponding exact analytic solution of Eq. (4.9) (since the figure implies $\frac{1}{r} > \omega$). The numerical solution falls off the analytic solution at late times, for $t > 10.5$ Gyr. Distinct from the analytic definition of "yields", stellar "yields" in our numerical model are a collection of abundances for each combination of initial stellar mass and metallicity (12, 13, 15, 18, 20, 22, 25, 30, 35, and 40 $M_{\odot}$, and 0, $10^{-4}$, $10^{-2}$, 0.1, 0.5, 1, and 2 $Z/Z_{\odot}$, from Woosley & Weaver (1995) [276]) inclusive of the ISM intake as the stars formed and freshly-produced material from stellar and explosive nucleosynthesis. Rather than average over the IMF for a stellar generation like the analytic model, the contamination of the ISM by these yields is dictated by the number and initial mass (see appendix D and appendix E) and metallicity of stars created during each time step. Because we do not possess yields for stars of
all initial masses and metallicities, the code embodying our numerical model carries out a bi-linear interpolation in $Z/Z_\odot$ and $M/M_\odot$ to approximate the intermediate yields.

To understand the fall-off, we must return to the time evolution of the primary mass fraction in the work of Tinsley and Clayton. To arrive at Eq. (4.4), they first considered the evolution of the gaseous primary mass:

$$\frac{d(Z_p M_G)}{dt} = -Z_p (1 - R) \Psi + y_z (1 - R) \Psi$$

$$\equiv -Z_p \Psi - R \Psi + y_z (1 - R) \Psi,$$

where the first term accounts for the gaseous primary mass consumed by forming stars, the second term accounts for the instantaneous return to the ISM of unprocessed primary mass, and the final term accounts for the newly-created or destroyed primary mass averaged over the IMF for a stellar generation. If $y_z > 0$, then this fresh mass is added to the mass of the species taken in as the star formed. If $y_z < 0$, then part of that initial gaseous primary mass the star forms with is destroyed and what is left in a given star is the difference between the initial and destroyed amounts.

In our model, however, we do not separately return the unprocessed material:

$$\frac{d(Z_p M_G)}{dt} = -Z_p \Psi + y_z (1 - R) \Psi,$$

(5.1)

where the interpolated "yield", $y_z$, is the mix of old (unprocessed) and new (stellar-produced) material ejected by instantaneously-dying stars of varying initial masses and metallicities. As the yields from Woosley & Weaver (1995) [276] contain the final abundances in a star of given initial mass and metallicity at the conclusion of nucleosynthesis, they may only take on positive values. If a particular species is not present, then it was never there to begin with or completely destroyed during a given star’s evolution. We may shed light on the evolution of the primary mass fraction through a simple re-arrangement of Eq. (5.1) with the assistance of Eq. (4.1):

$$\frac{dZ_p}{dt} = y_z \omega - Z_p \frac{R}{1 - R} \omega - Z_p \frac{f(t)}{M_G(t)},$$

(5.2)

indeed markedly different from Eq. (4.9) by the addition of the middle term. In the long-time limit,
we found in § 4.2.2 that \( \frac{f(t)}{\dot{M_G}(t)} \to 0 \). Thereby neglecting the final term of Eq. (5.2) culminates in
\[
Z_p(t) = y_z \frac{1 - R}{R} \left( 1 - e^{-\frac{R}{R} \omega t} \right)
\]
for the behavior of the primary mass fraction at late times, its value falling off from the linear growth of Eq. (4.10) in approaching the asymptotic value of \( y_z \frac{1 - R}{R} \). Had we extended the duration of our calculation in evolving the Galaxy, the fall-off of the red curve in Fig. (5.1) would surely have steepened as the \(^{16}\text{O}\) mass fraction leveled off in agreement with the late-time evolution of Eq. (5.3).

### 5.2 The Fix

#### 5.2.1 \(^{16}\text{O}\) Only

To remedy the discrepancy in the previous section and ensure the validity of our numerical model in aligning with the results of the analytic model in the limit of instantaneous lifetimes, consider the simplest scenario in which stars are composed of \(^{1}\text{H}\) and both the \(^{16}\text{O}\) they form with and produce during their evolution. No other isotopes are created or destroyed in the stars and ISM. Upon death, stars return the entirety of their mass and leave behind no remnants. Figure (5.2) illustrates the \(^{16}\text{O}\) yields for stars of varying initial masses and metallicities [276]. To simulate the averaging of the yields over the IMF for a stellar generation in the analytic model, I computed the average yield across all initial masses and metallicities denoted by the squares in Fig. (5.2).

A striking feature of the yields is their more or less apparent lack of dependence on the initial metallicity of a star of given initial mass, thus confirming the primary nature of \(^{16}\text{O}\). Disregarding initial metallicities of 0 and \(10^{-4} \frac{Z}{Z_\odot}\) due to the small yields for high initial masses, I defined that value of 0.0835694 as the average fraction of \(^{16}\text{O}\) produced by a star of given initial mass and metallicity. Although the mass fraction is identical, stars of different initial masses will, of course, eject different amounts of \(^{16}\text{O}\). For a star of given initial mass, assume an upper limit of 20 for initial \(Z/Z_\odot\). Since the ISM contains only \(^{3}\text{H}\) and \(^{16}\text{O}\), the initial metallicity (sum of mass fractions for isotopes heavier than hydrogen and helium) of the star as it forms is simply the ISM mass fraction of \(^{16}\text{O}\). When the star dies, the ejected yield, then, will be the sum of this unprocessed gaseous mass fraction (20\(Z_\odot\), or, 0.4) and newly-created mass fraction (0.0835694).
We next construct the following points, $(0, 0.0835694)$ and $(0.4, 0.4835694)$, and linearly interpolate to acquire the intermediate yields as a function of initial metallicity for a given initial mass:

$$y(Z) = 0.0835694 + 0.1Z.$$  

Once we know how the yields vary with initial metallicity for a given initial mass, we may interpolate in the “initial mass” direction to complete the so-called landscape of intermediate yields as a function of initial mass and metallicity bounded by the values of 1 and 40 for initial $M/M_\odot$ and aforementioned values of 0 and 20 for initial $Z/Z_\odot$. Figure (5.3) is the output from the endeavor, displaying the gaseous $^{16}$O mass fraction as a function of time for the analytic (blue circles) and our numerical (solid red curve) model. Per the discussion in § 4.2.2, the remarkable fit of the exact analytic solution to the data courtesy of the bi-linear interpolation is unsurprising since the short- and long-time limits of the gaseous $^{16}$O mass fraction are linear. With modest change between these limits, it is not difficult for the interpolation to succeed in approximating near-identical yields to
Figure 5.3: Mass fraction of $^{16}\text{O}$ in the gas for a single-zone IRA calculation (solid red curve) and the exact solution of Eq. (4.9) (blue circles). Those as predicted by the analytic solution.

5.2.2 $^{16}\text{O}$ and $^{17}\text{O}$

How does the gaseous mass fraction of a secondary species compare to the prediction from the exact analytic solution of Eq. (4.14)? In the short- and long-time limits, the behavior of the solution approaches that of a parabola. Choosing endpoints to bi-linearly interpolate the intermediate yields, as above, will therefore not suffice because the resulting line (along the “initial metallicity” or “initial mass” direction) is, by nature, not quadratic in time. The approximated yields will be grossly misrepresented. Multiple points, however, may serve our purpose, as many small line segments (or, “planes”, since the input is two-dimensional) connecting various initial masses and metallicities could suitably portray the landscape of intermediate yields. Likewise for the primary mass fraction, the endpoints here are easy to deduce. But what about yields for initial masses and metallicities between the endpoints. Somewhat of a cheat in a sense, yet preferably described as “reverse-engineering”, we must employ the analytic solution for the gaseous secondary mass fraction to fill in the remaining points of initial mass and metallicity.
For this scenario, then, stars are composed of $^1$H, both the $^{16}$O they form with and produce during their evolution, and both the $^{17}$O they form with and produce. No other isotopes are created or destroyed in the stars and ISM and dying stars return all mass. For stars that form from a gaseous reservoir with zero metallicity, the fraction of $^{16}$O they eject upon death is that mean value of 0.0835694. Because the yields of secondary isotopes require the presence of pre-existing primary metals, no $^{17}$O will be produced by such stars for a given initial mass. As the Galaxy evolves and stars form and die, enriching the ISM with their $^{16}$O and $^{17}$O content, the initial metallicity of newly-created stars will be the sum of the gaseous $^{16}$O and $^{17}$O mass fractions they form with in the absence of other heavy isotopes. We thereby compute the ejected $^{16}$O of dying stars as the sum of the initial fraction absorbed during the star’s formation (given by Eq. (4.9) and average freshly-synthesized yield (0.0835694). We compute the ejected $^{17}$O as the sum of the initial formation fraction (given by Eq. (4.14) and freshly-synthesized yield. Later stars having formed with the only primary metal, $^{16}$O, from the gas, we take the ejected freshly-synthesized yield of $^{17}$O as some factor, $\alpha$, of the initial $^{16}$O mass fraction in the star (Eq. (4.9)). To summarize,

$$^{16}\text{O}_{\text{yield}} = ^{16}\text{O}_{\text{gas}} + 0.0835694$$

$$= \frac{y_z \omega t}{1 - e^{-\beta t}} - \frac{y_z \omega}{\beta} + 0.0835694.$$ 

$$^{17}\text{O}_{\text{yield}} = ^{17}\text{O}_{\text{gas}} + \alpha^{16}\text{O}_{\text{gas}}$$

$$= \alpha y_z \omega \left( \frac{t^2}{2(1 - e^{\beta t})} - \frac{t}{\beta(1 - e^{\beta t})} + \frac{1}{\beta^2} \right) + \alpha \frac{y_z \omega t}{1 - e^{-\beta t}} - \alpha \frac{y_z \omega}{\beta},$$

where $y_z = 0.08375$, $\omega = 1.185 \times 10^{-10} \text{ yr}^{-1}$, and $\alpha = 1 \times 10^{-3}$ for the arbitrarily-chosen constants. The halo contributing mass to the ISM on a timescale of 1 billion years, the value for $\beta$ becomes $10^{-9} \text{ yr}^{-1} - 1.185 \times 10^{-10} \text{ yr}^{-1}$, or, $8.815 \times 10^{-10} \text{ yr}^{-1}$.

We are free to include as little or as many values for the $^{16}$O and $^{17}$O yields in the input file. As we add more and more values, we expect the analytic fit to the data to continually improve.
Figure 5.4: Mass fraction of $^{17}$O in the gas for a single-zone IRA calculation (solid red curve) and the exact solution of Eq. (4.14) (blue circles) for 5 mass-metallicity-yield points.

Figure 5.5: Mass fraction of $^{17}$O in the gas for a single-zone IRA calculation (solid red curve) and the exact solution of Eq. (4.14) (blue circles) for 8 mass-metallicity-yield points.
Figure 5.6: Mass fraction of $^{17}$O in the gas for a single-zone IRA calculation (solid red curve) and the exact solution of Eq. (4.14) (blue circles) for 14 mass-metallicity-yield points.

Figure 5.7: Mass fraction of $^{17}$O in the gas for a single-zone IRA calculation (solid red) and the exact solution of Eq. (4.14) (blue circles) for 27 mass-metallicity-yield points.
Figure 5.8: Disk gas mass for a single-zone IRA calculation (solid red) and the exact solution of Eq. (4.14) (blue circles).

As evidenced by Figs. (5.4), (5.5), (5.6), and (5.7) for the gaseous $^{17}$O mass fraction as a function of time in the analytic (blue circles) and our numerical (solid red curve) model, the yield from the data relaxes to the exact analytic value with more and more points for the code to interpolate between and better fit the tiny planes to the intermediate yields landscape. Again, the linear behavior of the primary $^{16}$O mass fraction at early and late times, with slight detour in between, removes any visible dependence on the number of mass-metallicity-yield points in the file. Although we manually contructed the yields of $^{16}$O and $^{17}$O as functions of initial metallicity for a given initial mass based on the exact analytic time evolution of said species in the ISM, the code still has much work to do in successfully mixing the stellar and ISM material after the number, initial mass, and location of stars are determined from the statistics of the processes. The agreement between the analytic and our numerical model is reassuring, to say the least. Figure (5.8) augments that agreement with the indistinguishable evolution of the disk gas mass in both models.
5.3 From Extreme (Instantaneous/Infinite) to Realistic (Finite) Lifetimes

Keeping all yields and parameters identical save for the stellar lifetimes, which are now gauged by

\[ t_{\text{main sequence}} \approx 10^{10} \left( \frac{M}{M_\odot} \right)^{-2.5} \text{yr} \]  

for stars on the main sequence [107]. Fig. (5.9) emphasizes the deviation in the gas mass of the Galactic disk when stars actually have time to evolve. Their mass remains locked up for millions (high-mass stars) or billions (low-mass stars) of years before it is finally returned to the ISM. Without that instantaneous addition early in the Galaxy, the gas mass cannot peak as high. Because the IMF is heavily weighted toward the creation of low-mass stars (on the order of 50% by mass for stars initially less than 1 $M_\odot$, as discussed in appendix E), much of the mass from dying stars is returned at least midway through the current evolution of the Galaxy, for $t > 6 \text{Gyr}$, and beyond. Following the peak in both calculations of Fig. (5.9), the gas mass of the non-IRA Galaxy declines at a slightly slower rate owing to this later return of stellar mass to the ISM. Had we extended the

Figure 5.9: Disk gas mass for a single-zone IRA (red) and non-IRA (blue) calculation.
Figure 5.10: Mass fraction of $^{16}\text{O}$ in the gas for a single-zone IRA (red) and non-IRA (blue) calculation.

duration of both calculations, surely the gas mass of the non-IRA calculation would have surpassed that of the IRA calculation as more and more low-mass stars extinguish their last flames in finally expelling mass back to the ISM billions of years later.

Figures (5.10) and (5.11) emphasize the deviation in the primary ($^{16}\text{O}$) and secondary ($^{17}\text{O}$) mass fractions of the Galactic disk when stars actually have time to evolve. The divergence of each isotope’s mass fraction from that of the IRA calculation begins early. But a glance at Fig. (5.9) suggests equivalent evolutions of the gas mass in both calculations up to roughly 750 million years. To clarify, we may zoom in on the time between 0 and 1 billion years, and even further between 0 and 200 million years. It is clear from Figs. (5.12) and (5.13) the equivalence breaks down after about 110 million years, hence the aforementioned immediate mass-fraction deviations.

Why does the output from the non-IRA calculation underestimate rather than overestimate that from the IRA calculation? From Eq. (5.4), the stellar main-sequence lifetime does not reach 500 million years for stars with initial mass greater than $3.3 \, M_\odot$. On the timescale of billions of years of Galactic evolution, the return of their mass millions of years later may as well be considered instantaneous and thus inconsequential in drastically impacting the gaseous composition relative to
Figure 5.11: Mass fraction of $^{17}$O in the gas for a single-zone IRA (red) and non-IRA (blue) calculation.

Figure 5.12: Disk gas mass for a single-zone IRA (red) and non-IRA (blue) calculation, zoomed in for $0 < t < 1$ Gyr.
that of the IRA calculation. The return of the low-mass stellar material, on the other hand, could arrive billions of years later. The instantaneous return of this material from many low-mass stars in the IRA calculation certainly increases the gas mass. That amount, however, pales in comparison to the mass of the ISM prior to enrichment, the size being on the order of $10^6 M_\odot$ in Fig. (5.9).

The increase in the mass of $^{16}$O and $^{17}$O during each time step as the instantaneously-dying stars eject their material far exceeds that of the corresponding increase in the gas mass. Holding back this stellar mass, then, as stars evolve for billions of years in the non-IRA calculation prevents the significant rise in the isotopic composition of the ISM as it gradually accumulates mass. The result is the reduced growth in the mass fractions of Figs. (5.10) and (5.11) when allowing stars time to evolve.

Figure 5.13: Disk gas mass for a single-zone IRA (red) and non-IRA (blue) calculation, zoomed in for $0 < t < 200$ Myr.
Chapter 6

Inhomogeneous GCE

A necessary first step before embarking on a series of calculations in pursuit of the project’s goals is a calibration of the code to determine the star-formation timescale. Observations yield a value of \( \approx 0.15 \) for the gas fraction of the Galactic disk at the current time of 13.5 Gyr \[43\]. To ensure compatibility with this value in augmenting the realism of our model, we conducted surveys characterized by one of a handful of star-formation timescales and the parameters hereunder. Beginning with the primordial composition of \(^1\)H, \(^2\)H, \(^3\)He, \(^4\)He, \(^6\)Li, \(^7\)Li, \(^9\)Be, and \(^{10}\)B \[68\][129][165][67], we allowed the Galaxy to evolve for 14 Gyr. For our particular study, we constructed a circular array of 32 zones to represent the Solar annulus, its mass growing by infall from a metal-poor halo on a timescale of 1 Gyr. Figure (6.1) provides a schematic of this structure and the mixing between components. A time-varying principle emulates the effect of 3 spiral arms of star formation \[54\][259] by proliferating mass in each zone 3 times every \( \approx 200 \) Myr \[114\], said zones, in turn, mixing with nearest neighbors on a timescale of 5 Myr. To clearly define the arms as tightly packed and highly peaked, we specified values of 100 and 200 for the amplitude and power, respectively, of the corresponding cosine function (see appendix F). Figure (6.2) provides a snapshot at 8.895 Gyr of this mass flow, the connection between the first and last zones completing the annular structure visible in Fig. (6.1). We allowed 1.66% of white-dwarf/low-mass-star binaries to explode as Type Ia supernovae on a timescale of 100 Myr and 100% of neutron-star/neutron-star binaries to merge on a timescale of 30 Myr.

Prior to running the surveys, we zeroed out the yields from dying stars. Instead of isotopic yields as discussed in chapter 3, stars simply returned ambiguous blobs of mass. Also, we did
Figure 6.1: Schematic of our Galactic structure consisting of 32 annular zones enclosing the halo zone and the ongoing mixing between them.
Figure 6.2: Snapshot of 3 spiral mass-density arms propagating across the Solar annulus.

not save any stars. Without the memory load attributable to keeping track of various isotopic abundances and long-lived stars as they formed, the code executed much faster in evolving the gas mass of the Galactic disk. Figures (6.3), (6.4), (6.5), (6.6), and (6.7) display the gas fraction of the Galactic disk at 13.5 Gyr as a function of the input star-formation timescale for a range of total disk masses. For increasing total mass, the gas fraction at 13.5 Gyr approaches a growth linear in the star-formation timescale. The wobble of points about the line for low total masses owes to the statistical fluctuations in the number of forming stars that smooth out as the total mass increases and more stars are created. As expected, the interpolated value for the correct star-formation timescale is nearly independent of the total disk mass in approaching a value of 1466 yr. With a Schmidt exponent of 1 (see appendix F), the star-formation rate as described in appendix D is proportional to the available gas mass of the Galactic disk. For a given star-formation timescale, then, more stars form from a reservoir of greater total mass (initially all gas). Although more gas of the ISM is consumed by the larger star formation, more of it is leftover relative to reservoirs of lower total mass such that the ratio to the total remains more or less fixed.

Only 1-2% of the mass of Giant Molecular Clouds (GMCs), the site of much star formation, condenses to create stars on a timescale of $10^7$ years. The low-mass bias of the initial mass function
results in many newborn stars having a mass similar to that of the Sun. Taking the mass of GMCs to be on the order of $10^5$-$10^6 \ M_\odot$, one may estimate the timescale for a star to form within the clouds as on the order of $10^3$ yr, in agreement with our value extracted from the simple ICE model. Such validation of our code boosts our confidence in its general applicability [87][187][280][191][141][32].

The pages following the surveys present a print-out of all options currently available for the user to tune ICE to his or her problem at hand, with default values listed where necessary.

Figure 6.3: Galactic-disk gas fraction at 13.5 Gyr as a function of star-formation timescale for $10^4 \ M_\odot$ of total mass.
Figure 6.4: Galactic-disk gas fraction at 13.5 Gyr as a function of star-formation timescale for $10^5 \, M_\odot$ of total mass.

Figure 6.5: Galactic-disk gas fraction at 13.5 Gyr as a function of star-formation timescale for $10^6 \, M_\odot$ of total mass.
Figure 6.6: Galactic-disk gas fraction at 13.5 Gyr as a function of star-formation timescale for 32 x 10^6 M☉ of total mass.

Figure 6.7: Galactic-disk gas fraction at 13.5 Gyr as a function of star-formation timescale for 10^7 M☉ of total mass.
All Allowed Options:

Help Options:
  --help                             print out usage statement and exit
  --example                          print out example usage and exit
  --response-file arg               can be specified with '@name', too
  --program_options arg             print out list of program options (help,
                                     general, output, yields, remnants,
                                     star_pop, graph, user, or all) and exit

General Options:
  --n_x_zones arg (=10)              Number of x zones
  --n_y_zones arg (=1)               Number of y zones
  --n_z_zones arg (=1)               Number of z zones
  --time arg (=0.)                   Initial time (years)
  --dt arg (=1.e5)                   Initial time step (years)
  --dtmax arg (=1.e5)                Maximum time step (years)
  --tend arg (=1.e9)                 Duration of calculation (years)
  --total_mass arg (=1.e8)          Total mass (solar masses)
  --seed arg                         Random number seed (optional)
  --small_abund arg (=1.e-25)        Small abundances threshold
  --small_rates arg (=1.e-25)        Small rates threshold
  --it_max arg (=100)                Maximum number of iterations in
                                     exponential solver
  --relative_tolerance arg (=1.e-8)  Relative tolerance for solutions
  --debug                            Print out debugging information about
                                     solutions (default: not set)
  --star_form arg (=1.e3)            star-formation timescale (years)
  --schmidt_exponent arg (=1.)       Schmidt exponent in star formation law
  --cloud_mix arg (=1.e6)            cloud-mixing timescale (years)
  --nuc_xpath arg                    XPath to select nuclei (default: all
                                     nuclides)
  --reac_xpath arg                   XPath to select reactions (default: all
                                     reactions)
  --zone_xpath arg                   XPath to select zones (default: all zones)
  --history_steps arg (=100)        History steps.
Output Options:
--steps arg (=50) Frequency of output to main hdf5 file.
--stars_hdf5_file arg Hdf5 file for star output:lower mass:upper mass (default: not set)

Yield options:
--yields_push_time arg Push time for yields in years (default: 0)
--solar_metallicity arg (=0.02) Solar metallicity (default: 0.02)
--zero_yields arg (=no) Zero the yields
--sn_r_proc_mass arg (=0) Mass of r process from a supernova

Remnants options:
--Ia_fraction arg (=0.05) Fraction of star/white dwarf systems that will become Ias
--Ia_time arg (=1.e8) Timescale (years) for Ia explosion on star/white dwarf system
--Ia_file arg Name of text file to record Ia events (default: not set)
--ns_merger_fraction arg (=0.01) Fraction of neutron star/neutron star systems that will merge
--ns_merger_time arg (=2.e8) Timescale (years) for neutron star/neutron star merger
--ns_merger_file arg Name of text file to record ns-ns merger events (default: not set)

Star Population Options:
--dev_file arg Name of text file for IMF deviate output (default: not set)
--imf_ml arg (=0.01) Lower limit of star mass for IMF
--imf_mu arg (=100) Upper limit of star mass for IMF
--mass_file arg Name of total mass output file
--pop_pts arg (=100) Number of mass points for POP output
--pop_file arg Name of text file for star population output (default: not set)

Graph Options:
--graph_file arg Name of dot file for output graph
--graph_step arg (=0) Time step for output graph

User-defined options:

General options:
--hot_mix arg hot-zone-mixing timescale in years (optional)
--halo_mix arg halo-zone-mixing timescale in years (optional)

X options:
--p_x arg power of cosine wave in x-direction (required if neither p_y nor p_z is set)
--A_x arg amplitude of cosine wave in x-direction (required if neither A_y nor A_z is set)
<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>--T_x arg</td>
<td>period of cosine wave in x-direction</td>
</tr>
<tr>
<td></td>
<td>(required if neither T_y nor T_z is set)</td>
</tr>
<tr>
<td>--m_x arg</td>
<td>multiplier of cosine wave in x-direction</td>
</tr>
<tr>
<td></td>
<td>(required if neither m_y nor m_z is set)</td>
</tr>
<tr>
<td>Y options:</td>
<td></td>
</tr>
<tr>
<td>--p_y arg</td>
<td>power of cosine wave in y-direction</td>
</tr>
<tr>
<td></td>
<td>(required if neither p_x nor p_z is set)</td>
</tr>
<tr>
<td>--A_y arg</td>
<td>amplitude of cosine wave in y-direction</td>
</tr>
<tr>
<td></td>
<td>(required if neither A_x nor A_z is set)</td>
</tr>
<tr>
<td>--T_y arg</td>
<td>period of cosine wave in y-direction</td>
</tr>
<tr>
<td></td>
<td>(required if neither T_x nor T_z is set)</td>
</tr>
<tr>
<td>--m_y arg</td>
<td>multiplier of cosine wave in y-direction</td>
</tr>
<tr>
<td></td>
<td>(required if neither m_x nor m_z is set)</td>
</tr>
<tr>
<td>Z options:</td>
<td></td>
</tr>
<tr>
<td>--p_z arg</td>
<td>power of cosine wave in z-direction</td>
</tr>
<tr>
<td></td>
<td>(required if neither p_x nor p_y is set)</td>
</tr>
<tr>
<td>--A_z arg</td>
<td>amplitude of cosine wave in z-direction</td>
</tr>
<tr>
<td></td>
<td>(required if neither A_x nor A_y is set)</td>
</tr>
<tr>
<td>--T_z arg</td>
<td>period of cosine wave in z-direction</td>
</tr>
<tr>
<td></td>
<td>(required if neither T_x nor T_y is set)</td>
</tr>
<tr>
<td>--m_z arg</td>
<td>multiplier of cosine wave in z-direction</td>
</tr>
<tr>
<td></td>
<td>(required if neither m_x nor m_y is set)</td>
</tr>
</tbody>
</table>
Chapter 7

Analysis of the Galactic Chemical Evolution of the Short-Lived Radioactivities

7.1 Halo + Single ISM Zone

Having considered only $^{16}$O and $^{17}$O in the simplified numerical IRA and non-IRA models of chapter 4 and chapter 5, we now replace the self-constructed yields with the full yields from chapter 3. In other words, we do not zero out the yields. Beginning with primordial composition, we evolve the Galaxy for nearly 12 Gyr. The metallicity of the ISM exceeded the largest value in the yield tables at that point and the calculation subsequently halted. With a star-formation timescale of 1450 yr, a value on the order of that acquired in the surveys of the previous chapter, total mass of $10^7 M_\odot$, Schmidt exponent of 1, and halo-infall timescale of 1 Gyr, we allowed 1.66% of white-dwarf/low-mass-star binaries to explode as Type Ia supernovae on a timescale of 100 Myr and 100% of neutron-star/neutron-star binaries to merge on a timescale of 30 Myr. As the ejecta from dying stars is too hot to mix instantaneously with the surrounding ISM, we first allowed the material to cool on a timescale of $10^7$ yr. What follows is a discussion of the gaseous mass-fraction evolution of various isotopes as compared to expectations from simple GCE.
7.1.1 $^{26}$Al and $^{27}$Al

Figure 7.1: Mass fractions of $^{26}$Al and $^{27}$Al in the gas for a single-zone, full-yield, non-IRA calculation with hot zones.

Figure (7.1) demonstrates the evolution of the $^{26}$Al and $^{27}$Al mass fractions in the gas of the ISM and Fig. (7.2) displays the corresponding ratio. While $^{26}$Al is a radioactive secondary species, its mass fraction approaching a steady-state value in the long-time limit [115], the stellar production of $^{27}$Al is characterized by both a primary and secondary component [62][220][64]. Its quadratically-growing mass fraction (alone in Fig. (7.3)) thereby reduces the overall ratio in Fig. (7.2) as time goes on.
Figure 7.2: Ratio of mass fractions of $^{26}$Al and $^{27}$Al in the gas for a single-zone, full-yield, non-IRA calculation with hot zones.

Figure 7.3: Zoomed-in mass fraction of $^{27}$Al in the gas for a single-zone, full-yield, non-IRA calculation with hot zones.
7.1.2 $^{60}$Fe and $^{56}$Fe

Figure 7.4: Mass fractions of $^{60}$Fe and $^{56}$Fe in the gas for a single-zone, full-yield, non-IRA calculation with hot zones.

Figure (7.4) demonstrates the evolution of the $^{60}$Fe and $^{56}$Fe mass fractions in the gas of the ISM. Similar to the growth of primary $^{56}$Fe, the mass fraction of radioactive $^{60}$Fe linearly increases in the long-time limit [115]. The corresponding ratio is therefore approximately constant at late times, as can be deduced from a quick inspection of Fig. (7.4).
7.1.3 $^{129}$I and $^{127}$I

Figure 7.5: Mass fractions of $^{129}$I and $^{127}$I in the gas for a single-zone, full-yield, non-IRA calculation with hot zones.

Figure (7.5) demonstrates the evolution of the $^{129}$I and $^{127}$I mass fractions in the gas of the ISM. As a primary radioactive species, we expect the mass fraction of $^{129}$I to approach a steady-state value in the long-time limit. However, the continuous contamination of the ISM by freshly-synthesized r-process material from merging neutron stars every 100-200 Myr, followed by decay on a timescale of the same order of magnitude, results in the oscillatory behavior of Fig. (7.5). The material from the mergers causes the mass fraction to peak but there is significant time shortly after for it to decay back down to a low level. Though the species may not achieve a constant mass fraction in the long-time limit, the average appears to do so.

A primary and secondary component contributing to its stellar production, the mass fraction of $^{127}$I in Fig. (7.6) thereby grows quadratically in time. By comparison to Fig. (7.3) for $^{27}$Al, the evolving mass fraction of $^{127}$I is not nearly as smooth. Since the nucleosynthetic contamination from dying stars is more frequent than that from merging neutron stars, the mass fraction of $^{127}$I becomes diluted by the former before rising again in the aftermath of the violent binary collisions. Hence, the growth takes on the jagged structure of Fig. (7.6). Beyond 7.5 Gyr, the occurrence of the mergers
Figure 7.6: Zoomed-in mass fraction of $^{127}\text{I}$ in the gas for a single-zone, full-yield, non-IRA calculation with hot zones.

Figure 7.7: Mass-fraction yield of multiple isotopes for Solar-metallicity stars of varying initial masses.
is more sparse and the dilution appears to strengthen as now the $^{127}\text{I}$ mass fraction suffers greater declines before increasing after each merger. Why the overpowering dilution? At these late times, dying low-mass stars finally return their low-metallicity mass to the ISM [115].

On a side note, massive stars also eject $^{129}\text{I}$ and $^{127}\text{I}$ with fractions on the order of $10^{-11}$ and $10^{-9}$, respectively. We averaged the yields per species across all initial stellar masses for the given initial Solar metallicity from Rauscher et al. (2002) [212] in Fig. (7.7) and allowed dying stars to eject amounts scaled to initial metallicity in addition to the yields as described in chapter 3. However, with fractions on the order of $10^{-3}$, the bulk of the yields for both species arrives as a consequence of the merging neutron stars.

### 7.1.4 $^{182}\text{Hf}$ and $^{180}\text{Hf}$

![Figure 7.8: Mass fractions of $^{182}\text{Hf}$ and $^{180}\text{Hf}$ in the gas for a single-zone, full-yield, non-IRA calculation with hot zones.](image)

The evolution of the $^{182}\text{Hf}$ and $^{180}\text{Hf}$ mass fractions in Fig. (7.8) is analogous to that of the $^{129}\text{I}$ and $^{127}\text{I}$ mass fractions, with $^{182}\text{Hf}$ in place of $^{129}\text{I}$ and $^{180}\text{Hf}$ in place of $^{127}\text{I}$. Yet, notice from Fig. (7.9) that the growth in the $^{180}\text{Hf}$ mass fraction is not influenced by the perpetual dilution from dying stars like $^{127}\text{I}$ in Fig (7.6). I can only offer the much less fraction of $^{180}\text{Hf}$ in the gas...
Figure 7.9: Zoomed-in mass fraction of $^{180}$Hf in the gas for a single-zone, full-yield, non-IRA calculation with hot zones.

relative to that of $^{127}$I, by a factor of a few or more, as the reason behind the reduced effect of the dilution on the $^{180}$Hf mass fraction.
7.2 Solar-Mass Stellar Composition: 1 ISM Zone vs. 32 ISM Zones

Likewise for the surveys to determine the star-formation timescale, we now consider Galactic evolution across 32 zones simulating the Solar annulus. All parameters specified in that first paragraph of chapter 6 are identical here, save for the inclusion of full yields. What follows is a comparison between the isotopic compositions of forming Solar-mass stars in the single- and multi-zone calculations. Each red dot in the forthcoming figures represents such a newborn star between 7 and 9 Gyr onward from the start of the Galaxy and the isotopic mass-fraction ratios it formed with. The x- and y-intercepts of the dashed lines are the values for the ratios inferred from meteoritic samples (see Tab. (1.1) of chapter 1)

7.2.1 Fe and Al

Figure 7.10: Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for 3 single-zone, full-yield, non-IRA calculations with hot zones and 1 without. The dashed lines represent the meteoritic values.
Figure 7.11: Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values.

The meteoritic values for the isotopic mass-fraction ratios of $^{60}\text{Fe}/^{56}\text{Fe}$ and $^{26}\text{Al}/^{27}\text{Al}$ in Figs. (7.10) and (7.11) are extracted from Refs. [84] and [146], respectively. The figures suggest a clear solution to the problem of the low iron mass-fraction ratio in the early Solar System. By implementing the instantaneous mixing of the hot stellar ejecta into a single ISM zone followed next by calculations in which we increase the cooling timescale prior to mixing, from 1 to 2 to $3 \times 10^7$ yr, we find that the iron ratio in many forming Solar-mass stars gradually descends toward and below a value about that measured in meteoritic samples.

Figure (7.11) provides the corresponding ratios in forming Solar-mass stars for the 32-zone calculation with a hot-ejecta cooling timescale of $10^7$ yr. The spatial extent of the annulus works in conjunction with the cooling timescale to allow for the Solar-mass stars to form with iron ratios closer to the “correct value”. Stars may now form in zones as near to or as far from the locations of recent dying stars, the average spatial correlation resulting in a bulk reduction of the iron ratios relative to those in forming Solar-mass stars of the single-zone calculation and a larger overall spread in the ratios. That spread to iron ratios between $4 \times 10^{-8}$ and $4 \times 10^{-7}$ corresponds to Solar-mass stars forming on the periphery or just outside of the high-density mass peaks as ejecta from dying stars mixes into low-mass valleys, their fractional compositions enhanced above those of the compressed peaks. Inside the peaks, however, the fraction of a particular species ejected by
dying stars diminishes by virtue of the sudden rise in total mass introduced by the propagating density waves and most Solar-mass stars here thereby form with ratios less than $4 \times 10^{-8}$.

Of course, the aluminum isotopic mass-fraction ratios in forming Solar-mass stars also plunge within the increased spread of the multi-zone calculation. Although these ratios are higher inside Solar-mass stars of the single-zone calculation in Fig. (7.10), they still fall well below the meteoritic value of $5 \times 10^{-5}$. Building out the structure of the Galaxy and enabling mixing between nearest neighbors only worsens the ratios. Neither the single- nor multi-zone calculation produces Solar-mass stars near the time of the Sun’s birth containing aluminum ratios in agreement with the value inferred from meteoritic samples.

### 7.2.2 Mn

![Figure 7.12](image)

**Figure 7.12:** Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the single-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values.
Figure 7.13: Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values.

From Fig. (7.12), Solar-mass stars near the time of the Sun’s birth form with too high a value for the $^{53}$Mn/$^{55}$Mn isotopic mass-fraction ratio in the single-zone calculation. The mixing within the greater spatial extent of the multi-zone annulus, on the other hand, ensures many Solar-mass stars form in zones as near to or as far from the locations of recent dying stars that contaminate their immediate surroundings with manganese and other isotopes, the average intake ratios reduced, about an overall spread, from those of the single-zone calculation. The forming Solar-mass stars of the spread, its cause discussed in § 7.2.1, consume matter comprising iron ratios in the aforementioned range of that subsection and manganese ratios between $5 \times 10^{-5}$ and $4 \times 10^{-4}$. Solar-mass stars created inside the high-density mass peaks acquire diminished fractional compositions relative to those of the single-zone calculation owing to attenuation from such large total masses, their manganese ratios above the meteoritic value but below $5 \times 10^{-5}$ for iron ratios about the “correct” value. Although no stars form with “correct” values for both ratios in Fig. (7.13), it is not difficult to imagine that further delaying the injection of the hot stellar ejecta into the ISM could allow for extra decay of $^{53}$Mn (as well as $^{60}$Fe) to levels in forming Solar-mass stars corresponding to both ratios being in agreement with the meteoritic values.
7.2.3 Ca

Figure 7.14: Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the single-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values.

Figure 7.15: Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values.
Opposite to the manganese isotopic mass-fraction ratios in Fig. (7.12) above, Solar-mass stars near the time of the Sun’s birth form with too low a value for the $^{41}\text{Ca}/^{40}\text{Ca}$ ratio in the single-zone calculation of Fig. (7.14). The net effect of the greater spatial extent in the multi-zone calculation, however, is the same: an average decrease in the calcium ratios, about an overall spread, relative to those in forming Solar-mass stars of the single-zone calculation. The bulk of the Solar-mass stars forming inside mass peaks encompass iron ratios about the “correct” value and calcium ratios below the meteoritic value but above $10^{-15}$ while the remainder defining the spread take in slightly higher ratios along both axes. Further delaying the mixing of the hot stellar ejecta into the ISM, while improving the manganese ratios, would only magnify the discrepancy between the results of our model and the meteoritic findings for the calcium ratios in Fig. (7.15).

7.2.4 Cl

Figure 7.16: Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the single-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values.
Figure 7.17: Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values.

The patterns for the $^{36}\text{Cl}/^{35}\text{Cl}$ isotopic mass-fraction ratios engulfed by forming Solar-mass stars near the time of the Sun’s birth in the single- and multi-zone calculations of Figs. (7.16) and (7.17), respectively, follow those of the calcium ratios above. Since the chlorine ratios inside Solar-mass stars of the single-zone calculation are too far under the meteoritic value, the overall spread enclosing their bulk decrease when expanding the spatial extent of the Galaxy is insufficient to account for Solar-mass stars with ratios near or at the “correct” value in Fig. (7.17) of the multi-zone calculation.
7.2.5 Pd

Figure 7.18: Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the single-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values.

Figure 7.19: Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values.
The middle case enclosed by the two bounds of the manganese and calcium isotopic mass-fraction ratios in Figs. (7.12) and (7.14) above, multiple Solar-mass stars near the time of the Sun’s birth form with the “correct” value for the $^{107}\text{Pd}/^{108}\text{Pd}$ ratio in the single-zone calculation of Fig. (7.18). The net effect of the greater spatial extent in the multi-zone calculation has now inverted to produce an average increase in the palladium ratios, about an overall spread, relative to those in forming Solar-mass stars of the single-zone calculation. The less-rapidly decaying $^{107}\text{Pd}$ survives in larger amounts of the ISM prior to star formation, its longer mean lifetime thereby counteracting its fractional attentuation by the high-density mass peaks. Despite much palladium production occurring in the r-process of binary neutron-star mergers, a significant component from massive-star shell nucleosynthesis emerges in the ejecta of dying stars. The source of that “floor” of the palladium ratios about $\approx 2 \times 10^{-5}$ and $\approx 5 \times 10^{-6}$ in the multi-zone calculation of Fig. (7.19) is the yields from this nucleosynthesis lifting the ratios in the long decay intervals between subsequent r-process events. The intensified star formation inside the mass peaks corresponds to a boost in the rate of Type II supernovae relative to that of the single-zone calculation, such constant contamination of the ISM accumulating the fractions of species relative to their initial compositions in the ejecta. The bulk of the Solar-mass stars thus form with palladium ratios between the minimum floor value of $3 \times 10^{-6}$ and $2 \times 10^{-2}$ for iron ratios about the “correct” value. The remainder form with ratios of the spread in Fig. (7.19).
7.2.6 I and Hf

Figure 7.20: Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the single-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values.

Figure 7.21: Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values.
From Figs. (7.20) and (7.21), it appears the greater spatial extent of the 32-zone annulus worked in favor of the iodine and hafnium isotopic mass-fraction ratios in lifting the latter inside Solar-mass stars to values about that inferred from meteoritic samples while creating more such stars containing the “correct” value for the former. As the mean lifetimes for $^{129}$I and $^{182}$Hf are on the order of tens of millions of years, similar to that for $^{107}$Pd, the enduring survival of these species opposes their fractional attenuation from the high-density mass peaks. Augmenting this resistance is the high ejection rate from dying stars of iodine and hafnium isotopes produced during massive-star shell nucleosynthesis, the frequent stellar explosions balancing the decay of $^{129}$I and $^{182}$Hf in the long intervals between subsequent r-process events that generate much of the yields for these species. The result is a range of iodine and hafnium ratios above minimum floor values (between $\approx 6 \times 10^{-6}$ and $\approx 3 \times 10^{-5}$ for the former and at $\approx 5 \times 10^{-5}$ for the latter) inside Solar-mass stars near the time of the Sun’s birth. The blue dots of Fig. (7.22) represent 330 Solar-mass stars, or, about 1.17% of all Solar-mass stars, containing iodine and hafnium isotopic mass-fraction ratios within a factor of 2 of the meteoritic values.

The blue dots of Figs. (7.20) and (7.21) are the output of a calculation in which we did not include iodine and hafnium isotopes with the ejected yields of dying stars. Such isotopes were only produced in the r-process of binary neutron-star mergers. To better understand this behavior,
Figure 7.23: Mass-fraction ratios from simple diffusion calculation for a mixing timescale of $10^6$ yr.

Figure 7.24: Mass-fraction ratios from simple diffusion calculation for a mixing timescale of $10^7$ yr.
we ran simple diffusion calculations for an annulus of 32 zones, each containing $10^6 M_\odot$ of Solar composition. We deposited 0.1 $M_\odot$ of Solar-distribution r-process material into zone 0 and allowed it to mix out on a timescale of $10^6$ yr, all other zones also permitted to mix with nearest neighbors on the same timescale. The curves of Fig. (7.23) replicate the behavior of the blue dots of Fig. (7.21), both patterns the sum of mixing and decay branches.

The mixing of material out of zone 0 is represented by the top-right component of the blue curve in Fig. (7.23). Soon, however, the decay of $^{129}$I and $^{182}$Hf kicks in and dominates as the blue curve bends slightly and the iodine and hafnium ratios decrease along a line until there is no more radioactive material in zone 0. As the material mixes out of and decays in zone 0, the iodine and hafnium ratios suddenly rise in zone 5 after the zone-0 material finally reaches this region. Again, though, the decay eventually dominates when the mixing “turns over” to it and the iodine and hafnium ratios decrease along the orange line until the radioactivities vanish. Because the material in zone 0 has to travel successively larger distances to zones 10 and 15, their iodine and hafnium ratios peak at successively smaller values owing to the longer time the zone-0 material has to decay before reaching said zones.

Figure (7.24) is the output from the same calculation but with a slightly longer mixing timescale of $10^7$ yr. That order of magnitude difference causes us to choose zones closer to zone 0 (1, 5, 10 vs. 5, 10, 15), as much more material would have decayed upon arrival at the far zones. The iodine and hafnium ratios in zones 5 and 10, in particular, though closer to zone 0, do not peak as high as the ratios in zones 10 and 15 of the calculation with the shorter mixing timescale.

The deposition of Solar-distribution r-process material into zone 0 and its mixing out into neighboring zones is representative of the ejection of r-process material from a binary neutron-star merger and its mixing out into the surrounding ISM in our multi-zone calculations of Fig. (7.21). For a given mixing timescale between adjacent zones of the Solar annulus, stars of a given zone will form with the rising iodine and hafnium mass-fraction ratios as the material from the merger reaches said zone. Likewise, stars of this zone will also form with the falling ratios after the decay has taken over. The different curves traced out by the blue dots for the mergers-only calculation of Fig. (7.21) correspond to forming Solar-mass stars in this and other zones in varying proximities to the location of that merger, the time of formation and distance from merger determining their isotopic compositions. Other mergers happening in separate zones lead to similar series of curves.

Without the floors of their ratios established by yields from massive-star shell nucleosynthe-
sis, our model cannot account for iodine and hafnium in the early Solar System. From Fig. (7.21), if these species are only produced in the r-process, then Solar-mass stars that form with the “correct” hafnium ratio also acquire too much iodine, as the longer mean lifetime of $^{129}$I prevents not nearly enough from decaying early. Solar-mass stars that form well after significant decay of $^{129}$I down to levels corresponding to agreement with the meteoritic ratio also take in too little hafnium. To compensate, the floor in the hafnium ratios lift these values in the ISM as Solar-mass stars form, their compositions reflecting a range of values due to steady stellar injection of the mass peaks but also the significant decay of $^{129}$I correlating to ratios about the meteoritic value.

The diffusion rooted in the curves of Figs. (7.23) and (7.24) accurately describes the behavior of the intake ratios of forming Solar-mass stars in the multi-zone calculation of Fig. (7.21). But the mathematics of the process imply material instantaneously arrives at all zones, whether near to or far from the location of a binary neutron-star merger. As this is clearly not realistic, does the approximation impact our results?

Suppose the annulus of the Galaxy has a radius of 8.5 kpc, or, $8.24 \times 10^{22}$ cm. A particle traveling at the speed of light would traverse halfway around the annulus in roughly 87,000 yr. As our annulus consists of 32 zones that mix with nearest neighbors on a timescale of 5 Myr (see chapter 6), a particle takes, on average, $16^2 \cdot 5$ Myr, or, 1.28 Gyr, to traverse halfway around. We may ignore the time prior to 87,000 yr because particles would be required to move at superluminal speeds. We may even ignore the time prior to 80 Myr since it takes 5 Myr to travel unimpeded between successive zones of our annulus. After this time, only a small amount of material, on average, would have mixed throughout half the annulus. Even though the mathematics dictate rapid mixing, those small initial amounts in all zones equivalent to the instantaneous results are irrelevant because, in our model, the annulus has not had adequate time to build-up steady-state ISM abundances from many generations of stellar birth and death. For our purposes, we are interested in the evolution of the Galaxy following a balance between stellar production and injection of fresh material into the ISM and its removal by decay and new episodes of star formation. The figures of § 7.1 indicate this could take close to 2 Gyr, well beyond the average time for material to traverse halfway around our annulus. Hence, we are not concerned about the mathematics governing early Galactic history in our model.
7.2.7 Other Isotopic Compositions of the 330 Solar-Mass Stars

The blue dots of Figs. (7.25), (7.26), (7.27), (7.28), and (7.29) represent the 330 Solar-mass stars that formed near the time of the Sun’s birth with iodine and hafnium mass-fraction ratios within a factor of 2 of the meteoritic values. In addition to forming with iron ratios about the meteoritic value, we find some of these stars also contain manganese and palladium ratios within a factor of a few of the meteoritic values. The aluminum, calcium, and chlorine ratios remain too low.

Figure 7.25: Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values.
Figure 7.26: Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values.

Figure 7.27: Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values.
Figure 7.28: Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values.

Figure 7.29: Mass-fraction ratios in forming Solar-mass stars near the time of the Sun’s birth for the multi-zone, full-yield, non-IRA calculation with hot zones. The dashed lines represent the meteoritic values.
Chapter 8

Analysis of the Galactic Chemical Evolution of the Long-Lived Radioactivities

Summary: Though my dissertation is on SLRs, I would like to include an analysis of my results for the long-lived radioactivities (LLRs), $^{40}$K, $^{235}$U, $^{238}$U, and $^{232}$Th. These isotopes have long been of interest for dating the age of the Galaxy. The new interest is in their influence on the internal heating of terrestrial-type exoplanets, which has a role, for example, in the outgassing of the planet’s atmosphere and possible techtonic activity. My introduction to LLRs came as a referee on the publication by M. Fatuzzo and F. Adams entitled ”Distributions of Long-lived Radioactive Nuclei Provided by Star-forming Environments” [88].

8.1 Potassium-40

$^{40}$K has an effective mean lifetime of $\approx 1,800,000$ years, the disintegration occurring 89.14% of the time by beta-minus decay to the ground state of $^{40}$Ca, 0.02% and 10.66% of the time by electron capture to the ground and an excited state of $^{40}$Ar, respectively, and 0.001% of the time by beta-plus decay (see appendix B) to an excited state of $^{40}$Ar. Figure (8.1) [158] encompasses all transitions. $^{40}$K is produced in massive stars during hydrostatic helium-core and -shell burning
via the s-process and explosive oxygen-shell burning via neutron-capture reactions from neutrons released in the breakdown of heavy nuclei \cite{276,62,153}.

### 8.2 Uranium-235 and Uranium-238

$^{235}$U has an effective mean lifetime of $\approx 1,015,000,000$ years, the disintegration occurring predominantly by alpha decay (see appendix B) to the excited states of $^{231}$Th highlighted in the energy-level diagram of Fig. (8.2) \cite{160}. Negligible fractions disintegrate via cluster decay ($8 \times 10^{-10}$\%) and spontaneous fission ($7 \times 10^{-9}$) \cite{99,51,29,162,207,144}. $^{238}$U has an effective mean lifetime of $\approx 6,446,000,000$ years, the disintegration occurring predominantly by alpha decay (see appendix B) to the ground and excited states of $^{234}$Th illustrated by the decay schemes of Figs. (8.3) \cite{161} and (8.4) \cite{50}. Small ($\approx 0.0000545\%$) and negligible ($2.2 \times 10^{-10}$\%) fractions disintegrate via spontaneous fission and the rare, neutrinoless, double-beta-minus decay, respectively \cite{29,162,207,144,100,251}. Both isotopes are produced solely in the r-process (see appendix H) \cite{252,73,153}.
Figure 8.2: Energy-level diagram for decay of $^{235}\text{U}$ [160].

Figure 8.3: Energy-level diagram for decay of $^{238}\text{U}$ [161].
8.3 Thorium-232

$^{232}$Th has an effective mean lifetime of $\approx 20,200,000,000$ years, the disintegration occurring predominantly by alpha decay (see appendix B) to the ground and excited states of $^{228}$Ra outlined by the various levels in Figs. (8.5) and (8.6). Negligible fractions disintegrate via cluster decay ($2.78 \times 10^{-10}$%) and spontaneous fission ($1.1 \times 10^{-9}$) [101][29][162][207][144]. $^{232}$Th is produced solely in the r-process (see appendix H) [252][73][153].

Figure 8.5: Energy-level diagram for decay of $^{232}$Th [159].
8.4 Future Analysis

Figure 8.6: Energy-level diagram for decay of $^{232}$Th [20].

Figure 8.7: Average mass fractions of $^{235}$U, $^{238}$U, and $^{232}$Th across all zones of the annulus as a function of time.
Chapter 9

Conclusions

From the results of chapter 7, the forming of Solar-mass stars near the time of the Sun’s birth with $^{60}\text{Fe}/^{56}\text{Fe}$ isotopic mass-fraction ratios about the meteoritic value appears to be a natural consequence of our model. Therefore, we can confidently accomodate the $^{60}\text{Fe}$ abundance in the early Solar System. To alleviate the low $^{26}\text{Al}/^{27}\text{Al}$ isotopic mass-fraction ratios inside these stars, we must resort to a special scenario, several of which are briefly discussed in chapter 1 and another I published with colleagues at the University of Chicago [84].

Our results confirm Solar-mass stars near the time of the Sun’s birth also form with agreeable iodine abundances in the wake of a rare binary neutron-star merger and a long decay afterwards. To balance an otherwise similar decay for $^{182}\text{Hf}$ in the ISM prior to star formation, ejecta containing freshly-synthesized abundances from massive-star shells raise the corresponding hafnium ratios to values about that inferred from meteoritic samples. Our model thus correlates the abundances

<table>
<thead>
<tr>
<th>Radionuclide</th>
<th>Model Succeeds</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{26}\text{Al}$</td>
<td>X</td>
</tr>
<tr>
<td>$^{36}\text{Cl}$</td>
<td>X</td>
</tr>
<tr>
<td>$^{41}\text{Ca}$</td>
<td>X</td>
</tr>
<tr>
<td>$^{53}\text{Mn}$</td>
<td>✓</td>
</tr>
<tr>
<td>$^{60}\text{Fe}$</td>
<td>✓</td>
</tr>
<tr>
<td>$^{107}\text{Pd}$</td>
<td>✓</td>
</tr>
<tr>
<td>$^{129}\text{I}$</td>
<td>✓</td>
</tr>
<tr>
<td>$^{182}\text{Hf}$</td>
<td>✓</td>
</tr>
</tbody>
</table>

Table 9.1

From the results of chapter 7, the forming of Solar-mass stars near the time of the Sun’s birth with $^{60}\text{Fe}/^{56}\text{Fe}$ isotopic mass-fraction ratios about the meteoritic value appears to be a natural consequence of our model. Therefore, we can confidently accomodate the $^{60}\text{Fe}$ abundance in the early Solar System. To alleviate the low $^{26}\text{Al}/^{27}\text{Al}$ isotopic mass-fraction ratios inside these stars, we must resort to a special scenario, several of which are briefly discussed in chapter 1 and another I published with colleagues at the University of Chicago [84].

Our results confirm Solar-mass stars near the time of the Sun’s birth also form with agreeable iodine abundances in the wake of a rare binary neutron-star merger and a long decay afterwards. To balance an otherwise similar decay for $^{182}\text{Hf}$ in the ISM prior to star formation, ejecta containing freshly-synthesized abundances from massive-star shells raise the corresponding hafnium ratios to values about that inferred from meteoritic samples. Our model thus correlates the abundances

89
of $^{129}\text{I}$ and $^{182}\text{Hf}$ in the early Solar System, a link previously unsubstantiated and worth future investigations. The $^{107}\text{Pd}/^{108}\text{Pd}$ isotopic mass-fraction ratios in the ISM also benefit from the added production from massive-star shells following merger ejection and decay of $^{107}\text{Pd}$ yet the values are just under the meteoritic ratio as Solar-mass stars form. To within a factor of a few, then, our model can accommodate the ESS abundance of $^{107}\text{Pd}$.

Also to within a factor of a few, our model can accommodate the ESS abundance of $^{53}\text{Mn}$. Though Solar-mass stars near the time of the Sun’s birth form with $^{41}\text{Ca}/^{40}\text{Ca}$ isotopic mass-fraction ratios ranging across many orders of magnitude, they do not reach as high as the meteoritic value, especially inside stars containing the Solar hafnium and iodine abundances. Because $^{41}\text{Ca}$, however, may be injected along with $^{26}\text{Al}$ [27], we do not stress about the lack of reconciliation within the framework of our model. Likewise, our model fails to accommodate the ESS abundance of $^{36}\text{Cl}$, the corresponding ratios inside Solar-mass stars too low. As this species may be produced by irradiation in the early Solar System [270], we again do not agonize over the disagreement with the corresponding meteoritic ratios.
Appendices
Appendix A

Nuclear and Atomic Masses and Binding Energies

A.1 Definition of Mass Defect and Binding Energy

Atomic masses have been measured to be less than the sum of the masses of the nucleus and electrons:

\[ m_{\left(\frac{A}{Z}X\right)} < m_{\text{nuc}} + Zm_e, \]

where \( Z \) is the atomic number, \( A \) is the mass number, and \( m_{\left(\frac{A}{Z}X\right)}, m_{\text{nuc}}, \) and \( m_e \) are the masses of the isotope of element, \( X \), containing \( A - Z \) neutrons, the corresponding nucleus, and the electron, respectively. Similarly, the masses of nuclei have been measured to be less than the sum of the masses of their constituent nucleons:

\[ m_{\text{nuc}} < Zm_p + (A - Z)m_n, \]

where \( m_p \) and \( m_n \) are the masses of the nucleus and proton, respectively, and \( A \) is the mass number. As the atomic, nuclear, and particle masses all correspond to rest energies of \( m_{\left(\frac{A}{Z}X\right)}c^2, m_{\text{nuc}}c^2, m_pc^2, m_nc^2, \) and \( m_ec^2 \), such mass differences guarantee conservation of energy and thereby prevent the spontaneous dissociation of atoms into nuclei and electrons or nuclei into protons and neutrons.
The equivalent energies of these mass defects, 

\[ B_{A^Z_X} = [(m_{\text{nuc}} + Zm_e) - m(A^Z_X)]c^2 \]  

(A.1)

and

\[ B_{\text{nuc}} = [(Zm_p + (A - Z)m_n) - m_{\text{nuc}}]c^2, \]  

(A.2)

are the electron and nuclear binding energies, respectively, denoted as \( B_{A^Z_X} \) and \( B_{\text{nuc}} \). Energies of \( B_{A^Z_X} \) and \( B_{\text{nuc}} \) are released upon formation of an atom from a nucleus and electrons and formation of a nucleus from protons and neutrons. Likewise, \( |B_{A^Z_X}| \) and \( |B_{\text{nuc}}| \) are the minimum energies required to break-up an atom into its nucleus and electrons and a nucleus into its protons and neutrons [77][118]. [145][245]

A.2 Binding Energy as Applied Work

Consider the binding energy of a nucleus. The strong nuclear force between the protons and neutrons ensures the stability of the nucleus. Energy must therefore be imparted to break-up the nucleus into its constituent protons and neutrons. Imagine doing work, \( W_1 \), in slowly removing one nucleon from the nucleus and displacing it far away, so that the nucleon remains nearly at rest with no kinetic energy while the work is being done. All the work goes into increasing the potential energy of the nucleon-nucleus system. An infinite distance apart, the nucleon and nucleus of the system gained a mass, \( W_1/c^2 \), equivalent to this potential-energy change, per Einstein’s principle. In other words, the additional mass stores this increase in the system’s energy.

Now do work, \( W_2 \), in slowly removing another nucleon from the nucleus and displacing it an infinite distance away as well. Again, with no change in kinetic energy, the work is transferred to the potential energy of the nucleon-nucleon-nucleus system and the system’s mass increases by an amount, \( W_2/c^2 \). The additional mass once more stores this excess energy. Continue to slowly remove and infinitely displace the remaining nucleons, each successive system gaining mass equivalent to the work done at each step and the work deposited into each system’s mass build-up. Infinitely separated, all nucleons are free from the effects of all forces. Such work, then, is the minimum energy required to disband the nucleus, or, the binding energy.

Running the process in reverse, our gradual applied work in changing the potential energy of
the system as we reassemble the nucleus corresponds to a decrease in said nuclear mass relative to the
sum of nucleon masses. We removed, from the system, energy equivalent to this mass loss. In other
words, mass is dispersed from the system in the form of this energy. Such work, then, is the energy
released upon formation of the nucleus, or, the negative of the binding energy [30][105][199][257].

A.3 Determination of Binding Energies and Nuclear Masses

As the measurement of nuclear masses requires the extraction of all electrons, atomic mass
measurements have proven less difficult [118][216]. Consequently, most resources list atomic masses.
Can such accessible values benefit the determination of nuclear binding energies? Examine Eq. (A.1)
in calculating the mass of a hydrogen atom:

\[ m(\text{\textsuperscript{1}H}) = (m_{\text{nuc}} + m_e) - \frac{B_{\text{\textsuperscript{1}H}}}{c^2} \]

\[ = (m_p + m_e) - \frac{B_{\text{\textsuperscript{1}H}}}{c^2}, \]

since the nucleus of a hydrogen atom is a single proton. Now, solve for the mass of the proton and
replace \( m_p \) of Eq. (A.2) with that expression:

\[ B_{\text{nuc}} = \left[ Z \left( m(\text{\textsuperscript{1}H}) - m_e + \frac{B_{\text{\textsuperscript{1}H}}}{c^2} \right) + (A - Z)m_n - m_{\text{nuc}} \right] c^2. \] (A.3)

From Eq. (A.1), the mass of the nucleus of isotope, \( ^{\text{A}}_{\text{Z}}\text{X} \), is

\[ m_{\text{nuc}} = \frac{B_{\text{\textsuperscript{A}X}}}{c^2} + m(\text{\textsuperscript{A}X}) - Zm_e. \] (A.4)

Using this expression for \( m_{\text{nuc}} \) in Eq. (A.3), we obtain the following:

\[ B_{\text{nuc}} = \left[ Zm(\text{\textsuperscript{1}H}) - Zm_e + Z \frac{B_{\text{\textsuperscript{1}H}}}{c^2} + (A - Z)m_n - \frac{B_{\text{\textsuperscript{A}X}}}{c^2} - m(\text{\textsuperscript{A}X}) + Zm_e \right] c^2 \]

\[ = \left[ Zm(\text{\textsuperscript{1}H}) + Z \frac{B_{\text{\textsuperscript{1}H}}}{c^2} + (A - Z)m_n - \frac{B_{\text{\textsuperscript{A}X}}}{c^2} - m(\text{\textsuperscript{A}X}) \right] c^2. \] (A.5)
Because the electron binding energy of isotope, $^{A}X$, and $Z$ times the electron binding energy of a hydrogen atom, range from $10^{-10}$ eV, while $m(^1H)c^2$, $(A - Z)m_n c^2$, and $m(^A X)c^2$ all range from $10^9$-$10^{11}$ eV, the corresponding contributions of the electron binding energies to the nuclear binding energy in Eq. (A.5) is negligible. For a simple example, the electron binding energy of $^4He$ is 24.6 eV and 2 times the hydrogen-atom electron binding energy is 27.2 eV [272]. Their difference is only a few eV. The rest energies of $^1H$, the neutron, and $^4He$ are $9.38783 \times 10^8$ eV, $9.39565 \times 10^8$ eV, and $3.7284 \times 10^9$ eV, respectively [142]. The binding energy of a helium nucleus becomes $2.8296 \times 10^7$ eV without the electron binding energy difference versus $2.82960026 \times 10^7$ eV with the electron binding energy difference, an error on the order of $10^{-6}$%, in other words, negligible. Eq. (A.5) thereby approximately reduces to

$$B_{nuc} \approx [Zm(^1H) + (A - Z)m_n] - m(^A X), \quad (A.6)$$

thus allowing one to calculate nuclear binding energies in terms of the atomic masses of hydrogen and isotope, $^{A}X$, and the neutron mass [228][279].

From Eq. (A.4), the calculation of the nuclear mass of isotope, $^{A}X$, includes the electron binding energy of that isotope. Again, however, this electron binding energy, being many orders of magnitude less than the rest energies of that same isotope and the electron (24.6 eV for the electron binding energy of $^4He$ compared to rest energies of $3.7284 \times 10^9$ eV and $5.11 \times 10^5$ eV for $^4He$ and the electron, respectively [142]) allows us to simplify said determination:

$$m_{nuc} \approx m(^A X) - Zm_e,$$

which is how one would naively assume to extract the mass of the object center when that object consists of the center and electrons surrounding it [77]. Like the previously-defined nuclear binding energy of Eq. (A.6), this calculation also ensures the utilization of the abundance of atomic mass resources.
A.4 Binding Energy per Nucleon and Causes of Observable Patterns

If we sum our work done in displacing each nucleon to infinity and then divide by the total number of nucleons, we can gauge the average minimum energy needed to displace a given nucleon, or, the average binding energy per nucleon:

\[
\frac{B_{\text{nuc}}}{A} = \frac{[(Zm_p + (A - Z)m_n) - m_{\text{nuc}}]c^2}{A}
\]

\[
\approx \frac{[Zm(\text{^1H}) + (A - Z)m_n - m(\text{^2X})]c^2}{A}.
\]

Small or large, this quantity provides a measure of the strength of nuclear bonds trapping a given nucleon inside the nucleus. The greater the energy input to free a given nucleon, the stronger the bonds and the more stable that particular nucleus. Figure (A.1) illustrates the average binding energy per nucleon experimentally ascertained for select nuclei across a multitude of mass numbers.

Figure A.1: Average binding energy per nucleon as a function of mass number for select nuclei [76].

Figure (A.2) plots the same quantity but includes additional nuclei not accounted for in Fig. (A.1). The average binding energy per nucleon is lowest for the deuterium nucleus in these figures, the value measured at 1.1122865 $\text{MeV/nucleon}$. The average binding energy per nucleon increases sharply
Figure A.2: Average binding energy per nucleon as a function of mass number emphasizing more nuclei and, in turn, the granularity, or, spikes, of the curve [257].

for rising mass number to a value of 7.07391825 $MeV$/nucleon attributable to the $^4He$ nucleus. The values soon begin oscillating with growing mass number, the fluctuations superimposed upon a net increase until the maximum value of 8.7944965967742 $MeV$/nucleon for the $^{62}_{28}Ni$ nucleus is achieved, as indicated in Fig. (A.2). Further increasing the mass number causes a gradual decline in the average binding energy per nucleon, the $^{238}_{92}U$ nucleus characterized by a value of 7.5701458067227 $MeV$/nucleon in Figs. (A.1) and (A.2).

Encompassing many nuclei, the mean of the average binding energy per nucleon adopts a value of roughly 8 $MeV$/nucleon. The “iron-peak” nuclei, $Ti−V−Cr−Mn−Fe−Co−Ni−Cu−Zn$, exhibit the largest average binding energies per nucleon with values between 8.75-8.8 $MeV$/nucleon. This peak is conspicuous in Fig. (A.3) after zooming-in on the curves of Figs. (A.1) and (A.2). As the average minimum energy required to extract a given nucleon is greatest for these nuclei, such nuclear species are the most tightly-bound of all. Distinguished by the maximum average binding energy per nucleon, the $^{62}_{28}Ni$ nucleus is exceedingly resilient [11][35]. The fusion of nuclei to the left of $^{62}_{28}Ni$ in Fig. (A.2) inherently results in a nucleus of higher mass number and, consequently, more stable configuration. Likewise, fission of nuclei to the right of $^{63}_{28}Ni$ creates lighter nuclei of, again, more stable configurations. In both instances, the mass defects are transformed as kinetic energy of the products and/or $\gamma$-rays. On a side note, for the longest time, the $^{56}_{28}Fe$ nucleus was assumed to
Figure A.3: Average binding energy per nucleon as a function of mass number highlighting the “iron-peak” nuclei [118].

comprise the maximum average binding energy per nucleon. The article of reference[90] discusses in detail the fascinating misconception [143][15].

What is the cause of the aforementioned broad pattern in the average binding energy per nucleon with increasing mass number? There are two forces at work within a given nucleus: the attractive, short-range, strong nuclear force and the repulsive, long-range, weak electrostatic force, the former about 100 times stronger than the latter and acting only on a scale of $\sim 10^{-15} m$. The stability of said nucleus is subject to the effects of both forces, which are contingent on the number and type of nucleons present. For small nuclei, the strong nuclear force acts independent of nucleon type, overpowering neutrons and protons alike in mutual attraction. Nuclei of increasingly larger size contain more protons and/or neutrons that experience enhanced attraction via this force; hence, the overall surge in average binding energy per nucleon for $A \leq 20$ in Figs. (A.1) and (A.2).

For $A > 20$, the strong nuclear force is unable to extend beyond nearest neighbors to the nucleon excess, namely, it has saturated. Since the maximum attraction is felt by most nucleons, we would expect the minimum energy required to extract a given nucleon to remain essentially
unchanged as more nucleons are added. However, the negligible long-range effects of the strong nuclear force in the more massive nuclei allow the repulsive electrostatic force between protons to take effect in dictating stability. Each added proton for progressively larger nuclei inflates the net repulsion experienced by all other protons, thereby counteracting the attraction from nearest neighbors and reducing the average binding energy per nucleon. Such reduction is visible in Figs. (A.1) and (A.2) as the surge is halted and the curve begins sloping downward at $A = 20$. For $A > 62$, the net repulsion from growing $Z$ escalates in proportion to the near-constant circumferential attraction and the average binding energy per nucleon now decreases slightly to the value for the $^{238}{\text{U}}$ nucleus. Because the electrostatic force is many orders of magnitude weaker than the strong nuclear force, this drop-off is much less steep than the previous rise for $A < 20$. For $A > 209$, specifically the $^{209}{\text{Bi}}$ nucleus, the net repulsion finally exceeds attraction and no nuclei of any configuration are capable of preserving stability indefinitely, eventually succumbing to spontaneous decay.

Up until $A = 40$, the number of protons and neutrons in stable nuclei is comparable, if not identical. For $A > 40$, though, the number of neutrons far exceeds that of protons ($N \approx 1.7Z$), as the neutron abundance serves to increase separation between protons and thus diminish repulsion. Otherwise, the repulsion becomes great enough to disrupt stability. [257][105][30][13][77][76]

A.5 Historical Formulation of Binding Energy and Nuclear Mass Equations

Attempts at conceptual models of the nucleus beginning in 1929 prevailed in the development of a formula to describe the broad pattern of average binding energy per nucleon displayed in Figs. (A.1) and (A.2). In February of that year, George Gamow introduced the idea of the nucleus as a “liquid drop”. Following the discovery of the neutron by James Chadwick several years later in 1932, Werner Heisenberg and Ettore Majorana expanded on the foundation of the “liquid drop” model via consideration of exchange forces. In late 1935, Neils Bohr and associates applied the model in exploration of the compound nucleus to explain nuclear processes such as fission. During this same year, Carl Friedrich von Weizscker exploited the earlier work of Heisenberg and Majorana in positing a semi-empirical nuclear-masss formula that would prove advantageous in probing nuclear binding energies. [41][232][12][49]

The liquid-drop model envisions the nucleus consisting of a sea of nucleons in constant
motion and collisions. By analogy to the cohesive forces sustaining the structural integrity of a liquid, the net attraction from competing strong nuclear and electrostatic forces retains the spherical shape of the nucleus. As the binding energy per nucleon in Figs. (A.1) and (A.2) is almost constant for $A > 50$, a first approximation for the total binding energy of the nucleus is to assume the strong nuclear force extends only to nearest neighbors, per the argument above. Because each nucleon feels the same circumferential effect from the strong nuclear force, a greater number of nucleons in heavier nuclei should result in a linear increase in the total binding energy of the nucleus, a contribution expressed as $a_1 A$ for some constant, $a_1$. Nucleons on the surface of the nuclear sphere, however, do not have as many neighbors as nucleons in the core. Denoting the radius of the nucleus as $R$ and since $R \propto A^{\frac{1}{3}}$, the number of surface nucleons grows relative to the surface area as $A^{\frac{2}{3}}$. The total nuclear binding energy must therefore lessen from that of the former assumption by an amount, $a_2 A^{\frac{2}{3}}$, for some constant, $a_2$.

The next effect to quantify is due to the repulsion between protons. If we regard the nucleus as a sphere of uniform charge density of radius, $R$, the total work done in assembling the $Z$ protons from infinity into increasingly-larger, concentric, thin, spherical shells up to radius, $R$, is given by the following:

$$W = \frac{3}{5} \frac{Z^2 e^2}{4\pi \epsilon_0 R}.$$  

For a single-proton nucleus, this equation reduces to

$$w = \frac{3}{5} \frac{e^2}{4\pi \epsilon_0 R},$$

where $e$ is the charge on the proton and $\epsilon_0$ is the permittivity of free space. But there is no work against repulsion necessary in moving a single proton from infinity. Such energy, then, is required to assemble an individual proton. As the protons already exist, we accordingly subtract the value of $w$ from $W$, and do so $Z$ times over to account for each proton:

$$W_{\text{total}} = \frac{3}{5} \frac{Z^2 e^2}{4\pi \epsilon_0 R} - Z \frac{3}{5} \frac{e^2}{4\pi \epsilon_0 R}$$

$$= \frac{3}{5} \frac{Z(Z - 1)e^2}{4\pi \epsilon_0 R}.$$

100
Referring to the definition of nuclear binding energy that initiated our discussion at the top of the appendix, $W_{total}$ is another contribution, rewritten as $a_3 \frac{Z(Z-1)}{A^{1/3}}$ with all constants embedded in $a_3$ and, again, $R \propto A^{1/3}$, that lessens the total.

The 3 classical effects described above are unable to elucidate the exceptional stability of lighter ($A < 20$) nuclei with $N = Z$, the peaks hidden in Figs. (A.1) and (A.2) yet revealed in Figs. (A.4) and (A.5) as experimental values of the average binding energy per nucleon for various isotopes and isotones. A perturbation to such stability, a consequence of quantum effects, occurs in nuclei with any significant imbalance between $N$ and $Z$, the drop-off in average binding energy per nucleon on either side of $N = Z$ nuclei in Figs. (A.4) and (A.5) accentuating these disruptions. The strength of the $N/Z$ correlation may be expressed as $a_4 \frac{(N-Z)^2}{A}$ for some constant, $a_4$, one combined outcome of squaring the difference between $N$ and $Z$ in the numerator and having $A$ in the denominator being a prominent reduction in the total nuclear binding energy for lighter nuclei with large discrepancies between $N$ and $Z$. Recalling from the prior analysis of Figs. (A.1) and (A.2) that $N \approx 1.7Z$ for heavier nuclei, another outcome of this term is the corresponding minimal binding-energy reduction for similar $N/Z$ discrepancies in nuclei with $A > 40$. For $N = Z$ nuclei,
the term goes away and there is no decline in the total nuclear binding energy, again in agreement with the behavior of the nuclei in Figs. (A.4) and (A.5).

The exceptional stability arising from quantum effects extends, as well, to even-even nuclei, those possessing an even number of both neutrons and protons. Observations convey the highest abundances in nature for these nuclei, a reflection of said stability. On the other hand, observations betray a dearth of odd-odd nuclei, indicative of their poor stability. Nuclei with even $N$ and odd $Z$ or odd $N$ and even $Z$ inhabit an intermediate stability range. The inclusion of a term, $\pm a_5 A^{-\frac{2}{3}}$, to the total nuclear binding energy allows for an accurate fit for even-even and odd-odd nuclei, with the positive sign (greater binding energy and, thus, stability) chosen for the former and negative sign (less binding energy) for the latter. For odd-$A$ nuclei, either even-$N$/odd-$Z$ or odd-$N$/even-$Z$, $a_5$ vanishes because the rest of the terms prove adequate in describing their total nuclear binding energy.

Together as a single equation, the 5 terms constitute the semi-empirical formula for the
Figure A.6: Ratio of measured to predict average binding energy per nucleon as a function of atomic number for select nuclei [228].

total nuclear binding energy:

\[ B_{\text{nuc}} = a_1 A - a_2 A^{\frac{5}{3}} - a_3 \frac{Z(Z-1)}{A^{\frac{2}{3}}} - a_4 \frac{(N-Z)^2}{A} \pm a_5 A^{-\frac{7}{4}}. \] (A.7)

For \( A > 14 \), the values, \( a_1 = 15.7 \text{ MeV} \), \( a_2 = 17.8 \text{ MeV} \), \( a_3 = 0.71 \text{ MeV} \), and \( a_4 = 23.6 \text{ MeV} \), produce an excellent fit of the theoretical expression to the experimental values of Figs. (A.1), (A.2), (A.4), and (A.5). Solely in terms of \( A \) and \( Z \), we can anticipate the determination of a wide range of nuclear masses via a rearrangement of Eq. (A.2):

\[ m_{\text{nuc}} = Zm_p + (A-Z)m_n - \frac{a_1}{c^2} A + \frac{a_2}{c^2} A^{\frac{5}{3}} + \frac{a_3}{c^2} \frac{Z(Z-1)}{A^{\frac{2}{3}}} + \frac{a_4}{c^2} \frac{(A-2Z)^2}{A} \pm \frac{a_5}{c^2} A^{-\frac{7}{4}}, \]

where \( N = A-Z \). This semi-empirical mass formula is ascribed to Carl Friedrich von Weizsacker for the work he carried out in the early 1930s. Comparison of theoretical binding-energy values computed employing Eq. (A.7) and experimental values acquired in the measurements of atomic masses by Eq. (A.6) demonstrate the relevance of the theoretical formula in simplifying the deduction of nuclear stability. Other models, like the shell model, further expound on these differences as presented in Fig. (A.6). As my intention here is to provide a summary of nuclear and atomic masses and binding energies, I shall leave supplementary investigations to the reader [261][262][203][77][228][181].
Appendix B

Nuclear Decay

B.1 Origins of the Radioactive Decay Law

The radioactive decay law as we know it today has its origins in the work of Ernest Rutherford and Frederick Soddy on thorium samples from the early 1900s [48][210][209], and later in the interpretations of Egon von Schweidler. Based on a fit of only 8 observations plotted in Fig. (B.1), Rutherford and Soddy concluded the “activity of $^{224}$Ra decreases very approximately in a geometrical progression with the time, i.e. if $I_0$ represent the initial activity and $I_t$ the activity after time $t$,

$$\frac{I_t}{I_0} = e^{-\lambda t}, \quad (B.1)$$

where $\lambda$ is a constant and $e$ the base of natural logarithms” and each “activity” is a current consisting of ions produced per second by particles projected from the sample in the apparatus. From Eq. (G.3), they then derived the relation between the initial number of “systems” and number at time, $t$, in the thorium samples:

$$\frac{N_t}{N_0} = e^{-\lambda t}, \quad (B.2)$$

where $N_0$ and $N_t$ are the numbers initially and at time, $t$, respectively. By differentiation of $N_t$,

$$\frac{dN_t}{dt} = -\lambda N_t, \quad (B.3)$$
Rutherford and Soddy (1902)

Figure B.1: Decay of thorium X and recovery of thorium vs. time for observations by Rutherford and Soddy.

Rutherford and Soddy found that “the rate of change of the system at any time is always proportional to the amount remaining unchanged”, where $dN$ is the differential change in $N_t$ during the differential time, $dt \equiv (t + dt) - t$, $N_t$ is the amount of the system at time, $t$, and $\lambda$ is the constant of proportionality describing the “proportional amount of radioactive matter that changes in unit time”. Coined the “radioactive constant”, $\lambda$ today is known to be unique to each radioactive nucleus, or, radionuclide, and mode of decay, independent of the radionuclide’s age, and impervious to changes by any physical or chemical means as well as temperature or pressure variations, though questions concerning the validity of constancy still linger [240]. The first and last of these properties of $\lambda$ suffered no arguments to the contrary in the experiments of Rutherford and Soddy [3][4][23][34][231].

Rutherford and Soddy alluded to the discrete nature of radioactive decay when describing in a publication “the expulsion of a charged particle” as the change that occurs [4][264], yet proceeded to embody said process with the empirical formula of Eq. (B.2). It was not until a couple of years later in 1905 that Egon von Schweidler considered fluctuations in the radioactive constant for small samples and was rewarded with confirmation via the experimental results of Fritz Kohlrausch. Von Schweidler understood the stochastic nature of radioactivity in which it was not possible to determine if and when a given radioactive atom will decay within a given time interval. Only a probability
may be associated with its decay in that duration. Analogously, the mean decay behavior for a large number of identical radioactive atoms may accurately be anticipated.

Von Schweidler interpreted $\lambda dt$ as the probability inherent to each radioactive atom for decaying within an infinitesimal time interval, a value independent of the sample size, and, subsequently, $e^{-\lambda t}$ as the corresponding probability for survival until time, $t$. From Eq. (B.3), the proportional, or, fractional, change in $N_t$, $\left| \frac{dN}{N_t} \right|$, represents how many atoms decay (favorable number of events) from that initial amount of $N_t$ (total number of events) and, thus, the probability of decay for a given atom during $dt$. From Eq. (B.2), $\frac{N_t}{N_0}$ represents how many atoms remain (favorable number of events) from that initial amount of $N_0$ (total number of events) and, thus, the probability of survival until time, $t$, for a given atom. In agreement with the deductions by Rutherford and Soddy, Von Schweidler hence successfully attributed the behavior of radioactive decay to a statistical phenomenon [23][69][172][22][186][235].
B.2 Numerics of the Radioactive Decay Law

It thereby follows that the radioactive constant, $\lambda$, gauges the instantaneous probability of decay per unit time for a given radioactive nucleus:

$$\lambda \equiv \lim_{\Delta t \to 0} \frac{\Delta N/N_t}{\Delta t}. \quad (B.4)$$

A measure of the radioactive constant during such infinitesimal time intervals will undoubtedly result in fluctuations (visible in Fig. (B.2)) that, when averaged across a hypothetical infinite number of experiments, diminish in accession to the true $\lambda$ value. Also, I switch to “nucleus” from “atom” in the previous discussion because in the time of Rutherford and Soddy, the nature of the atom and the effects of radioactive decay on its structure were still evolving.

Fundamental to exponential decline or growth processes, like radioactive decay, are constant timescales for some fraction of the sample to fall or rise. Specifically, the time for half of a radioactive sample to decay is determined by replacing $N_t$ with $N_0/2$ in Eq. (B.2) and solving for $t$:

$$e^{-\lambda T_{1/2}} = \frac{N(T_{1/2})}{N_0}$$

$$= \frac{N_0}{2N_0} \equiv \frac{N_0}{N_0}$$

$$\Rightarrow T_{1/2} = \frac{\ln(2)}{\lambda}. \quad (B.5)$$
After $n$ half-lives,

$$N(nT_{1/2}) = N_0 e^{-\lambda nT_{1/2}}$$

$$= N_0 \left( e^{-\frac{\lambda T_{1/2}}{2}} \right)^n$$

$$= N_0 \left( \frac{N_0}{2N_0} \right)^n$$

$$N(nT_{1/2}) = \frac{1}{2^n} N_0,$$

the initial number, $N_0$, of radionuclides in the sample has decreased by a factor of $2^n$. The remaining fraction, $\frac{N(nT_{1/2})}{N_0} \equiv f$, survived the passage of $-\ln(f) / \ln(2)$ half-lives of time:

$$N(nT_{1/2}) = \frac{1}{2^n} N_0$$

$$\Rightarrow 2^n = \frac{1}{f}$$

$$\Rightarrow n = -\frac{\ln(f)}{\ln(2)}.$$

By rearrangement of Eq. (B.5), the radioactive decay law of Eq. (B.2) may be expressed in terms
of the half-life:

\[
\frac{N_t}{N_0} = e^{-\frac{\ln(2)}{T_{1/2}} t}
\]

\[
= (e^{\ln(2)})^{-\frac{t}{T_{1/2}}}
\]

\[
= 2^{-\frac{t}{T_{1/2}}}
\]

\[
= \frac{1}{2^{\frac{t}{T_{1/2}}}}
\]

\[
\frac{N_t}{N_0} = \left(\frac{1}{2}\right)^{\frac{t}{T_{1/2}}}.
\]

What is the mean lifetime of a radionuclide in a sample? Originally ascertained by Egon von Schweidler in his 1905 statistical analysis and easily derived from the starting assumption of \(\lambda dt\) for the decay probability of a radionuclide within a small-enough time interval, a radionuclide’s survival probability until time, \(t\), is computed as \(e^{-\lambda t}\). Its total probability for decay at or before time, \(t\), must therefore be \(1 - e^{-\lambda t}\), the sum of individual decay probabilities within successive infinitesimal time intervals from 0 to time, \(t\). Put another way, \(1 - e^{-\lambda t}\) is the total probability that the random variable, time, is less than or equal to \(t\), or, from appendix C, the cumulative distribution function:

\[
C(t) = \int_0^t p(t')dt'
\]

\[
= 1 - e^{-\lambda t}.
\]
By the second part of the Fundamental Theorem of Calculus,

\[
\frac{dC(t)}{dt} = \frac{d}{dt} \int_0^t p(t')dt' = p(t) = \lambda e^{-\lambda t}
\]

for the probability density function of radioactive decay [205][235][108].

Recalling the review of appendix C, the mean value for \( t \) from \( p(t) \) is

\[
A_C = \int_0^\infty p(t)t \, dt
\]

since \( t \) cannot take on negative values. As \( p(t)dt \) is the probability for decay of a radionuclide between times \( t \) and \( t + dt \), or, the fraction of the sample that decays between times \( t \) and \( t + dt \), the time value associated with this probability in Eq. (B.6) corresponds to the time of “death” of that fraction of radionuclides, or, in other words, their age. Summing across all time thus provides
the mean age of a radionuclide in the sample:

\[ A_C = \int_0^\infty \lambda e^{-\lambda t} dt \]

\[ = \lim_{a \to \infty} \left( -e^{-\lambda t} \bigg|_0^a + \int_0^a e^{-\lambda t} dt \right) \]

\[ = \lim_{a \to \infty} \left( -e^{-\lambda a} - \frac{1}{\lambda} e^{-\lambda t} \bigg|_0^a \right) \]

\[ = \lim_{a \to \infty} \left( -\frac{e^{-\lambda a}}{\lambda} - \frac{1}{\lambda^2} + \frac{1}{\lambda} \right) \]

\[ A_C = \frac{1}{\lambda} \equiv \tau \]

\[ \Rightarrow \tau = \frac{T_{1/2}}{\ln(2)}, \]

where \( \tau \) is the conventional symbol for the mean lifetime and the last step utilizes Eq. (B.5).

Some radionuclides decay via multiple modes, each characterized by a distinct radioactive constant. The differential equation governing the time rate of change of such a radionuclide’s abun-
dance due solely to decay becomes

$$\frac{dN_{t,D}}{dt} = D_1 + D_2 + \ldots$$

$$= \frac{dN_{t,1}}{dt} + \frac{dN_{t,2}}{dt} + \ldots$$

$$= (-\lambda_1 N_t) + (-\lambda_2 N_t) + \ldots$$

$$= -(\lambda_1 + \lambda_2 + \ldots)N_t$$

$$= -\left(\sum_i \lambda_i\right)N_t$$

$$\frac{dN_{t,D}}{dt} \equiv -\lambda_e N_t,$$  \hspace{1cm} (B.7)

where \(dN_{t,i}\) is the differential change in \(N_t\) during \(dt\) due to the \(i\)th mode of decay, \(\lambda_e\) is the effective radioactive constant as the sum of constants of all modes, and \(\left|\frac{dN_{t,D}}{dt}\right|\) is the total number of radionuclides of the sample that decay per unit time across all modes. Thus, the fraction of radionuclides that decay, or, the probability of decay, via the \(i\)th mode is

$$f_i = \frac{|dN_{t,i}|}{|dN_{t,D}|} = \frac{|\frac{dN_{t,i}}{dt}|}{|\frac{dN_{t,D}}{dt}|} = \frac{\lambda_i N_t}{\lambda_e N_t} = \frac{\lambda_i}{\lambda_e}.$$
The total probability of decay is given by

\[ f_{total} = \sum_i f_i \]

\[ = \sum_i \frac{\lambda_i}{\lambda_e} \]

\[ = \frac{1}{\lambda_e} \sum_i \lambda_i \]

\[ = \frac{1}{\lambda_e} \lambda_e \]

\[ f_{total} = 1, \]

as expected for the sum of all probabilities. Solving Eq. (B.7) for \( N_{t,D} \) yields

\[ \frac{N_{t,D}}{N_0} = e^{-\lambda_e t}, \]  

(B.8)

where \( N_0 \) and \( N_{t,D} \) are the numbers of radionuclides initially and at time, \( t \), respectively. Now, however, \( N_{t,D} \) accounts for the survival of possibly more than one decay mode, thereby generalizing Eq. (B.2).

As the half-life and mean lifetime of a radionuclide in a sample both arose out of manipulations of Eq. (B.2), the same analysis on Eq. (B.8) culminates in the effective half-life and effective
mean lifetime since the two equations have identical forms:

\[
T_{1/2,e} = \frac{\ln(2)}{\lambda_e}
\]

\[
= \frac{\ln(2)}{\sum_i \lambda_i}
\]

\[
= \frac{\ln(2)}{\sum_i \frac{1}{\tau_i}}
\]

\[
\tau_e = \frac{T_{1/2,e}}{\ln(2)}
\]

\[
= \frac{1}{\sum_i \frac{1}{\tau_i}}
\]

the two formulas in terms of the mean lifetimes for survival against individual decay modes. One example of a radionuclide with numerous decay paths is $^{64}\text{Cu}$, which has a 17.4% probability of transmuting to $^{64}\text{Zn}$ by $\beta^+$ decay, a 39.0% probability of transmuting to $^{64}\text{Ni}$ by $\beta^-$ decay, and, finally, a 43.6% probability of capturing an electron en route, as well, to $^{64}\text{Ni}$ [156][231][77][170][21].

**B.3 Types and Energetics of Radioactive Decay**

A convenient summary, Fig. (B.3) outlines the most common types of radioactive decay. Preceding additional details for many of them in the forthcoming discussion, consider the following conservation laws governing nuclear reactions:

- **Conservation of Charge** In a reaction, the sum of elementary charges of the reactants must equal the sum of elementary charges of the products.

- **Conservation of Nucleon, or, Mass, Number** In a reaction, the sum of protons and neutrons of the reactants must equal the sum of protons and neutrons of the products.

- **Conservation of Baryon Number** In a reaction, the sum of baryon numbers of the reactants must equal the sum of baryon numbers of the products.
Table 5.1: Summary of important types of radioactive decay. The parent atom is denoted as P and the product or daughter atom by D.

<table>
<thead>
<tr>
<th>Decay Type</th>
<th>Reaction</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>gamma (γ)</td>
<td>$\frac{4}{2}P^* \rightarrow \frac{4}{2}P + \gamma$</td>
<td>An excited nucleus decays to its ground state by the emission of a gamma photon.</td>
</tr>
<tr>
<td>alpha (α)</td>
<td>$\frac{4}{2}P \rightarrow \frac{4}{2-2}D + \alpha$</td>
<td>An α particle is emitted leaving the daughter with 2 fewer neutrons and 2 fewer protons than the parent.</td>
</tr>
<tr>
<td>negatron (β⁻)</td>
<td>$\frac{4}{2}P \rightarrow z+1D + \beta^- + \bar{\nu}$</td>
<td>A neutron in the nucleus changes to a proton. An electron (β⁻) and an anti-neutrino ((\bar{\nu})) are emitted.</td>
</tr>
<tr>
<td>positron (β⁺)</td>
<td>$\frac{4}{2}P \rightarrow z-1D + \beta^+ + \nu$</td>
<td>A proton in the nucleus changes into a neutron. A positron (β⁺) and a neutrino ((\nu)) are emitted.</td>
</tr>
<tr>
<td>electron capture (EC)</td>
<td>$\frac{4}{2}P + e^- \rightarrow z-1D^* + \nu$</td>
<td>An orbital electron is absorbed by the nucleus, converts a nuclear proton into a neutron and a neutrino ((\nu)), and, generally, leaves the nucleus in an excited state.</td>
</tr>
<tr>
<td>proton (p)</td>
<td>$\frac{4}{2}P \rightarrow \frac{4-1}{2-1}D + p$</td>
<td>A nuclear proton is ejected from the nucleus.</td>
</tr>
<tr>
<td>neutron (n)</td>
<td>$\frac{4}{2}P \rightarrow \frac{4-1}{2}D + n$</td>
<td>A nuclear neutron is ejected from the nucleus.</td>
</tr>
<tr>
<td>internal conversion (IC)</td>
<td>$\frac{4}{2}P^* \rightarrow [\frac{4}{2}P]^+ + e^-$</td>
<td>The excitation energy of a nucleus is used to eject an orbital electron (usually a K-shell) electron.</td>
</tr>
</tbody>
</table>

Shultis and Faw (2018)

Figure B.3: (caption at top)

- **Conservation of Lepton Number** In a reaction, the sum of lepton numbers of the reactants must equal the sum of lepton numbers of the products.
• **Conservation of Total Relativistic Energy, or, Mass-Energy** In a reaction, the total relativistic energy of the reactants must equal the total relativistic energy of the products.

• **Conservation of Total Linear Momentum** In a reaction, the total linear momentum of the reactants must equal the total linear momentum of the products.

• **Conservation of Total Angular Momentum** In a reaction, the total angular momentum of the reactants must equal the total angular momentum of the products.

### B.3.1 Reaction Q-Value

In particular, for the alpha decay (see § B.3.4 below) of a parent nucleus into its daughter nucleus with the emission of an alpha particle, conservation of relativistic energy states

\[ Mpc^2 = K_D + m_Dc^2 + K_\alpha + m_\alpha c^2, \]

where \(K_i\) and \(m_ic^2\) are the kinetic and rest energies, respectively, of the daughter nucleus/alpha particle and \(Mpc^2\) is the rest energy of the parent nucleus, assuming it is initially at rest. The rest energy of the parent nucleus contains a potential energy of interaction between said nucleus and the as-yet emitted alpha particle residing inside it. Also, if the products are not sufficiently separated when measuring their energies, a potential energy of interaction will exist between them as well. Hence,

\[ (m_D + m_\alpha + \frac{U_{D\alpha,0}}{c^2})c^2 = K_D + K_\alpha + (m_D + m_\alpha + \frac{U_{D\alpha,f}}{c^2})c^2, \]

(B.9)

where the rest energy of the parent nucleus explicitly shows the contribution from the particle-nucleus potential energy of interaction \((U_{D\alpha,0})\), as does the rest energy of the products explicitly includes their potential energy of interaction \((U_{D\alpha,f})\). If the products are indeed sufficiently separated when measuring their energies so that the system’s electrostatic potential energy is negligible, \(U_{D\alpha,f} \rightarrow 0\) and we find

\[ Q \equiv (m_D + m_\alpha + \frac{U_{D\alpha,0}}{c^2})c^2 - (m_D + m_\alpha)c^2 = K_D + K_\alpha. \]

The increase in mass of the parent nucleus attributable to the particle-nucleus potential energy of interaction is transformed into the kinetic energies of the products, again assuming they have moved far enough apart from each other [60][132].
An everyday macroscopic example is a system consisting of two masses connected to opposite ends of a compressed spring. By analogy to Eq. (B.9),

\[(m_1 + m_2 + \frac{U_{12,0}}{c^2})c^2 = K_1 + K_2 + (m_1 + m_2)c^2\]

\[\Rightarrow Q \equiv (m_1 + m_2 + \frac{U_{12,0}}{c^2})c^2 - (m_1 + m_2)c^2 = K_1 + K_2,\]

where \(U_{12,0}\) now denotes the contribution to the rest energy of the system from the potential energy of the compressed spring. This corresponding increase in the rest mass of the system is transformed into the kinetic energies, \(K_1\) and \(K_2\), of the charge-neutral masses upon release of the spring.

Similarly, instead of a locked spring keeping the masses together in place, imagine a completely inelastic collision:

\[K_1 + K_2 + (m_1 + m_2)c^2 = (m_1 + m_2 + \frac{T_{12,0}}{c^2})c^2\]

\[\Rightarrow Q \equiv (m_1 + m_2)c^2 - (m_1 + m_2 + \frac{T_{12,0}}{c^2})c^2 = -(K_1 + K_2),\]

where \(T_{12,0}\) now denotes the contribution to the rest energy of the system from the thermal energy due to heat of the collision. The initial kinetic energies, \(K_1\) and \(K_2\), of the masses are transformed into this corresponding increase in the rest mass of the system. Since these additional energies are usually not distinguished from that of the rest of the nucleus/spring-masses/masses systems, we may succinctly rewrite the conservation of energy and Q-value as

\[M_0c^2 \Leftrightarrow K_1 + K_2 + (m_1 + m_2)c^2\]

\[\Rightarrow Q \equiv \pm M_0c^2 \mp (m_1 + m_2)c^2 = \pm (K_1 + K_2),\]

where the mass of the system, \(M_0\), includes any contributions from energy transformations and the double arrow and plus-minus symbol allow for the interaction to proceed from left to right or right to left, depending on if the system breaks apart or comes together [149][78].

In general, for an interaction of nucleus/particle, \(a\), with nucleus/particle, \(b\), producing
nuclei/particles, $c$ and $d$, assuming the reactants and products are sufficiently separated before and after said interaction prior to measurements so that the system’s electrostatic potential energy is negligible, conservation of total relativistic energy states

$$K_a + m_a c^2 + K_b + m_b c^2 = E_c + m_c c^2 + E_d + m_d c^2$$

$$\Rightarrow Q \equiv (m_a + m_b)c^2 - (m_c + m_d)c^2 = E_c + E_d - (K_a + K_b),$$

where $K_i$ and $m_i c^2$ are the kinetic and rest energies, respectively, of the nucleus/particle, $i$, and $E_i$ is also a kinetic energy unless the particle is a gamma photon. Then $E_i$ is the energy of the photon. The Q-value emphasized repeatedly above is the difference in rest energies between the initial and final states of the system or the gain or loss of gamma-photon/kinetic energies of the final state. If the initial rest mass is greater ($Q > 0$), then part of that mass is transformed into an increase of the gamma-photon/kinetic energies of the products, and the nuclear reaction is therefore exothermic. If, on the other hand, the final rest mass is greater ($Q < 0$), then part of the photon/kinetic energies of the reactants is transformed into that additional mass, resulting in a decrease in the corresponding energies of the products. The nuclear reaction is, in turn, endothermic [121].

### B.3.2 Macroscopic Illusions and Long Half-Lives

The increased masses of the aforementioned macroscopic systems are not noticeable when attempting to measure them. Why is that? Consider one last macroscopic example of a car battery rated to move $600 \, A \cdot h$ of charge at $12.0 \, V$. To fully charge an empty battery, an electrostatic potential energy of $qV \equiv (600 A \cdot h)(12.0 V)$ is converted into $2.88 \times 10^{-10} \, kg$ of mass, extremely small indeed. Given an initial battery mass of $20.0 \, kg$, this increase is a mere $1.44 \times 10^{-9} \%$, again extremely small. By contrast, the mass transformed in fueling a nuclear reactor is a significant percentage and, thus, more than enough to be measured [86].

The requirement of large-enough sample sizes also factors into measuring the half-life of a long-lived radionuclide. Uranium-238, for example, has a half-life of $4.468 \, Gyr$, or, mean lifetime of $6.446 \, Gyr$. If theory tells us it takes almost 5 billion years for half of a sample of $^{238}\text{U}$ to decay, how will we ever have enough time to experimentally confirm this half-life?

The probability for decay of $^{238}\text{U}$ within a time, $t$, previously reasoned to be $1 - e^{-\frac{t}{\tau}}$, may
be estimated as $\frac{1}{\tau}$ in the limit of a long mean lifetime. In 1 year, then, the $^{238}\text{U}$ nuclide has a 1-in-a-
6.446-billion chance, or, $\sim 1.55 \times 10^{-8}$ % probability, of decaying. If a sample contains more than 1 $^{238}\text{U}$ nuclide, this probability is gauged by the number of decays, $\Delta N_t$, in time, $t$ (favorable number of events) per the initial number of nuclides, $N_0$ (total number of events, assuming a negligible change in $N_t$ during $t$):

$$\frac{t}{\tau} = \frac{\Delta N_t}{N_0} \quad (B.10)$$

$$\Rightarrow \Delta N_t = \frac{N_0 t}{\tau},$$

as evident from Eq. (B.2) in extracting the expression for $\Delta N_t \equiv N_0 - N_t$ and simplifying in the limit of a long mean lifetime. If a sample contains 6.446 billion $^{238}\text{U}$ nuclides, then the number of decays within a year becomes $\frac{1}{6.446 \times 10^9} \cdot 6.446 \times 10^9 \equiv 1$. On average, one nuclide from this sample will decay within a year. If a sample contains $\sim 2.353$ trillion $^{238}\text{U}$ nuclides, then the number of decays within a day becomes $\frac{1}{6.446 \times 10^9} \cdot 2.353 \times 10^{12} \equiv 1$. On average, one nuclide from this sample will decay within a day. If a sample contains $\sim 56.467$ trillion $^{238}\text{U}$ nuclides, then the number of decays within an hour becomes $\frac{1}{6.446 \times 10^9} \cdot 56.467 \times 10^{12} \equiv 1$. On average, one nuclide from this sample will decay within an hour. If a sample contains $\sim 3.388$ quadrillion $^{238}\text{U}$ nuclides, then the number of decays within a minute becomes $\frac{1}{6.446 \times 10^9} \cdot 3.388 \times 10^{15} \equiv 1$. On average, one nuclide from this sample will decay within a minute. If a sample contains $\sim 203.049$ quadrillion $^{238}\text{U}$ nuclides, then the number of decays within a second becomes $\frac{1}{6.446 \times 10^9} \cdot 203.049 \times 10^{15} \equiv 1$. On average, one nuclide from this sample will decay within a second. And so on [92].

From Eq. (B.3), the disintegration rate of a radioactive sample is proportional to the sample size. Increasing the sample size thereby results in more decays within a given time interval. Statistically speaking, each $^{238}\text{U}$ nuclide has a probability for decay at any moment in time and may therefore decay right away or 6 billion years from now. By adding more of these nuclides to the sample, there is the chance that more decay within the specified duration (although, again, these additional nuclides may just as well decay much later). That is why, regardless of the long mean lifetime, decaying $^{238}\text{U}$ nuclides may be detected for successively-smaller time intervals above as the sample size increases.
In terms of the half-life, we may recast Eq. (B.10) as

\[
\frac{t}{T_{1/2}} \ln(2) = \frac{\Delta N_t}{N_0}
\]

\[\Rightarrow T_{1/2} = \frac{N_0 \cdot t \cdot \ln(2)}{\Delta N_t}. \tag{B.11}\]

From appendix D, sample masses ranging from 1 microgram to 1 gram of \(^{238}\text{U}\) contain on the order of \(10^{15}-10^{21}\) nuclides [211], up to many orders of magnitude greater than the numbers used above. For even a sample as small as 1 microgram, the detection of multiple decays and (from Eq. (B.11) subsequent determination of the time for half that mass to decay is possible within hours. The acquisition of greater masses highly feasible, the half-life determination only becomes more efficient and accurate as the sample size increases and more decays are detected. Extending the detection duration for a given sample size and careful measurement of the number of nuclides in the sample also improve said determination.

### B.3.3 Gamma Decay

Not a primary process, gamma decay occurs in reaction products containing a nucleus in an excited state. The complete transition to the ground state usually proceeds rapidly within \(10^{-9}\) s accompanied by the emission of one or more gamma photons. An excited state lasting longer than 1 ns is called a metastable or isomeric state (denoted by \(m\)), the nucleus in such a state called an isomer, and the associated gamma decay called an isomeric transition. The energy-level diagram of Fig. (B.4) illustrates the gamma decay of the metastable \(^{97m}\text{Tc}\) nucleus by the release of a 96.56-\(keV\) gamma photon in transition to the ground state.

From its reaction equation in Fig. (B.3) and assuming the parent nucleus is initially at rest, conservation of total relativistic energy for gamma decay states

\[
M(\frac{1}{2}P^*)c^2 \equiv M(\frac{1}{2}P)c^2 + E^* = M(\frac{1}{2}P)c^2 + K_P + E_\gamma
\]

\[\Rightarrow Q \equiv M(\frac{1}{2}P)c^2 + E^* - M(\frac{1}{2}P)c^2 = K_P + E_\gamma, \tag{B.12}\]
where $E^*$ is the excitation energy relative to a lower excited or the ground state of the parent nucleus, $E\gamma$ the gamma-photon energy, $K_P$ the recoil kinetic energy of the lower-excited- or ground-state nucleus. For non-relativistic particles/nuclei, conservation of total linear momentum states

\[
\frac{E_\gamma}{c} = \sqrt{2M(\frac{A}{2}P)K_P}
\]

\[\Rightarrow K_P = \frac{E_\gamma^2}{2M(\frac{A}{2}P)c^2}, \quad \text{(B.13)}\]

as the still parent nucleus dictates the gamma photon and lower-excited-/ground-state nucleus move in opposite directions with equal magnitudes of momentum. Substitution of Eq. (B.13) into Eq. (B.12) yields

\[
E_\gamma = Q \left[1 + \frac{E^*}{2M(\frac{A}{2}P)c^2}\right]^{-1}. \quad \text{(B.14)}
\]

As the maximum value of $E_\gamma$ in these transitions is no more than 10 $MeV$ [208][116][157] or 20 $MeV$ [231] and $2M(\frac{A}{2}P)c^2 \geq 4000MeV$, we may approximate the exponentiated term on the right side of Eq. (B.14) as $1 - \frac{E^*}{2M(\frac{A}{2}P)c^2}$. For the aforementioned range of gamma energies, this factor is close enough to 1 that the emitted photon essentially acquires just about all of the energy in the decay equal to the difference in energy between the excited and lower-excited/ground states (i.e., $E_\gamma \simeq Q \equiv E^*$ from Eq. (B.12). Consequently, the kinetic energy of the lower-excited-/ground-state nucleus is negligible [77].
B.3.4 Alpha Decay

Briefly touched upon in § B.3.1, alpha decay is the spontaneous disintegration of a parent nucleus to its daughter nucleus through the emission of an alpha particle, a process leaving the daughter with 2 fewer protons and 2 fewer neutrons. From its reaction equation in Fig. (B.3) and assuming the parent nucleus is initially at rest and the products sufficiently separated when measuring their energies ($U_{D\alpha, f} \to 0$), conservation of total relativistic energy for alpha decay states

$$M(A_Z P) c^2 = M(A_Z - 4 D) c^2 + K_D + m_\alpha c^2 + K_\alpha$$

(B.15)

$$\Rightarrow Q \equiv M(A_Z P) c^2 - [M(A_Z - 4 D) c^2 + m_\alpha c^2] = K_D + K_\alpha,$$

where $P$ and $D$ denote the rest/kinetic energies of the parent/daughter nuclei and $m_\alpha c^2$ and $K_\alpha$ are the rest/kinetic energies of the alpha particle. For non-relativistic particles/nuclei, conservation of total linear momentum states

$$M(A_Z - 4 D) v_D = m_\alpha v_\alpha$$

$$\Rightarrow v_D = \frac{m_\alpha}{M(A_Z - 4 D)} v_\alpha,$$

as, like gamma decay, the still parent nucleus dictates the daughter nucleus and alpha particle move in opposite directions with equal magnitudes of momentum.

With this relation between the speeds of the daughter nucleus and alpha particle, the Q-
value and the kinetic energy of the alpha particle correlate via a function of the product masses:

\[ Q = K_D + K_\alpha \]

\[ = \frac{1}{2} M(\frac{A-4}{Z-2}D)v_D^2 + \frac{1}{2} m_\alpha v_\alpha^2 \]

\[ = \frac{1}{2} M(\frac{A-4}{Z-2}D) \left[ \frac{m_\alpha}{M(\frac{A-4}{Z-2}D)} v_\alpha \right]^2 + \frac{1}{2} m_\alpha v_\alpha^2 \]

\[ = \left( \frac{m_\alpha}{M_D} + 1 \right) \frac{1}{2} m_\alpha v_\alpha^2 \]

\[ Q = \left( \frac{m_\alpha}{M_D} + 1 \right) K_\alpha \quad \text{(B.16)} \]

\[ \Rightarrow K_\alpha = \left( \frac{M_D}{m_\alpha + M_D} \right) Q \]

\[ \Rightarrow K_D = Q - K_\alpha = \frac{m_\alpha}{M_D} K_\alpha \equiv \left( \frac{m_\alpha}{m_\alpha + M_D} \right) Q. \]

As kinetic energy is an inherently-positive quantity, Eq. (B.16) implies \( Q > 0 \) and, thus, alpha decay is an exothermic process. Also, for massive nuclei in which \( \frac{m_\alpha}{M_D} \ll 1 \), the alpha particle carries off most of the kinetic energy. Although atomic masses (by adding identical electron masses to both sides and neglecting negligible differences in electron binding energies of the parent, daughter, and \(^4\text{He} \) atoms in Eqs. (B.15) or nuclear masses may be employed in computing the Q-value of Eq. (B.16), mass numbers prove a most straightforward and satisfactory approximation since protons and neutrons, near identical in mass at roughly 1 \( \text{amu} \), are many orders of magnitude more massive than electrons. Without the small mass of electrons, the mass of an atom or a nucleus estimates to
Figure B.5: Alpha decay of a $^{238}\text{U}$ nucleus and gamma decay of its daughter [16].

$A \cdot 1\text{ amu}$, or, numerically speaking, the mass number. Hence,

$$Q \simeq \left( \frac{A}{A - 4} \right) K_\alpha \quad \text{(B.17)}$$

$$\Rightarrow K_\alpha \simeq \left( \frac{A - 4}{A} \right) Q$$

$$\Rightarrow K_D = Q - K_\alpha \simeq \frac{4}{A - 4} K_\alpha \equiv \frac{4}{A} Q,$$

where $A$ is the mass number. Please refer to appendix A for a reminder of binding-energy scales and differences.

Measurements of the alpha decay for a particular radionuclide usually convey the detection of several alpha particles of distinct energies, sometimes accompanied by the emission of a gamma photon. The parent nucleus may decay directly to the ground state of the daughter nucleus or to any of its excited states. The latter eventually culminates in the former by successive gamma decays, as described in § B.3.3. The visual of (B.5) encapsulates the consecutive alpha and gamma decays of $^{238}\text{U}$ and $^{234}\text{Th}$ nuclei, respectively. Consider two different alpha decays of a parent nucleus, one to an excited state, $^\ast\ast$, of the daughter and the other to the next lower excited state, $^\ast$. Letting $^\ast\ast$
de-excite to $^*$, the Q-values for each are

$$Q^{**} = M(\frac{A}{2} P)c^2 - [M(\frac{A-4}{Z-2} D^{**})c^2 + m_\alpha c^2]$$

$$= M(\frac{A}{2} P)c^2 - [M(\frac{A-4}{Z-2} D^*)c^2 + E^{**} + m_\alpha c^2],$$

$$Q^* = M(\frac{A}{2} P)c^2 - [M(\frac{A-4}{Z-2} D^*)c^2 + m_\alpha c^2]$$

$$\Rightarrow Q^* - Q^{**} = E^{**} \equiv E_\gamma^{**} \rightarrow ^*,$$

where the equivalency in the last step follows from § B.3.3 and the gamma photon emitted in the de-excitation of $^{**}$ to $^*$ has an energy equal to that level difference. A quick determination of the Q-value from Eq. (B.17) for each detected alpha-particle kinetic energy accordingly allows illumination of a radionuclide’s alpha-decay energy-level structure. Such a structure is highlighted in Fig. (B.6) for $^{226}$Ra [77][231][131].

![Energy-level diagram for alpha decay of $^{226}$Ra.](image)

Shultis and Faw (2018)

Figure B.6: Energy-level diagram for alpha decay of $^{226}$Ra.

**B.3.5 Beta-Minus Decay**

Beta-minus decay is the spontaneous disintegration of a typically neutron-rich parent nucleus to its daughter nucleus through the transmutation of a neutron into a proton antecedent to the emission of an electron and electron anti-neutrino. The emission of $-1$ e of charge by a down quark
in the parent nucleus transforms the down quark into an up quark. An extremely small probability then exists for the $W^-$ boson carrying the $-1\ e$ of charge to decay within $10^{-26}\ s$ into an electron and electron anti-neutrino prior to the charge’s re-absorption by the up quark (transforming it back into a down quark). Schematics of these transformations are shown in Figs. (B.7), (B.8), and (B.9).

Figure B.7: (caption at top) [2]

Figure B.8: (caption at top) [2]

Figure B.9: Net result of processes outlined in Figs. (B.7) and (B.8) [2].
For a neutral neutron to transmute into a positively-charged proton, conservation of charge dictates that one or more particles must also be produced whose total charge sums to \(-1\) in order to balance the \(+1\) charge gain of the proton. That produced particle is the electron. Likewise, for a neutron (lepton number = 0) to transmute into a proton (lepton number = 0) with the emission of an electron (lepton number = 1), conservation of lepton number dictates that one or more particles must also be produced whose total lepton number sums to -1 in order to balance the +1-lepton-number gain of the electron. That produced particle is the electron anti-neutrino [8].

From its reaction equation in Fig. (B.3) (under “negatron”) and assuming the parent nucleus is initially at rest and the products sufficiently separated when measuring their energies \((U_{D e^-,f} \rightarrow 0)\), conservation of total relativistic energy for beta-minus decay states

\[
M_{(A^ZP)}c^2 = M_{(A^{Z+1}D)}c^2 + K_{D} + m_{e^-}c^2 + K_{e^-} + m_{\bar{\nu}_{e^-}}c^2 + K_{\bar{\nu}_{e^-}}
\]

\[
\Rightarrow Q \equiv M_{(A^ZP)}c^2 - \left[ M_{(A^{Z+1}D)}c^2 + m_{e^-}c^2 + m_{\bar{\nu}_{e^-}}c^2 \right] = K_{D} + K_{e^-} + K_{\bar{\nu}_{e^-}},
\]

where \(M_{(A^ZP)}c^2\) and \(M_{(A^{Z+1}D)}c^2\) are the rest energies of the parent and daughter nuclei, \(m_{e^-}c^2\) and \(m_{\bar{\nu}_{e^-}}c^2\) the rest energies of the electron and electron anti-neutrino, and \(K_i\) the corresponding kinetic energies. The sum of positive kinetic energies above implies \(Q > 0\) and, thus, beta-minus decay is an exothermic process. As the mass of the daughter nucleus is typically much larger than that of the electron and electron anti-neutrino, its recoil kinetic energy can be neglected to achieve the following approximation for the Q-value:

\[
Q \approx K_{e^-} + K_{\bar{\nu}_{e^-}}
\]

\[
\Rightarrow K_{e^-,max} \simeq Q,
\]

the electron attaining maximum kinetic energy in the near-absence of any for the electron anti-neutrino.

Reminiscent of alpha decay, the parent nucleus may beta-minus decay directly to the ground state of the daughter nucleus or to any of its excited states. The latter eventually culminates in the former by successive gamma decays, as described in § B.3.3. The visual of Fig. (B.10)
encapsulates the consecutive beta-minus and gamma decays of $^{234}\text{Th}$ and $^{234}\text{Pa}$ nuclei, respectively. The difference in Q-values between adjacent excited-state decays to the daughter nucleus informs us of a radionuclide’s beta-minus-decay energy-level structure:

$$Q^{**} = M(\frac{A}{2}P)c^2 - [M(\frac{A}{2+1}D^{**})c^2 + m_e c^2 + m_{\nu_e} c^2]$$

$$= M(\frac{A}{2}P)c^2 - [M(\frac{A}{2+1}D^{*})c^2 + E^{**} + m_e c^2 + m_{\nu_e} c^2],$$

$$Q^* = M(\frac{A}{2}P)c^2 - [M(\frac{A}{2+1}D^{*})c^2 + m_e c^2 + m_{\nu_e} c^2]$$

$$\Rightarrow Q^* - Q^{**} = E^{**} \equiv E_\gamma \rightarrow ^*,$$

an example afforded by Fig. (B.11) for $^{38}\text{Cl}$ [77][231].
From appendix A, we may recast Eqs. (B.18) in terms of binding energies and particle masses:

\[
(Zm_p + (A - Z)m_n)c^2 - B_2^A = [(Z + 1)m_p + (A - Z - 1)m_n]c^2 - B_{Z+1}^A + K_D + m_e - c^2 + K_{e^-} + m_{\bar{\nu}_e} - c^2 + K_{\bar{\nu}_e} - c^2,
\]

where \(B_i^j\) is the binding energy of the nucleus with \(j\) protons and \(i - j\) neutrons and \(m_p\) and \(m_n\) are the masses of the proton and neutron, respectively. Ignoring the negligible mass of the electron anti-neutrino, \((m_n - m_p - m_e)c^2 \approx 782\text{ keV}\). If the sum of kinetic energies of the product particles/daughter nucleus is less than this amount, then \(B_{Z+1}^A - B_2^A \lesssim 0\) and the daughter is not as stable as the parent [116].

**B.3.6 Beta-Plus Decay**

The mirror process of beta-minus decay, beta-plus decay ("positron" in Fig. (B.3) is the spontaneous disintegration of a typically proton-rich parent nucleus to its daughter nucleus through the transmutation of a proton into a neutron antecedent to the emission of a positron and electron neutrino. The emission of \(+1\ e\) of charge by an up quark in the parent nucleus transforms the up quark into a down quark. An extremely small probability then exists for the \(W^+\) boson carrying the
+1 e of charge to decay within $10^{-26}$ s into a positron and electron neutrino prior to the charge’s re-absorption by the down quark (transforming it back into an up quark).

The equations of §B.3.5 for conservation of total relativistic energy and the Q-value apply here with $e^-$ changed to $e^+$, $\bar{\nu}_e$ changed to $\nu_e$, and $Z + 1$ of the daughter nucleus changed to $Z - 1$. In beta-plus decay, an exothermic process, it is the positron that may acquire the maximum kinetic energy (equivalent to the Q-value) in the near-absence of any for the electron neutrino. The energy-level diagram of Fig. (B.12) displays the beta-plus decays of $^{22}$Na to the ground state and an excited state of the daughter, the structure revealed in the difference of Q-values as emphasized in §B.3.5.

For a positively-charged proton to transmutate into a neutral neutron, conservation of charge dictates that one or more particles must also be produced whose total charge sums to +1 e in order to balance the +1 − e charge loss of the proton. That produced particle is the positron. Likewise, for a proton (lepton number = 0) to transmutate into a neutron (lepton number = 0) with the emission of a positron (lepton number = -1), conservation of lepton number dictates that one or more particles must also be produced whose total lepton number sums to +1 in order to balance the -1-lepton-number gain of the positron. That produced particle is the electron neutrino [8][17][77][231][192].

From appendix A, we may recast Eqs. (B.18) (with the necessary aforementioned changes)
in terms of binding energies and particle masses:

\[
(Zm_p + (A - Z)m_n)c^2 - B^3_2 = [(Z - 1)m_p + (A - Z + 1)m_n]c^2 - B^4_{Z-1} + K_D + m_{e^+}c^2 + K_{e^+} + m_{\nu_e}c^2 + K_{\nu_e}
\]

\[
\Rightarrow Q \equiv K_D + K_{e^+} + K_{\nu_e} = (B^4_{Z-1} - B^4_Z) - (m_n + m_{e^+} + m_{\nu_e} - m_p)c^2.
\]  

(B.19)

Ignoring the negligible mass of the electron neutrino, \((m_n + m_{e^+} - m_p)c^2 \approx 1.804\) MeV. As the process is exothermic, it will only proceed spontaneously if \(B^4_{Z-1} - B^4_Z > 0\), or, in other words, the stability of the daughter exceeds that of the parent by more than 1.804 MeV. This minimum binding-energy requirement is a consequence of the mass increase from the transmutation of the proton into the neutron, a re-arrangement of Eq. (B.19) providing enlightenment:

\[
(B^4_{Z-1} - B^4_Z) = (m_n + m_{e^+} + m_{\nu_e} - m_p)c^2 + Q.
\]

Energy must be released from the parent nucleus to create the more stable daughter, an amount, \(B^4_{Z-1} - B^4_Z\), driving the decay by allocation between the particles’ rest-energy increase and the kinetic energies of the products [116][106].

Without this energy as the impetus for decay, per a violation of the conservation laws, an isolated free proton will not spontaneously transmute into a neutron coincident to the emission of a positron and electron neutrino. Although grand unification models predict the decay of the proton, experiments have yet to yield conclusive results confirming such a process. All that may be theorized is the mean lifetime of the proton must be larger than 10^{32} years. An isolated free neutron, on the other hand, has been established to decay with the latest measurements estimating the mean lifetime at \(\sim 14.63\) minutes [224][194][204].

**B.3.7 Electron Capture**

A competing process to beta-plus decay, electron capture is the spontaneous disintegration of a typically proton-rich parent nucleus to its daughter nucleus through the transmutation of a proton into a neutron antecedent to the emission of an electron neutrino. The emission of +1 e of charge by an up quark in the parent nucleus transforms the up quark into a down quark. An
extremely small probability then exists for the $W^+$ boson carrying the +1 $e$ of charge to interact with a nearby electron, usually from the inner K-shell, in the creation of an electron neutrino prior to the charge’s re-absorption by the up quark (transforming it back into a down quark) [85][2][77].

Considering the parent nucleus captures one of the atom’s orbital electrons, now envision $M(\frac{A}{2}P)$ and $M(\frac{A}{2}Z-1D)$ as the masses of the parent and daughter atoms, respectively, in the energy-conservation equation by adding $Z-1$ electron masses to both sides and neglecting negligible differences in electron binding energies of the parent and daughter atoms (see appendix A) and the negligible neutrino mass. In the immediate aftermath of the decay, the daughter has 1 less electron (lost in the capture) and 1 less proton. From its reaction equation in Fig. (B.3) and assuming the parent atom is initially at rest, conservation of total relativistic energy for electron capture states

$$M(\frac{A}{2}P)c^2 - B^A_Z = M(\frac{A}{2}Z-1D)c^2 - B^A_{Z-1} + K_D + m_{\nu_e}c^2 + K_{\nu_e}$$

$$\Rightarrow M(\frac{A}{2}P)c^2 - M(\frac{A}{2}Z-1D)c^2 = K_D + K_{\nu_e} + m_{\nu_e}c^2 + B^A_Z - B^A_{Z-1}$$

$$\Rightarrow Q_{EC} \approx M(\frac{A}{2}P)c^2 - M(\frac{A}{2}Z-1D)c^2 > 0.$$

Similarly, for the beta-plus decay of § B.3.6,

$$M(\frac{A}{2}P)c^2 - B^A_Z = M(\frac{A}{2}Z-1D)c^2 - B^A_{Z-1} + m_e c^2 + K_D + m_{e^+}c^2 + K_{e^+} + m_{\nu_e}c^2 + K_{\nu_e}$$

$$\Rightarrow M(\frac{A}{2}P)c^2 - [M(\frac{A}{2}Z-1D)c^2 + 2m_e c^2] = K_D + K_{e^+} + K_{\nu_e} + m_{e^+}c^2 + m_{\nu_e}c^2 + B^A_Z - B^A_{Z-1}$$

$$\Rightarrow Q_{e^+} \approx M(\frac{A}{2}P)c^2 - M(\frac{A}{2}Z-1D)c^2 - 2m_e c^2 > 0,$$

where the leftover electron mass from the mass approximation of the daughter atom is combined with the positron mass as the sum of 2 electron masses since both particles have the same mass. Hence, achieving stability by the reduction of 1 proton is only possible by electron capture if the rest-energy difference between the parent and daughter atoms is less than that of 2 electrons, or, 1.022 MeV. Otherwise, both processes are possible and in competition with each other [230].
Upon removal of the inner K-shell electron, the atom will re-configure in pursuit of greater stability by having an outer-shell electron shift from a higher-energy state to the lower K-shell state, another outlying electron shift to fill the void of that outer-shell electron, and so on. The loss in energy of the transitioning electrons is carried away by photons as “X-rays”, their energy equal to the difference between the initial and final electron states. Or, outer-shell electrons may absorb these photons, the transfer of energy causing the electrons’ emission from the atom as “Auger electrons”. Once freed, the energy of the Auger electron decreases by an amount binding it to the atom. Figure (B.13) encompasses a schematic of electron capture and the resulting emissions while the energy-level diagram of Fig. (B.14) displays the electron-capture decays of $^7$Be to the ground state and an excited state of the daughter. Either decay in Fig. (B.14) expels less than 1.022 MeV of energy, thus eliminating the rival beta-plus process from occurring [143].
Appendix C

Sampling a Probability Distribution

C.1 From Discrete to Continuous Random Variables

During each time step of our calculations, we sample values from the Poisson distribution function. For a general probability distribution or probability density function, what does it mean to sample from it and how may we proceed in doing so? The following example proves illuminating. If we had 1 gram of a radioactive material and counted the number of emitted particles in a 10-second interval, and repeated this measurement for the next 5 minutes, the results would be different each time and distributed per the Poisson distribution of appendix D. To sample from the Poisson distribution, then, means to retrieve the number of emitted particles in one of these 10-second measurements. By extension, to sample from a general probability distribution or probability density function means to retrieve a value corresponding to one of the measurements or trials [243][236].

Before examining one method of sampling, a reminder and additional extension are necessary. As described in appendix D, the cumulative distribution function for a discrete random variable, $x$, is defined by the following sum:

$$ F(x) = \sum_{i=0}^{x} p(i), \quad (C.1) $$
where \( p(i) \) is the probability of obtaining the value, \( i \), for \( x \) in any given measurement or trial. Thus, \( F(x) \) is the total probability of obtaining a value equal to or less than \( x \). But \( p(i) \) is the fraction of measurements or trials of \( x \) giving the value, \( i \). Hence, the sum over all trials of the product of that fraction and matching \( i \) value is the mean value for \( x \):

\[
A_F = \sum_{i=0}^{x} p(i)i.
\]

For a continuous random variable, \( x \), the probability distribution function, \( p(x) \), becomes a probability density function. While \( p(x) \) for discrete \( x \) represents the probability of obtaining a value of \( x \), \( p(x) \) for continuous \( x \) represents the probability per unit of \( x \). Only within a specified interval may we acquire a probability for continuous \( x \).

For an infinitesimal interval, \( dx \), \( p(x)dx \) thereby denotes the probability of \( x \) falling between \( x \) and \( x + dx \). Integration yields the probability for greater ranges:

\[
P_{ab} = \int_a^b p(x)dx,
\]

where \( P_{ab} \) denotes the probability of \( x \) falling between the values of \( a \) and \( b \). For a particular upper limit, \( b = x \), the corresponding analog to Eq. (D.2) introduces

\[
C(x) = \int_{-\infty}^{x} p(x')dx'
\]

as the total probability of producing a value for the random variable up to and including \( x \), assuming said variable takes on both positive and negative values. Otherwise, the lower limit of the integral is 0 [61][248]. Similarly,

\[
A_C = \int_{-\infty}^{\infty} p(x)x\,dx
\]

is the mean value for \( x \) from a probability density, assuming the random variable takes on both positive and negative values. Otherwise, the lower limit of the integral is 0.
C.2 Steps for Sampling

Assuming the probability density function, \( p(x) \), is normalized such that

\[
\int_{-\infty}^{\infty} p(x) dx = 1,
\]

since the value of \( x \) will have to take on some value with 100% certainty in any given measurement or trial, the first step in sampling from \( p(x) \) is to invert it. Consider the Rayleigh density function:

\[
p(x) = \begin{cases} 
0 & x < 0 \\
\frac{x}{\sigma^2} e^{-\frac{x^2}{2\sigma^2}} & x \geq 0
\end{cases}
\]

and find its cumulative distribution function:

\[
C(x) = \int_{-\infty}^{x} p(x') dx'
\]

\[
= \lim_{a \to -\infty} \left( \int_{a}^{0} 0 \, dx' \right) + \int_{0}^{x} \frac{x'}{\sigma^2} e^{-\frac{x'^2}{2\sigma^2}} dx'
\]

\[
\Rightarrow C(x) = 1 - e^{-\frac{x^2}{2\sigma^2}}. \tag{C.2}
\]

Both the Rayleigh probability density and cumulative distribution functions are plotted in Fig. (C.1) for a value of unity for \( \sigma \).

Now set \( y \) equal to \( C(x) \) and solve for \( x \) to arrive at the expression for the sampled value of \( x \):

\[
y = 1 - e^{-\frac{x^2}{2\sigma^2}}
\]

\[
\Rightarrow x = \sigma \sqrt{-2 \ln(1 - y)}. \tag{C.3}
\]

As the values of \( y \) in Eq. (C.3) are the values of \( C(x) \) in Eq. (C.2), the domain of \( x \) is simply the set of uniformly-distributed real numbers, \([0, 1]\). For use in computational algorithms, we may thus
sample from the probability density function, \( p(x) \), by replacing \( y \) in Eq. (C.3) with a uniformly-distributed random-number generator, an example of which is acknowledged in appendix E. This inverse-transform method is one of many to sample from a probability density or probability distribution function \([226][218][46][104]\).

The inverse-transform method also applies to discrete probability distribution functions but invites further complications since the sums in many of the corresponding cumulative distribution functions do not exist as simple analytical expressions. Finding the inverse values, then, amounts to choosing which random variate of the probability distribution function that the drawn (from, say, a generator) random number should take on by either rounding down or rounding up. For instance, in Fig. (C.2), should we choose the value of 18 or 19 for the random variate of the discrete probability distribution function to correlate with a total probability, \( P \), of 0.05? Please see that and other discussions in Refs. [155], [31], [79], [260], and [83]. The inverse-transform method and PTRD algorithm of appendix D are among a category of algorithms called “Monte Carlo” \([133][174]\).
Figure C.2: Cumulative distribution function for discrete $x$ demonstrating the uncertainty in determining the value of the random variate [155].
Appendix D

The Poisson Distribution

D.1 The Poisson Process and Examples

A Poisson process is a random process of discrete events occurring at a constant mean rate, per time or space interval, that satisfies the following conditions:

1. The numbers of events in non-overlapping time or space intervals are independent of each other.

2. For a sufficiently small time or space interval, the probability of one event is proportional to that interval.

3. The probability of more than one event in a sufficiently small time or space interval is negligible.

In our calculations, the formation of stars during each time step is a Poisson process. Other examples include babies born in a hospital across 3 days, telephone calls arriving at a switchboard between breakfast and lunch, $\gamma$-rays emitted by a source of radioactive $^{137}$Cs nuclei in 8 seconds, vehicles passing through an intersection amid rush hour, aircrafts arriving at an airport on a Tuesday morning, customers arriving at a bank on Thursday afternoon, “hits” received by a webpage in a week, grammar or spelling errors made by a typesetter on a single page, red blood corpuscles in 2 ml of disease-ridden blood, factory accidents in a month, railway accidents in a year, micro-organisms or tadpoles in 0.5 l of pond water, mildewed peaches in a carton of 250 individually-packed peaches, roadkill discovered on a 10-mile stretch of the interstate highway, or salmon caught in a drift net. The
Poisson distribution, to be derived shortly, is a discrete distribution for determining the probability of observing \( r \) events in a specified time or space interval of a Poisson process. As the foundation of my work is the time evolution of the Galaxy, I will focus on time intervals in the following discussion.

\( \text{[150][255][254][239][201][80][102]} \)

### D.2 Derivation Methods for the Poisson Distribution

There are multiple methods one may employ in deriving the Poisson distribution. From the conditions at the top of this appendix, proof by induction produces the Poisson distribution by assuming knowledge of the probability of \( N \) events in time, \( t \), as a springboard for expressing the successive probability in time, \( t + \Delta t \) [47][71]. A second method is to find the limit of the binomial distribution, which provides the probability of observing \( r \) successes in \( N \) independent trials for an experiment defined by only two possible outcomes of each trial, either “success” or “failure”. Example trials include the tossing of a coin that lands either heads up (success) or tails up (failure), the rolling of a 6-sided die that lands either on a chosen value (success) or on one of the other 5 values (failure), or asking a group of people if each either voted for (success) or against (failure) Donald Trump [95]. The probability is dictated by the formula,

\[
P(r, N) = \binom{N}{r} p^r q^{N-r} = \frac{N!}{r!(N-r)!} p^r q^{N-r},
\]

where \( p \) and \( q \) are the probabilities of success and failure, respectively, in each trial, the two values correlating via \( p = 1 - q \) [273].

In the limit of a large number of trials, \( N \), and a small success probability, \( p \), such that the mean, \( Np \) [89], remains unchanged, it can be shown Eq. (D.1) approximates to

\[
P(\mu, r) = \frac{\mu^r e^{-\mu}}{r!},
\]

with \( \mu \) denoting a mean identical to that of the binomial distribution [57][55][71]. Multiple sources suggest conflicting “rules of thumb” for the cut-off in suitable approximation of the Poisson distribution to the binomial distribution, from \( N > 50 \) and \( p < 0.1 \), \( N \geq 20 \) and \( p \leq 0.05 \), \( N \geq 100 \) and \( Np \leq 10 \), \( N > 20 \) and \( Np \leq 7 \), or \( N \geq 100 \) and \( p \leq 0.05 \) [256][45][42][239]. I leave it to the reader to decide the range of parameters for the applicability of the Poisson distribution to the problem at
Meanwhile, Fig. (D.1) illustrates the Poisson distribution function for 4 values of \( \mu \) ("LAMBDA" in the figure), its spread increasing with the ascension of \( \mu \) due to the standard deviation’s dependence on the mean value [10][71]. For these same values of \( \mu \), Fig. (D.2) depicts the associated cumulative distribution function [10]. If \( \mu = 15 \), the cumulative distribution function, \( F(x; 15) \), is retrieved from the Poisson distribution function by the following sum:

\[
F(x; 15) = \sum_{i=0}^{x} \frac{\mu^i}{i!} e^{-\mu}.
\]

In other words, \( F(x; \mu) \equiv P \) is the total probability, \( P \), of observing \( x \) or less successes in a Poisson process averaging \( \mu \) successes. Also called the quantile function or percent point function, the inverse of the cumulative distribution function, \( F^{-1}(P; \mu) \equiv x \), is the value for \( x \) in \( F(x; \mu) \) generating that particular total probability, \( P \). Figure (D.3) embodies the Poisson percent point function for the preceding \( \mu \) values, the sum of Eq. (D.2) non-existent in simple closed form and, hence, only
computed numerically in mapping to the inverse function (see appendix C) [108][103][24][96][258][10].

D.3 Spontaneous Radioactive Decay

An example that immediately comes to mind is the spontaneous decay of the aforementioned radioactive $^{137}$Cs source, a single nucleus characterized by a mean lifetime, $\tau$, of 43.3963 years, or,
\(\sim 1.3670 \times 10^9\) seconds \[119\]. The probability a particular radioactive nucleus will decay at some instant in a time, \(t\), is computed as \(1 - e^{-\frac{t}{\tau}}\). For \(\tau \gg t\), this probability approaches a value, \(\frac{t}{\tau}\), much less than 1 \[235\][40]\[148\]. In the observation time of 8 seconds, then, the probability of decay for a \(^{137}\)Cs nucleus is \(\sim 5.84 \times 10^{-7}\) \%, extremely small indeed. And sample masses ranging from 1 microgram to 1 gram of \(^{137}\)Cs contain on the order of \(10^{15}-10^{21}\) nuclei \[211\], extremely large indeed.

To determine the probability of observing \(r\) successes, or, decays, in \(N\) independent trials, or, \(^{137}\)Cs nuclei, during that 8 seconds, we therefore resort to the Poisson distribution of Eq. (D.2) rather than the binomial distribution of Eq. (D.1). Rutherford, Geiger, and Bateman discovered this obedience of radioactive decay to the Poisson distribution in 1910 when measuring 10,097 counts from a polonium source across 2,608 successive intervals of 7.5 \(s\) each \[219\].

As stated above, the mean number of decays in a time, \(t\), is \(Np\), or, \(N\frac{t}{\tau}\). Because the mean lifetime for a radioactive nucleus is the reciprocal of its decay constant, \(\lambda\), the mean is similarly expressed as \(N\lambda t\). But \(N\lambda\), in assuming a negligible change in \(N\) during \(t\), is the mean rate of disintegration for the sample (see appendix B), a quantity deduced in experiments from “counts” received by detectors. If these experiments are repeated many times and their count rates averaged, knowledge of the number of nuclei in the sample is unnecessary since the Poisson distribution is a function of \(\mu\) only. Of course, an infinite number of experiments are required to obtain the true value of the mean. Otherwise, an associated error dependent on the number of experiments accompanies the estimated mean \[148\][109][248].

The meaning of \(N\) in Eq. (D.1) is open to interpretation. The prior discussion considered \(N\) as the quantity of a material object. However, \(N\), just as well, may refer to the quantity of a temporal object, specifically, a time interval. Re-evaluating the spontaneous decay of the radioactive \(^{137}\)Cs sample, divide the previous 8-second interval into \(N\) sub-intervals, \(\Delta t\), of equal length. The observation time is thus \(N\Delta t\). If the \(N\) sub-intervals are small enough and the sample contains \(M\) nuclei, there will be, at most, 1 decay per sub-interval with the probability of success given by \(M\lambda\Delta t\) since \(M\) decay possibilities exist within each sub-interval. The binomial distribution of Eq. (D.1) then determines the probability of observing \(r\) successes, or, decays, in \(N\) independent trials, or, time sub-intervals, for that 8 seconds. In the limit of a large number of sub-intervals, their corresponding length diminishes as \(\frac{\Delta t}{N}\) along with the decay probability for a cesium nucleus within it. The probability of observing \(r\) decays in 8 seconds is thereby more easily accessible via the Poission distribution of Eq. (D.2), the mean number of decays, \(Np = NM\lambda\Delta t = M\lambda t\), consistent
with that of the previous interpretation of \( N \) \cite{123,126}.

Outside of \( \Delta t \), though, our assumption of a constant activity no longer holds up as variations in the probability of decay for a given radioactive nucleus become significant with time and the approximation of Eq. (D.2) invalid \cite{265,148}. A return to Eq. (D.1), having computed the initial number of nuclei in the sample, yields the distribution of decays at time, \( t \), the probability of success in each trial, or, nucleus, increasing exponentially as \( 1 - e^{-\frac{t}{\tau}} \) \cite{113}. Said probability is small, and the Poisson distribution valid, for those nuclei in which \( \tau \gg t \). Equation (D.2) then provides the probability that exactly \( r \) nuclei disintegrate during an observation period averaging \( \mu \) decays.

### D.4 Application to Star Formation

In our calculations, the mean number of forming stars during each time step is proportional to the initial amount of gas mass and length of said time step, i.e.,

\[
\Delta N_{stars} \propto M_g(t) \Delta t,
\]

where \( \Delta N_{stars} \) is the mean increase in the number of stars during the time step, \( \Delta t \), and \( M_g(t) \) is the local gas mass (in units of \( 10^6 M_\odot \), or, \( MM_\odot \)) at the beginning of \( \Delta t \). If the gas is allowed to evolve over a longer time, more stars are bound to condense out of it. And if there is more material (i.e., gas mass) from which stars may form, more will inevitably do so. In other words, for a constant of proportionality, \( \lambda \),

\[
\Delta N_{stars} = \lambda M_g(t) \Delta t,
\]

so long as \( \Delta t \) is short enough that injection of new mass into the ISM from dying stars is minimal and the gas mass does not deplete. A simple re-arrangement highlights the mean rate of change in the number of stars across \( \Delta t \):

\[
\frac{\Delta N_{stars}}{\Delta t} = \lambda M_g(t),
\]

a quantity having units of inverse time. The reciprocal of the mean rate, \( \frac{1}{\lambda M_g(t)} \), has units of time, informing us of the mean time until the formation of a star. If, for instance, the mean star-formation rate is 0.001 \( yr^{-1} \), a star forms, on average, every 1000 years.

To acquire the mean rate on the right-hand side of Eq. (D.3), the constant, \( \lambda \), must represent
the mean star-formation rate in 1 $MM_\odot$ of gas. Conversely, what is the meaning of $\frac{1}{\lambda}$? A proper interpretation emerges via the corresponding replacement of $\lambda$ in the inversion of Eq. (D.3):

$$\frac{\Delta t}{\Delta N_{\text{stars}}} = \frac{\Delta M_{M_\odot}}{\Delta t} \frac{1}{M_g(t)}$$

$$= \frac{\Delta t}{\Delta M_{M_\odot}} \frac{1}{M_g(t)}.$$

If the reciprocal of $\lambda$ has a value of, say, 1500 yr $MM_\odot$, then it takes, on average, 1500 years for 1 star to form per 1 $MM_\odot$ of gas [66]. For ease of reading, we will symbolize this interpretation of $\frac{1}{\lambda}$ as $\tau_{MM_\odot}$ in Eq. (D.3):

$$\frac{\Delta N_{\text{stars}}}{\Delta t} = \frac{M_g(t)}{\tau_{MM_\odot}}.$$  

(D.4)

In a 1-$MM_\odot$ reservoir, we thus expect a star to form, on average, every 1500 years, as confirmed by the reciprocal of $\frac{\Delta N_{\text{stars}}}{\Delta t} \equiv \frac{1}{1500 \text{ yr } MM_\odot}$. In a larger reservoir of 2 $MM_\odot$, the mean time to form a star should decrease by a factor of 2 since we expect, on average, twice as many stars to form from the twice-as-large reservoir in that 1500 years. Again, our suspicions are confirmed by the reciprocal of $\frac{2 \text{ } MM_\odot}{1500 \text{ yr } MM_\odot} \equiv \frac{2}{1500 \text{ yr } MM_\odot}$. In a smaller reservoir of 0.5 $MM_\odot$, the mean time to form a star should increase by a factor of 2 since we expect, on average, half as many stars to form in that 1500 years, the reciprocal of $\frac{0.5 \text{ } MM_\odot}{1500 \text{ yr } MM_\odot} \equiv \frac{0.5}{1500 \text{ yr } MM_\odot}$ providing confirmation.

The value of $\tau_{MM_\odot}$ is a free parameter in our code and scales accordingly with the mass of each zone. As the mean lifetime and typical mass of giant molecular clouds, the site of much star formation, is on the order of $10^7$ years and between $10^5$-$10^6 M_\odot$, respectively, only 1-2% of the mass of a giant molecular cloud collapses to form stars, and most ($\sim$94%) newly-created stars contain no more than 1 $M_\odot$ of matter, the mean time to form a star within these clouds is on the order of $10^3$ years. Remembering it is the mean time to form a star per $10^6 M_\odot$ of gas (or, per giant molecular cloud), we acquire such a value for $\tau_{MM_\odot}$ in the simulations discussed in chapter 6 [266][87][187][280][191][141][140][32][238].

Consider $N$ as the quantity of a temporal object by dividing an arbitrary observation time step of 200,000 years into $N$ equal sub-intervals of length $\Delta t$. If the $N$ sub-intervals are small enough, there will be, at most, 1 forming star per sub-interval with the probability of success given by $\frac{\Delta N_{\text{stars}}}{N}$, as $\Delta N_{\text{stars}}$ (favorable number of events) of the $N$ (total number of events) sub-intervals, on average,
will form a star \[205\]. The binomial distribution of Eq. (D.1) then determines the probability of observing \( r \) successes, or, forming stars, in \( N \) independent trials, or, time sub-intervals, for that 200,000 years. In the limit of a large number of sub-intervals, their corresponding length diminishes as \( \frac{N}{\Delta t} \) along with the formation probability for a star within it. The probability of observing \( r \) forming stars in 200,000 years is thereby more easily accessible via the Poisson distribution of Eq. (D.2), the mean number of forming stars obtained in the product of the mean star-formation rate and time step: \( \frac{M_g(t)}{7 M_M} \Delta t \).

During each time step of our calculations, Boost utilizes a pseudo-random number generator [166] as input to the PTRD algorithm [117] in sampling (see appendix C) from the Poisson distribution function of Eq. (D.2). Constituting the number of forming stars, the PTRD algorithm extracts non-uniform random variates of the Poisson distribution function by a combination of the inverse-transform and acceptance-rejection methods [226][218], the former directly involving the Poisson percent point function of Fig. (D.3) with \( \mu \) as inferred above. Next, calls to the initial mass function (see appendix E) distribute some or all of the local gas mass to these stars.
Appendix E

The Initial Mass Function

E.1 Definition and Normalization

To distribute the masses of newly-created stars during each time step of our calculations, we sample from the multi-part power-law initial mass function (IMF) that Pavel Kroupa derived from data compilations of Scalo (1998) and observations by Muench, Lada, & Lada (2000). The initial mass function is the total number of stars that have ever formed per square or cubic parsec and per unit logarithmic mass:

\[ \xi(\log m) = \frac{d(N/L^x)}{d(\log m)} = \frac{dn}{d(\log m)}. \]  

(E.1)

where \( N \) is the number of newly-created stars, \( L^x \) represents area or volume for \( x = 2 \) or \( x = 3 \), respectively, \( n \) is the area or volume density, and \( m \) is the mass. Miller & Scalo (1979) state that “in the case of a time-constant IMF (as assumed here), the IMF at any given time has the same shape as the IMF at any other time and therefore the same shape as the IMF of all stars ever formed.” My interpretation of this clarification is that as the IMF characterizes the number density of stars per unit logarithmic mass that have ever formed up to a particular time, and not the actual number of stars per unit logarithmic mass, the shape of the IMF at a later time may well resemble the shape of the IMF at an earlier time because the increase in forming stars since the last IMF adds to the volume occupied by stars of a given initial mass range. The number of stars of a given initial mass range increases, but so does the amount of space they take up. The number density of stars in this mass range, or, IMF, thus remains unchanged in time.
For stars with mean main-sequence lifetimes greater than the age of the host galaxy, their
distribution has not changed over time and hence the initial and present-day mass functions for
these stars are identical. For stars with mean main-sequence lifetimes less than the age of the host
galaxy, their distribution today reflects the number that have evolved off the main sequence as red
giants, white dwarfs, neutron stars, or black holes since the host galaxy’s birth. Consequently, such
a distribution deviates from the initial mass function.

Expressing the differential, \( d(\log m) \), as \( \frac{1}{m(\ln 10)} dm \) similarly translates Eq. (E.1) to
\[
\xi(\log m) = \frac{dn}{dm} m(\ln 10) \equiv \xi(m) m(\ln 10)
\]
\[
\Rightarrow \xi(m) = \frac{1}{m(\ln 10)} \xi(\log m),
\tag{E.2}
\]
where \( \xi(m) \) is the total number of stars that have ever formed per square or cubic parsec and per
unit mass. Therefore, \( \xi(m) dm \) is the number of stars per area or volume born with mass between
\( m \) and \( m + dm \) while integrating said quantity across a range of stellar masses from, say, \( m_1 \) to \( m_2 \)
yields the number of stars that have ever formed per area or volume with \( m_1 \leq m \leq m_2 \):
\[
n_{m_1 - m_2} = \int_{m_1}^{m_2} \xi(m) dm.
\tag{E.3}
\]
Integrating \( \xi(m) dm \) across all possible stellar masses yields the total number of stars that have ever
formed per area or volume:
\[
n_{\text{total}} = \int_{m_l}^{m_u} \xi(m) dm,
\tag{E.4}
\]
where \( m_l \) and \( m_u \) are the lower and upper limits, respectively, of initial stellar masses. Division of
both sides of Eq. (E.4) by \( n_{\text{total}} \) provides the familiar normalization to unity:
\[
1 = \int_{m_l}^{m_u} \frac{\xi(m)}{n_{\text{total}}} dm
\]
\[
= \int_{m_l}^{m_u} \xi'(m) dm,
\tag{E.5}
\]
where \( \xi'(m) dm \) is the fraction of stars per area or volume born with mass between \( m \) and \( m + dm \).
By extension of Eq. (E.3),

\[ f_{m_1 - m_2} = \int_{m_1}^{m_2} \xi'(m)dm \]  

(E.6)
is the fraction of stars that have ever formed per area or volume born with \( m_1 \leq m \leq m_2 \) [188][56].

### E.2 The Alpha-Plot

Figure (E.1) highlights the data accumulated by Kroupa in the form of an alpha-plot. The value for alpha results from a shift in the power-law index of \( \Gamma \rightarrow \alpha = 1 - \Gamma \), where \( \Gamma \) is defined as the slope of the log-log plot of \( \xi(log m) \) vs. \( log m \). The data includes Milky-Way and Large-Magellanic-Cloud clusters and OB associations as well as Orion-Nebula clusters. In the brown-dwarf regime \( (m/M_\odot < 0.08) \), the thick horizontal long-dashed line corresponding to \( \alpha = 0.3 \) (the thin long-dashed lines above and below denoting the limits of uncertainty) represents a reasonable fit to the data. The thick short-dashed lines for \( 0.08 \leq m/M_\odot \leq 1.0 \) represent the single-star IMF of Kroupa, Tout, & Gilmore (1993), the change in \( \alpha \) near \( 0.5 M_\odot \) a key feature. There is large scatter in the shaded regions for \( 0.08 < m/M_\odot < 0.15 \) and for \( 0.8 < m/M_\odot < 2.5 \) from complications in IMF derivations attributable to unknown stellar ages, as further discussed in Ref. [140]. An average value of 2.3 for \( \alpha \) across the entire mass range from 3.0 to 120.0 \( M_\odot \) fits the data well to within an uncertainty of 0.7, the points, seemingly, randomly scattered inside these bounds without concentration toward a particular \( \alpha \) value.

Kroupa summarizes the above to describe his adopted multi-part power-law IMF:

\[
\xi(m) \propto m^{-\alpha_i},
\]

\[
\alpha_0 = +0.3 \pm 0.7, \quad 0.01 \leq m/M_\odot < 0.08
\]

\[
\alpha_1 = +1.3 \pm 0.5, \quad 0.08 \leq m/M_\odot < 0.5
\]

\[
\alpha_2 = +2.3 \pm 0.3, \quad 0.50 \leq m/M_\odot < 1.00
\]

\[
\alpha_3 = +2.3 \pm 0.7, \quad 1.00 \leq m/M_\odot,
\]

(E.7)
evidence existing for only 2 changes in \( \alpha \) near 0.08 and 0.5 \( M_\odot \). For stars born per area or volume with \( 0.01 \leq m/M_\odot \leq 50.00 \), the mean stellar mass of the IMF is 0.36 \( M_\odot \). Its distribution of stellar populations by number and mass percent for this mass range is listed in Tab. (E.1). Adding up the numbers unveils the fascinating property that just under half of the mass (49.3%) is in stars born
Figure E.1: The alpha-plot for Milky-Way and Large-Magellanic-Cloud clusters and OB associations as well as Orion-Nebula clusters.

per area or volume with $0.01 \leq m/M_\odot \leq 1.00$ while just over half is in stars born per area or volume with mass between 1 and 50 $M_\odot$ [222][136].

<table>
<thead>
<tr>
<th>Type</th>
<th>Number %</th>
<th>Mass %</th>
<th>Mass Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brown Dwarfs</td>
<td>37 %</td>
<td>4.3 %</td>
<td>0.01 - 0.08 $M_\odot$</td>
</tr>
<tr>
<td>M Dwarfs</td>
<td>48 %</td>
<td>28 %</td>
<td>0.08 - 0.50 $M_\odot$</td>
</tr>
<tr>
<td>‘K’ Dwarfs</td>
<td>8.9 %</td>
<td>17 %</td>
<td>0.50 - 1.00 $M_\odot$</td>
</tr>
<tr>
<td>Intermediate-Mass</td>
<td>5.7 %</td>
<td>34 %</td>
<td>1.00 - 8.00 $M_\odot$</td>
</tr>
<tr>
<td>‘O’ Stars</td>
<td>0.37 %</td>
<td>17 %</td>
<td>&gt; 8.00 $M_\odot$</td>
</tr>
</tbody>
</table>

Table E.1: Number and mass percents for stellar objects of the IMF.

### E.3 Possible Causes for Alpha Scatter

Contrary to fundamental arguments indicative of diverse conditions in an array of star-formation environments, no convincing evidence prevails in support of a variable IMF. Kroupa (2001)
sought to interpret the scatter in the alpha-plot as due to statistical noise from undersampling of the IMF, star loss from dynamical evolution of clusters, and unreliable mass estimates from lack of resolution of binary systems. Sampling from the IMF for a population of $10^2$-$10^3$ stars does indeed reproduce the systematic scatter for $m/M_\odot > 3.0$. Only a few percent of the total number of stars fill 10 mass bins in the model, producing a flattening of the IMF equivalent to near-identical numbers of stars in each bin and, thus, zero extraction of useful information. As such population sizes of $10^2$-$10^3$ stars are typical of star-count samples, undersampling poses a problem that may mask true variations in the IMF.

Beginning with 100% of stars born into binary systems, simulations of cluster evolution significantly underestimate the value of $\alpha_0$ by $\approx 1.1$ at $t = 0$ but only slightly at $t = 3, 70$ Myr since most of the Brown Dwarf-Brown Dwarf (BD) and star-BD systems eventually disband. That slight underestimation becomes even less in the absence of the incorrect assumption of perfect efficiency for binary births. At $t = 0$, the values of $\alpha_{1,2}$ are also significantly underestimated by $\approx 0.6$ and $\approx 0.8$, respectively. At the later times of 3 and 70 Myr, a considerable fraction of binaries still survive to maintain that underestimation of $\alpha_{1,2}$ by $\approx 0.5$ and $\approx 0.6$, respectively. For $m/M_\odot > 1.00$, the scatter in $\alpha$ is comparable to the observed scatter in Fig. (E.1) because the random sampling from the IMF mostly produces very-low-mass secondary stars paired with massive primaries. These secondaries surely contribute to the low-mass regime of the IMF but cannot have any affect on the $\alpha$ values for $m/M_\odot > 1.00$. It is clear, then, that corrections must be applied to the $\alpha$ values of very-low-mass stars to infer the single-star IMF in young stellar populations.

As the models incorporate unrealistically-extreme cluster densities, the typically-lower densities will result in a slower disruption rate of binaries and, in turn, a higher fraction surviving cluster evolution for longer durations. The models also do not account for triple, quadruple, and other higher-order systems, their unknown numbers further increasing the systematic error inherent to the observational estimates for $\alpha$ of Fig. (E.1). The errors present in this study by Kroupa (2001) must therefore encompass the minimum corrections to $\alpha$, both the statistical noise from small sample sizes, and lack of resolution of higher-order systems as clusters evolve, a hindrance to more accurate determinations for the shifted power-law index [136].
The Milky-Way clusters in Fig. (E.1) are between several and 100 million years old and thereby depict the latest episode of star formation in the Galaxy. The aforementioned corrections at the later times revise the IMF of Eq. (E.7) to

$$\xi(m) \propto m^{-\alpha_i},$$

$$\alpha_0 = +0.3 \pm 0.7, \; 0.01 \leq m/M_\odot < 0.08$$

$$\alpha_1 = +1.8 \pm 0.5, \; 0.08 \leq m/M_\odot < 0.5$$

$$\alpha_2 = +2.7 \pm 0.3, \; 0.50 \leq m/M_\odot < 1.00$$

$$\alpha_3 = +2.3 \pm 0.7, \; 1.00 \leq m/M_\odot$$

for the present-day star-formation IMF of said clusters. The following is its number and mass percents of the associated stellar (0.01 \leq m/M_\odot \leq 50.00) populations:

<table>
<thead>
<tr>
<th>Type</th>
<th>Number %</th>
<th>Mass %</th>
<th>Mass Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brown Dwarfs</td>
<td>50 %</td>
<td>10 %</td>
<td>0.01 - 0.08 M_\odot</td>
</tr>
<tr>
<td>M Dwarfs</td>
<td>44 %</td>
<td>39 %</td>
<td>0.08 - 0.50 M_\odot</td>
</tr>
<tr>
<td>'K' Dwarfs</td>
<td>4.3 %</td>
<td>14 %</td>
<td>0.50 - 1.00 M_\odot</td>
</tr>
<tr>
<td>Intermediate-Mass Stars</td>
<td>2.3 %</td>
<td>24 %</td>
<td>1.00 - 8.00 M_\odot</td>
</tr>
<tr>
<td>'O' Stars</td>
<td>0.15 %</td>
<td>12 %</td>
<td>&gt; 8.00 M_\odot</td>
</tr>
</tbody>
</table>

Table E.2: Number and mass percents for stellar objects of the PDMF.

the average stellar mass being 0.20 M_\odot and 'O' and 'IM' stars contributing 36% to the total [136].

Final Thoughts on Kroupa (2001) Study

There is much to unpack in this study by Kroupa (2001) that is beyond the scope of my work. I stumbled upon this study while researching the background of the IMF and find the alpha-plot quite fascinating as it relates to possible as-yet compelling evidence for variations in the IMF. To think that the number of stars that have ever formed per area or volume and per unit logarithmic mass up to some particular time in the past is the same as the number of stars that have ever formed per area or volume and per unit logarithmic mass up to some later time, regardless of where, is unbelievably remarkable. As I am sure more work has been completed since 2001 on the nature of the IMF, I look forward to continuing my review in the future.
E.6 The IMF Plot

Figure E.2: Initial mass function vs. stellar mass.

Figure (E.2) displays the normalized initial mass function of Kroupa (2001) as a function of stellar mass in units of Solar masses and Fig. (E.3) displays the corresponding log-log plot, Eqs. (E.1) and (E.2) emphasizing their correlation. From Eq. (E.6), the area under the curve of Fig. (E.2) across a range of stellar masses is the fraction of stars that have ever formed per area or volume with mass in that range. Proving difficult to obtain a sense of the area under the curve, let’s zoom in twice on Fig. (E.2) by reducing the x-axis range to [0, 5] and [0, 1]. The ambiguity of Fig. (E.2) vanishes in light of the apparent dominant area under the curve of Fig. (E.5) for stars born per area or volume with mass less than 1 Solar mass. Such bias of the IMF toward very-low-mass stars, at least for the range of stellar masses up to 50 $M_\odot$, was previously illuminated by Tab. (E.1) in which most ($\sim$94%) of the stars were born per area or volume with mass less than 1 Solar mass.

A complement to Fig. (E.5) and Tab. (E.1), the bar plot of Fig. (E.6) augments the deduced conclusions with a sampling from the IMF for 10,000 newly-created stars per area or volume. The bias for $0.08 \leq m/M_\odot \leq 1.00$ is visible as the thick black blob of indistinguishable bars while the
Kroupa (2001)

Figure E.3: Log of initial mass function vs. log of stellar mass.

Kroupa (2001)

Figure E.4: Initial mass function vs. stellar mass for reduced mass range.
Figure E.5: Initial mass function vs. stellar mass for even-further reduced mass range.

Figure E.6: Number of stars born per area or volume as sampled from the IMF for 10,000 stars.
bars for $m/M_\odot > 1.00$ are barely discernible. Let’s zoom in twice as before, reducing the y-axis range to $[0, 10]$ and then the x-axis range to $[10, 100]$ with that reduced y-range. The number of newly-created stars per area or volume may now be easily counted in Fig. (E.8) since each of the bars from 10 to 100 $M_\odot$ has a height of 1 in these zoomed-in plots, thus confirming once more that the IMF produces mostly very-low-mass stars per area or volume. Such counting gives 26 stars born per area or volume with $10.00 \leq m/M_\odot \leq 100.00$, only 0.26% of the 10,000. Corroborating the findings in Tab. (E.1) are the 9,345 stars, or, $\sim94\%$, born per area or volume with mass less than 1 Solar mass.
E.7 Normalizing the Kroupa (2001) IMF

Prior to sampling from the IMF, normalization per Eq. (E.5) is required:

\[ 1 = \int_{m_i}^{m_u} \xi'(m) dm \]

\[ \equiv \int_{0.01 M_\odot}^{0.08 M_\odot} C_1 m^{-0.3} dm + \int_{0.08 M_\odot}^{0.5 M_\odot} C_2 m^{-1.3} dm + \int_{0.5 M_\odot}^{100 M_\odot} C_3 m^{-2.3} dm, \]

where \( C_1, C_2, \) and \( C_3 \) are the normalization constants and the piece-wise nature of \( \xi'(m) \) dictates the break-up of the integral. Although evidence [75] opposes the theoretical restrictions for stellar masses in excess of 120 \( M_\odot \) [139], we chose 100 \( M_\odot \) as the upper limit in our calculations because the IMF samples a negligible percentage of masses beyond this value. The constants are determined...
from continuity conditions:

\[
\lim_{m \to 0.08^-} C_1 m^{-0.3} = \lim_{m \to 0.08^+} C_2 m^{-1.3}
\]

\[\Rightarrow C_1 (0.08)^{-0.3} = C_2 (0.08)^{-1.3}\]

\[\Rightarrow C_2 = 0.08 C_1\]

\[
\lim_{m \to 0.5^-} C_2 m^{-1.3} = \lim_{m \to 0.5^+} C_3 m^{-2.3}
\]

\[\Rightarrow C_2 (0.5)^{-1.3} = C_3 (0.5)^{-2.3}\]

\[\Rightarrow C_3 = 0.5 C_2\]

\[\Rightarrow C_3 = 0.04 C_1.\]

Hence,

\[
1 = \int_{m_1}^{m_u} \xi'(m) dm
\]

\[
\equiv C_1 \left[ \int_{0.01 M_\odot}^{0.08 M_\odot} m^{-0.3} dm + 0.08 \int_{0.08 M_\odot}^{0.5 M_\odot} m^{-1.3} dm + 0.04 \int_{0.5 M_\odot}^{100 M_\odot} m^{-2.3} dm \right]
\]

\[
= C_1 \left[ \frac{1}{0.7} m^{0.7} \int_{0.01}^{0.08} - \frac{0.08}{0.3} m^{-0.3} \int_{0.08}^{0.5} - \frac{0.04}{1.3} m^{-1.3} \int_{0.5}^{100} \right]
\]

\[\Rightarrow C_1 = \frac{1}{0.503233}\]
E.8  Cumulative Distribution Functions of the IMF

From appendix C, the cumulative distribution function of the IMF for a given stellar mass, \(0.01 \leq m/M_\odot < 0.08\), is

\[
C_1(m) = C_1 \int_{0.01 M_\odot}^{m} m'^{(-0.3)} dm' = C_1 \frac{1}{0.7} [m^{0.7} - (0.01)^{0.7}]. \tag{E.8}
\]

If \(m = 0.08 M_\odot\), then \(C_1(0.08 M_\odot)\) is the total probability of producing a stellar mass, per area or volume, up to and including 0.08 \(M_\odot\):

\[
C_1(0.08 M_\odot) = \frac{1}{0.503233} \frac{1}{0.7} [(0.08)^{0.7} - (0.01)^{0.7}]
= 0.371488,
\]

or, a probability of \(\sim 37.15\%\). Similarly, for a given stellar mass, \(0.08 \leq m/M_\odot < 0.5\), the cumulative distribution function is

\[
C_2(m) = C_1(0.08 M_\odot) + C_2 \int_{0.08 M_\odot}^{m} m'^{(-1.3)} dm' = 0.371488 - C_1 \frac{0.08}{0.3} [m^{-0.3} - (0.08)^{-0.3}]. \tag{E.9}
\]

If \(m = 0.5 M_\odot\), then \(C_2(0.5 M_\odot) + C_1(0.08 M_\odot)\) is the total probability of producing a stellar mass, per area or volume, up to and including 0.5 \(M_\odot\):

\[
C_2(0.5 M_\odot) + C_1(0.08 M_\odot) = -\frac{1}{0.503233} \frac{0.08}{0.3} [(0.5)^{-0.3} - (0.08)^{-0.3}] + 0.371488 = 0.849602,
\]
or, a probability of \( \sim 84.96\% \). Finally, for a given stellar mass, \( 0.5 \leq m/M_\odot < 100 \), the cumulative distribution function is

\[
\begin{align*}
C_3(m) &= C_1(0.08 \, M_\odot) + C_2(0.5 \, M_\odot) + C_3 \int_{0.5 \, M_\odot}^{m} m'(-2.3) \, dm' \\
&= 0.849602 - C_1 \frac{0.04}{1.3} \left[m^{-1.3} - (0.5)^{-1.3}\right].
\end{align*}
\] (E.10)

If \( m = 100 \, M_\odot \), then \( C_3(100 \, M_\odot) + C_2(0.5 \, M_\odot) + C_1(0.08 \, M_\odot) \) is the total probability of producing a stellar mass, per area or volume, up to and including \( 100 \, M_\odot \):

\[
C_3(100 \, M_\odot) + C_2(0.5 \, M_\odot) + C_1(0.08 \, M_\odot) = - \frac{1}{0.503233} \frac{0.04}{1.3} \left[(100)^{-1.3} - (0.5)^{-1.3}\right] + 0.849602
\]

\[
= 1,
\]

or, a probability of 100\%, as expected from the normalization.

### E.9 Sampling from the IMF

We are now ready to sample from the IMF. To do so as described in appendix C, we must invert Eqs. (E.8), (E.9), and (E.10):

\[
C_1^{-1}(m) = \left[\frac{0.7}{C_1}C_1(m) + (0.01)^{0.7}\right]^{\frac{1}{0.7}}
\] (E.11)

\[
C_2^{-1}(m) = \left[-\frac{0.3}{0.08C_1}[C_2(m) - C_1(0.08 \, M_\odot)] + (0.08)^{-0.3}\right]^{-\frac{1}{0.3}}
\] (E.12)

\[
C_3^{-1}(m) = \left[-\frac{1.3}{0.04C_1}[C_3(m) - C_1(0.08 \, M_\odot) - C_2(0.5 \, M_\odot)] + (0.5)^{-1.3}\right]^{-\frac{1}{1.3}}.
\] (E.13)

As \( C_1(m) \), \( C_2(m) \), and \( C_3(m) \) all represent probabilities (per area or volume) with values less than 1, the domain of each inverse function above is simply the set of uniformly-distributed real numbers,
During each time step of our calculations, Boost utilizes a pseudo-random number generator as input to a distribution function that returns uniformly-distributed floating-point values on the aforementioned range. We thus sample from the IMF by replacing $C_1(m)$, $C_2(m)$, and $C_3(m)$ with this distribution function. If the floating-point value, $x$, is less than $C_1(0.08 \, M_\odot)$, we apply Eq. (E.11) to acquire a stellar mass, $0.01 \leq m/M_\odot < 0.08$. If $C_1(0.08 \, M_\odot) \leq x < C_2(0.5 \, M_\odot)$, we apply Eq. (E.12) to acquire a stellar mass, $0.08 \leq m/M_\odot < 0.5$. And if $C_2(0.5 \, M_\odot) < x \leq C_3(100 \, M_\odot)$, we apply Eq. (E.13) to acquire a stellar mass, $0.5 \leq m/M_\odot < 100$. In our calculations, star formation is governed only by the amount of mass in each zone as outlined in appendix D [137].

Mixing at zonal boundaries influences this amount independent of any prescribed size for a given zone. Material that mixes into a given zone during each time step instantaneously homogenizes throughout that zone. Volume thus has no affect on zonal mass distributions. We thereby allocate a unit cubic volume to each zone for ease of stellar mass determinations. All mentions of “per area or volume” or “per square or cubic parsec” above may now simply be ignored.
Appendix F

The Inhomogeneous Chemical Evolution Tool

The workhorse of the chemical evolution calculations is the ICE (Inhomogeneous Chemical Evolution) code [183]. ICE is built on top of NucNet Tools [184] and, in particular, the multi-zone components of that code suite. ICE allows us to model the evolution of isotopes in the Galaxy as a multi-zone nuclear-reaction network. The user must supply the following code modules for ICE (all written as header files with .h or .hpp suffixes). The names of the modules are the default versions. A user can rewrite and choose different names as desired.

- **star.h** This module defines stars and multiple-star systems in ICE. Stars are C++ classes that have methods to store, return, and update properties such as formation time, end time, mass, initial metallicity, and location. StarSystem is a class to store Stars. The principal data structure in a StarSystem is a priority queue of Stars (instantiated as a fibonacci heap). The stars in the system are ordered according to their end time (the time they will die) such that the star on the top of the heap will die earliest. Removing a star is simply a matter of "popping" it from the queue, an operation that is logarithmic in time in a fibonacci heap. Insertion of stars into a star-system heap is constant in time for a fibonacci heap. A user defines stellar properties, such as stellar lifetime, in the Star class. A user typically does not modify the StarSystem class.
• **star.hpp** This module defines and keeps track of stellar populations. It is here that the user defines the initial mass function (IMF), that is, the distribution of the number of forming stars as a function of their mass. The default IMF for ICE is currently that of Ref. [138]. This module can also keep track of the current star population as a function of mass, a distribution that differs from the IMF due to the varying lifetimes of the stars. Please see appendix E for a detailed discussion of both distributions.

• **yields.hpp** This module defines and keeps track of stellar yields. The default version of this module is to read yields in from an XML file, the preferred format for the underlying NucNet Tools modules.

• **remnants.hpp** This module defines and keeps track of stellar remnants. More precisely, it defines what happens to a star after it dies. In the default version, for example, if a stellar system has two low-mass stars, when the more massive of the two dies, it leaves behind a white dwarf. The system is thus a white-dwarf/low-mass-star binary. The user can specify a timescale for mass to transfer from the low-mass star to the white dwarf and then for the white dwarf to explode as a Type Ia supernova.

• **cos_wave_halo.hpp** This module defines the structure of the multi-zone Galaxy and rules for mixing between its various components. The default module arranges multiple zones in a circular array to represent the Solar annulus in the Galaxy with another zone representing the Galactic halo. A number of spiral density waves go through the annulus giving episodes of star formation on user-defined timescales.

Once the essential modules are defined, the code operates as follows. The Galaxy is allowed to evolve over a user-defined interval. Stars form in user-defined zones in proportion to mass according to a Schmidt law [130] with an exponent of 1, a choice that motivates code diagnostics while preserving simplicity. A survey of the residual gas in the ISM at the current Galactic time (taken as 13.5 Gyr) identifies a star-formation timescale of 1466 yr as the culprit for the current Galactic gas fraction of ≈0.15 [43]. As input to the PTRD algorithm [117], the star-formation rate and a Boost random-number generator [168] determine the number of stars created during each time step. Additional calls to the random-number generator obey the IMF in distributing the newly-created stellar masses and spawn uniformly-distributed random variates between 0 and 1 for depositing the stars,
either single or comprising a system (i.e., binary in current ICE version), in one of the user-defined zones.

Stars are binned in mass, meaning, for example, that all stars born in the mass range, \( M_1 \) to \( M_2 \), in a particular region of the Galaxy are grouped together as a single “star” with mass given by the average mass of the stars in the bin. The binning also keeps track of the number of stars in each bin; thus, when this “star” dies, it gives off the ejected mass for such a star times the total number of stars. In this way, the code is able to avoid storing huge numbers of low-mass stars. Also, if the lifetime of a star is longer than the duration of the calculation, the star is considered “inactive” and not, in fact, added to the priority queue. Rather, its mass is simply added to the total mass of “inactive” stars.

During each time step, ICE checks whether a star in a system will die by iterating over the priority queue of Stars (see `star.h` above). Each star that does die is popped from the queue. Its status is then determined from the remnants module. If, for example, it becomes a neutron star, it is re-inserted into its star system with changed status. The mass ejected by the dying star is returned to the local part of the Galaxy with isotopic abundances specified in the yields module.

A star system that has evolved to a white-dwarf/low-mass-star binary could potentially become a thermonuclear (Type Ia) supernova. The user can input the fraction of such systems that explode and the timescale on which they do. Similarly, a massive-star system may evolve to a neutron-star/neutron-star binary. The user can input the fraction of such systems that merge (and eject r-process matter) and the timescale on which they do. Please see appendix H for a brief history of the r-process and where binary neutron-star mergers fit in.

The calculation proceeds with data saved as often as specified by a user-defined quantity. The chosen format is the Hierarchical Data Format (version 5), that is, HDF5. ICE uses the NucNet Tools library of HDF5 routines to output zone data at each data dump. ICE also saves the composition of any stars that form (filtered by initial-mass and formation-time ranges).

To solve the evolution of abundances in the various Galactic phases, ICE sets up a multi-zone reaction network with the construction of a large vector \( \vec{M}(t) \). The length of \( \vec{M} \) is \( (N_{\text{nuc}}+1) \times N_{\text{zones}} \), where \( N_{\text{nuc}} \) is the number of nuclear species in the network and \( N_{\text{zones}} \) is the number of zones in the calculation. If a given zone \( i \) has mass \( M_i \), then the entries \( M_{(i-1) \times (N_{\text{nuc}}+1)} + j \) of \( \vec{M} \) have values \( M_i X^j \), where \( X^j \) is the mass fraction of species \( j \) in zone \( i \). Of course, \( j \) runs from 1 to \( N_{\text{nuc}} \). The entry \( M_{i \times (N_{\text{nuc}}+1)} \) is \( M_i \). In other words, to fill the vector, we loop over all species in the first zone,
then loop over all species in the second zone, and so on across all remaining zones while reserving an extra element per zone for that zone’s mass.

As reactions among nuclei involve nuclear decays, dependent only on the abundances of the decaying species, and mixing between zones, taken as proportional to the zone mass, the resultant network is purely linear. Hence, the governing differential equation for the time evolution of masses in the network is

\[ \frac{d\vec{M}}{dt} = A\vec{M}. \]  

(F.1)

The matrix $A$ linking species within and among zones is quite sparse since not all species and zones interact. ICE thereby takes advantage of the sparse-matrix storage scheme of NucNet Tools to break up $A$ into a sum of submatrices $A \equiv \sum_i A_i$, each comprising elements of $A$ representing decays in, and the mixing of mass into and out of, zone $i$. The matrix multiplication of Eq. (F.1) may thus be written as a sum of matrix multiplications:

\[ A\vec{M} = \sum_i A_i\vec{M}. \]

ICE harnesses the OpenMP parallelization of the Palmetto Cluster [169] in carrying out the individual matrix multiplications and subsequent sum (reduction). The advantage of the parallel computations is an increase in performance speed by at least a factor of 8. To solve for $\vec{M}(t + \Delta t)$ from $\vec{M}(t)$ through the finite-differencing of Eq. (F.1), ICE applies SPARSKIT2’s matrix exponentiator [221] that requires only the aforementioned matrix multiplications of $A$ on the current guess for $\vec{M}$. Once the masses are determined in the ISM phases at $t + \Delta t$, ICE creates new stars and allows dying stars to ejecta their matter, as described above.
Appendix G

Fictitious Species

G.1 Definition and Naming

- **Bojazium**: A fictitious element that is added to a nuclear-reaction network to track its subsequent evolution in the model. It can have any atomic number not reserved for real species in the calculations and any number of isotopes. In practice, Bojazium has as many isotopes as needed for tracing sources in the model.

In our network, we arbitrarily chose stable Bojazium to have an atomic number of 150 with isotopes spanning a range of mass numbers from 300 to as high as 500. For the forthcoming results to be discussed, our calculation evolved the abundances of 44 isotopes between $^{300}\text{Upn}$ and $^{343}\text{Upn}$, the element symbol short for a name, “Unpenthilium”, as adopted per the IUPAC system [173]. Since we are particularly interested in the production of $^{129}\text{I}$ by the r-process, each isotope of Unpenthilium is produced in and expelled by the merger of two neutron stars [59][82], i.e., merger 1 is responsible for $^{300}\text{Upn}$, merger 2 for $^{301}\text{Upn}$, merger 3 for $^{302}\text{Upn}$, merger 4 for $^{303}\text{Upn}$, and so on. The tracer isotopes could easily originate from Type Ia or Type II supernovae or some other source as part of the s-, r-, or n-processes, for instance, their subsequent evolution in the Galaxy tracking the creation and distribution of various astronomical events and the contributions of each to the compositions of forming stars. To avoid interference with real species evolution, each merger yields a small fraction of $10^{-8}$ of its ejected mass for each fictitious isotope.
G.2 Ejection of Stable Masses and Resultant Contributions

To quantify the relative contribution of each merger to the composition of forming stars during the calculations, first consider Fig. (G.1). The set of symbols correspond to 3 different Solar-mass stars that form near the time of the Sun’s birth at 8.504 Gyr, 8.751 Gyr, and 8.998 Gyr post Big Bang. For a given star, each point on the plot represents a merger and its associated isotope, the time of merger occurrence on the x-axis and fractional contribution on the y-axis. What is meant by “fractional contribution”?

The fractional contribution, \( f^{(i)} \), is acquired as follows:

\[
f^{(i)} = \frac{M^{(i)}}{M_{Upn}} \equiv \frac{X^{(i)}}{\sum_j X^{(j)}},
\]

where \( X^{(i)} \) is the mass fraction of isotope \( i \) in the ejected merger material, or, the ejected mass of \( i \) divided by the total ejected mass in the merger, and the sum in the denominator is the ejected mass of Unpentnilium isotopes divided by the total ejected mass in the merger. The cancellation of this total ejected merger mass in the numerator and denominator allows determination of the mass of each Unpentnilium isotope \( (M^{(i)}) \) relative to the sum of all Unpentnilium masses \( (M_{Upn}) \). Because our calculation computes and stores \( X^{(i)} \), though, we must use these values to arrive at \( f^{(i)} \).

In monitoring each isotope’s relative mass fraction, we may ascertain the contribution of the associated merger’s mass to the composition of the 3 forming Solar-mass stars. Figure (G.1) highlights a low fractional contribution (near 0.01) of mergers occurring early in our calculation. From appendix D and appendix E, the mean star-formation rate is proportional to the available gas mass and the initial mass function is heavily weighted toward low-mass stars, respectively. As the available gas mass rises to a peak early in the evolution of the Galaxy (see chapter 4), a likely explanation, then, for such a low contribution is the amplified formation of long-lived, low-mass stars around this time that take up the ejected mass in the mergers and, while still present in the Galaxy, have yet to return it.

The last merger occurred at 8.471 Gyr post Big Bang. About 33 million years later, the star represented by the red circles in Fig. (G.1) formed. Notice the continual growth in the merger contribution with time is interrupted by the drop-off from the final 2 mergers, a phenomenon absent for the other 2 stars. These final mergers occur in zones 23 and 25 while the red-circle star formed in
Figure G.1: Fractional contribution to late-forming Solar-mass stars as a function of merger time.

Figure G.2: Fractional contribution to late-forming Solar-mass stars as a function of merger time.
zone 6. Due to the close temporal proximity of the merger and star-formation events, there was not enough time for the merger material to mix across at least 13 zones in becoming a significant part of the composition of the forming red-circle star. Hence, these final mergers contribute a minimal amount of mass to that star. The other two forming stars, on the other hand, are hundreds of millions of years away from the final merger, leaving plenty of time for the merger material to homogenize throughout the zones prior to their formation. An appreciable contribution to the red-circle star, though, emerges from the merger at 8.426 Gyr post Big Bang. Occurring in zone 27 and earlier than the previously-discussed mergers, enough time must have passed for much of this material to reach zone 6 prior to its homogenization across all zones.

Similar to Fig. (G.1), the red circles of Fig. (G.2) now correspond to a Solar-mass star that formed at 8.505 Gyr post Big Bang. Albeit close in formation time to the red-circle star of Fig. (G.1), this star, having been born in zone 28, is many zones nearer to the aforementioned final merger events. Such close spacial and temporal proximity is the source of the appreciable contributions to the red-circle star in Fig. (G.2), as there is just the right amount of time for much merger material to mix into zone 28 without yet homogenizing throughout the remainder of the zones.

G.3 Ejection of Radioactive Masses and Resultant Contributions

Is it also possible to track the evolution of radioactive species like $^{129}$I? Absolutely! To do so, a quick review is necessary:

\[ M_g = nM_{g/mole}, \]

\[ n = \frac{N_{part}}{N_A} \]

\[ \Rightarrow N_{part} = \frac{M_g}{M_{g/mole}N_A}, \quad (G.2) \]

where $M_g$ and $M_{g/mole}$ are the mass in grams and mass in grams in a mole, respectively, of a sample composed of a single element and $n$, $N_{part}$, $N_A$ are the number of moles, number of particles, and
Avogadro’s number, respectively, for the sample \([76]\).[227]. In terms of the mass of the sample, the radioactive decay law of appendix B then becomes

\[ e^{-\frac{t}{\tau}} = \frac{N_t}{N_0} = \frac{M_{g,t}}{M_{g,0} N_A} \]

where the assumed initial time of Eq. (G.3) is 0. As Eq. (G.1) already contains the numerator in terms of the mass of the isotope (divided by the total ejected merger mass), we may express \(X^{(i)}\) for radioactive species as

\[ X^{(i)} = \frac{M^{(i)}}{M_{\text{merger}}} = \frac{M_{g,0} e^{-\left(t_{\text{form}} - t^{(i)}\right)/\tau}}{M_{\text{merger}}}, \quad \text{(G.4)} \]

where the numerator now accounts for the contribution of radioactive mass ejected from merger, \(i\), by the difference in time between the birth of the star \(t_{\text{form}}\) and merger event \(t^{(i)}\). The larger this difference, the more time that mass has to decay and, in turn, contribute less to the composition of the soon-to-form star. Summing the expression of Eq. (G.4) across all mergers, \(j\), in the denominator of Eq. (G.1) provides the total ejected radioactive mass of the species under consideration. The ratio of the radioactive mass ejected from merger, \(i\), to the total ejected radioactive mass gauges the relative contribution of each merger to the forming star.

With a mean lifetime of \(\approx 22.65\) million years, Fig. (G.3) prominently illustrates the relative contribution of radioactive \(^{129}\text{I}\) mass from each merger to the 3 forming Solar-mass stars of Fig. (G.1). The spacial and temporal patterns of that figure have vanished here, as the final 2 mergers generate the greatest contribution to each star. Mergers occurring before \(\approx 8.40\) Gyr post Big Bang offer negligible \(^{129}\text{I}\) mass to the composition of the forming stars. On the scale of billions of years...
of Galaxy evolution, the mean lifetime of $^{129}$I is too short for any but the most recent mergers to contribute to the $^{129}$I mass of stars forming near the time of the Sun’s birth.

The contribution from each successive merger beyond 8.40 Gyr post Big Bang approaches 0.55, a value almost 14 times the peak contribution of the stable species in Fig. (G.1). Each merger produces a mass of $^{129}$I less than the corresponding stable mass by the exponential factor above. But the sum of Unpentnilium masses in the denominator of Eq. (G.1) for $^{129}$I will be significantly less than that for a stable species because most of the $^{129}$I masses in the sum will have decayed away. The decrease in the $^{129}$I mass due to decay and/or lack of mixing from zonal disparity between events (red-circle star), then, is offset by the greater decrease in the summed masses, yielding a larger overall contribution from the most recent merger events.

For the long-lived radioactive isotope, $^{238}$U, the contribution to each Solar-mass star in Fig. (G.4) seems only minimally larger than negligible for many of the mergers. However, upon zooming in, that gradual rise in contribution from each successive merger of Fig. (G.1) is visible in Fig. (G.5) for the long-lived species. Characterized by a mean lifetime ($\approx$4.468 Gyr) on the order of
Figure G.4: Fractional contribution to late-forming Solar-mass stars as a function of merger time for radioactive $^{238}$U.

Figure G.5: Zooming in on Fig. (G.4).
the age of the Solar System, the decay of radioactive $^{238}$U ejected from each merger is far less rapid than that of $^{129}$I. The effect attributable to the reduction of early ejected $^{238}$U masses in the sum of the denominator of Eq. (G.1) allows for the mergers beyond $6 \, \text{Gyr}$ post Big Bang to slightly overtake those mergers of Fig. (G.1) in contributing to the composition of the forming stars. The mean lifetime of $^{238}$U, however, is too long for the removal of the spacial and temporal patterns of Fig. (G.1) for the red-circle star, the contributions from the final 2 mergers marginally larger in Fig. (G.4) for the radioactive $^{238}$U mass.

### G.4 Mean Isotope Age

The age of material emanating from a particular merger and embedded within the star of interest upon its formation is computed as $t_{\text{form}} - t^{(i)}$, the amount of time between the birth of the star and merger event. To extrapolate to the mean age of material emanating from all merger events influencing the star’s composition as it forms, the following sum,

$$\langle t_{\text{age}} \rangle = \sum_i \frac{[t_{\text{form}} - t^{(i)}] N_i}{N_{\text{upn}}}, \quad \text{(G.5)}$$

shall prove useful since the mean, by definition, is a sum over all values divided by the total number of values, or, more concisely in Eq. (G.5), the sum over all unique values multiplied by how many times each occurs and then divided by the total number of values. In our calculation, each merger ejects some number of particles of a particular isotope (say, $^{127}$I or $^{129}$I) at time, $t^{(i)}$, post Big Bang. Of those, an amount, $N_i$, is later taken up by the forming star at time, $t_{\text{form}}$, post Big Bang, each particle having lived $t_{\text{form}} - t^{(i)}$ years as the star is born. As the early Solar System is of paramount interest to us, we home in on the 171 Solar-mass stars born between 8.5 and 9 Gyr post Big Bang.

To extract the mean age from the quantities in our calculation, rewrite Eq. (G.5) with the
help of Eq. (G.2) as

\[
\langle t_{age} \rangle = \sum_i \left[ t_{form} - t^{(i)} \right] \frac{N_i}{N_{UPn}}
\]

\[
= \sum_i \left[ t_{form} - t^{(i)} \right] \frac{N_i}{\sum_j N_j}
\]

\[
= \sum_i \left[ t_{form} - t^{(i)} \right] \frac{M_{g,i}}{M_{g/mole,i}} N_A \frac{1}{\sum_j \frac{M_{g,j}}{M_{g/mole,j}} N_A}
\]

The molar mass is identical for all particles of a single isotope ejected by the mergers. Thus,

\[
\langle t_{age} \rangle = \sum_i \left[ t_{form} - t^{(i)} \right] \frac{M_{g,i}}{M_{g/mole,i}} \frac{N_A}{\sum_j \frac{M_{g,j}}{M_{g/mole,j}} N_A}
\]

\[
\equiv \sum_i \left[ t_{form} - t^{(i)} \right] \frac{1}{M_{g/mole,i}} N_A M_{g,i} \frac{1}{M_{g/mole,i}} N_A \sum_j M_{g,j}
\]

\[
\langle t_{age} \rangle = \sum_i \left[ t_{form} - t^{(i)} \right] \frac{M_{g,i}}{\sum_j M_{g,j}}
\]

\[
\equiv \sum_i \left[ t_{form} - t^{(i)} \right] \frac{M^{(i)}}{M_{UPn}}
\]

\[
\equiv \sum_i \left[ t_{form} - t^{(i)} \right] f^{(i)}
\]

the final steps incorporating Eq. (G.1) and the \(X^{(i)}\) values in our calculation.

Figure (G.6) is an exhibit of the mean isotope age for a stable species taken up by the 171 Solar-mass stars as they form. The mean age peaks at 3.49661 Gyr with 50 stars containing material from the mergers at a mean age between 3.37143 Gyr and this peak value. The distribution itself peaks around 3.18 Gyr with 54 stars containing material from the mergers at a mean age between 3.11429 and 3.24286 Gyr (Fig. (G.7)). The aforementioned disappearance of merger material early
in the history of the Galaxy by the formation of low-mass stars shifts the ejection of said material nearer, on average, to the birth of the Sun.

The mean isotope age for a radioactive species is achieved by appending the exponential factor of Eq. (G.4) to both the numerator and denominator of Eq. (G.6):

$$\langle t_{age} \rangle = \sum_i \left[ t_{form} - t^{(i)} \right] \frac{M_{g,i} e^{-(t_{form} - t^{(i)})/\tau}}{\sum_j M_{g,j} e^{-(t_{form} - t^{(j)})/\tau}} \equiv \sum_i \left[ t_{form} - t^{(i)} \right] f^{(i)}_{rad}.$$ 

Figure (G.8) is an exhibit of the mean isotope age for $^{129}$I taken up by the 171 Solar-mass stars as they form. Providing confirmation of the previous conclusions, the short mean lifetime of $^{129}$I restricts its mean age to within 534 million years of the birth of the Sun, or, its origin to the most recent merger events. The mean age peaks at 0.53315 Gyr with 50 stars containing material from the mergers at a mean age between 0.41425 Gyr and this peak value (Fig. (G.9)). The distribution also peaks for mean ages in this range. The youngest, or, rawest, material is only 37.89 million years old, a single star containing material from the mergers at this mean age while a mere 2 other stars contain material at a mean age not exceeding 40 Myr.
Figure G.8: Mean isotope age for $^{129}$I inside newly-created Solar-mass stars.

Figure (G.10) is an exhibit of the mean isotope age for $^{238}$U taken up by the 171 Solar-mass
stars as they form. The long mean lifetime of $^{238}$U restricts its mean age by only half a billion years or so relative to that of the stable species. The mean age peaks at 2.64658 Gyr with 33 stars containing material from the mergers at a mean age between 2.57143 Gyr and this peak value while the distribution itself peaks around 2.38 Gyr with 54 stars containing material from the mergers at a mean age between 2.31429 and 2.44286 Gyr (Fig. (G.11)). The youngest, or, rawest, material is $\approx 1.82$ billion years old, a single star containing material from the mergers at this mean age while 3 other stars contain material at a mean age not exceeding 1.85 Gyr.
Figure G.10: Mean isotope age for $^{238}$U inside newly-created Solar-mass stars.

Figure G.11: Zooming in on Fig. (G.10).
Appendix H

Homing in on the Site of r-Process Nucleosynthesis

H.1 r-Process Inside Wind-Produced Hot Bubbles

I wrote this section prior to 08/17/17 as a summary of the most likely candidate for the site of r-process nucleosynthesis. At the time, I believed the innermost regions of a massive star, those layers of the iron core above the mass cut and just outside of the developing proto-neutron star, proved to be a promising locale for the r-process. Up until the late ’90s and early ’00s, models of the neutrino-driven hot bubbles produced following shock passage during a Type II supernova explosion provided nucleosynthetic yields in close agreement with the heavy Solar r-process abundances. The next 3 subsections detail the mechanisms at work to reproduce the Solar r-process abundance distribution in these models.

H.1.1 En Route to Core Collapse

Toward the completion of silicon-core burning, owing to the high temperature and density of the core, all reactions achieve nuclear statistical equilibrium and advance at the same rate in synthesizing various abundances of the exceedingly-stable iron-peak nuclei. The most stable and abundant of these nuclei, $^{56}\text{Fe}$, cannot fuse with another $^{56}\text{Fe}$ nucleus unless energy is provided in catalyzing the reaction, as the value for the binding energy per nucleon of an $^{56}\text{Fe}$ nucleus, 8.7903 MeV, is near
the peak value of 8.7945 MeV of a $^{62}$Ni nucleus and the fusion of two $^{56}$Fe nuclei would thereby produce a larger and less-stable nucleus. Before the temperature and density of the core attain the high values necessary for such fusion, the iron-peak nuclei will have already begun breaking-down into lighter nuclei, $\alpha$-particles, protons, and neutrons via photo-disintegration reactions, as the photons are energetic enough to overcome the binding energy of nuclei and decompose them. The net process is designated as $^{56}$Fe $+ \gamma = 13\alpha + 4n$ and occurs as the temperature and density approach on the order of $10^{10}$ K and $10^{9}$ g/cm$^3$, respectively. The cessation of energy production via fusion reactions hinders matter pressure support by impeding the build-up of kinetic energy while the sapping of thermal energy from the radiation field for photo-disintegration reactions reduces radiation pressure. As the temperature and density of the core increase during collapse, the rate of photo-disintegration reactions also increases, thereby diminishing matter and radiation pressure support even more.

Also aiding in the reduction of pressure support against gravitational collapse are capture reactions on protons of nuclei and free protons by the vast sea of degenerate electrons via $e^- + p \Rightarrow n + \nu_e$, the free protons having been released in the photo-disintegrations of heavy nuclei. For core densities on the order of $10^{10}$ g/cm$^3$, the Fermi energy of the electrons exceeds the threshold energy for capture of electrons by $^{56}$Fe, $^{32}$Si, and $^{28}$Si. For example, a core density of $\approx 10^{10}$ g/cm$^3$ corresponds to a Fermi energy of electrons of $m_e c^2 + 3.7$ MeV, or, the threshold energy for $^{56}$Fe $+ e^- \Rightarrow 56$Mn $+ \nu_e$. Since the mass of the core is comprised mostly of $^{56}$Fe nuclei, this reaction is the dominant source of electron destruction. As the electrons are consumed in these reactions, their degeneracy pressure decreases, thus further breaching the balance of gravity and accelerating the collapse of the core. Like the photo-disintegration reactions, the rate of these capture reactions also increases as the temperature and density of the core increase during collapse.

Various neutron-rich nuclei are unstable against $\beta$-decay and free neutrons $\beta$-decay with a mean lifetime of $\approx 15$ minutes. However, deep in the interior of a collapsing massive star, $\beta$-decays are averted because, by the Pauli exclusion principle, there are no available energy states for the electrons produced in such decays to occupy. All states having an energy of these decay-product electrons are filled by the gas of degenerate electrons. Hence, for the extreme densities of the core during collapse, the opposite process, also known as inverse $\beta$-decay, continues to thrive as the matter density and, in turn, electron Fermi energy, increase. The rise in Fermi energy results in more and more electrons having enough energy to capture onto nuclei and free protons, thus accelerating the rate of these capture reactions and, in turn, the collapse of the core. As inverse $\beta$-decays
produce increasingly neutron-rich nuclei and a significant abundance of free neutrons, their activation acquired the moniker, "neutronization". Photo-disintegration reactions and neutronization also occur post core-bounce as the shock wave propagates out from the core.

The bountiful electron neutrinos produced in these capture reactions initially escape from the core but become trapped for core densities in excess of $10^{11} - 10^{12}$ g/cm$^3$. In such dense matter, the core matter compresses so tightly that the diffusion velocity of neutrinos lags the velocity of collapse of the infalling matter. The timescale for neutrino diffusion from the core is thereby longer than that for core collapse and the neutrinos become trapped. As the core density approaches the large values during collapse, the mean free path of neutrinos decreases to less than the radius of the core. The neutrinos are therefore unable to freely escape from the core and instead must undergo multiple nuclear charged-current and coherent neutral-current scatterings before the possibility of escape. The "neutrino trapping surface" separates the interior region of neutrino production, where neutrinos are trapped, from the exterior region of neutrino freedom, where newly-created neutrinos are able to escape the core freely or diffuse out via nuclear scatterings since the mean free path of such neutrinos produced beyond the "neutrino sphere" is greater than the distance to the core surface.

H.1.2 Shock Propagation and Stalling

Upon collapse, the gravitational binding energy, on the order of $10^{53}$ ergs, of the newly-formed neutron star is stored as thermal energy of the core and eventually transferred to the kinetic energy of neutrinos, each flavor carrying approximately $10^{51}$ ergs/s of power. Neutrino-pair production occurs via electron-positron pair annihilation as $e^+ + e^- \Rightarrow \bar{\nu}_x + \nu_x$ (x = e, μ, τ), as the core abounds with electrons and positrons. Neutrino pairs are also produced by the electron-nucleon and nucleon-nucleon bremsstrahlung processes, $e^+ + N \Rightarrow e^+ + N + \bar{\nu}_x + \nu_x$ and $N + N \Rightarrow N + N + \bar{\nu}_x + \nu_x$, respectively, where N represents a nucleon. Plasmon decay via $\gamma \Rightarrow \bar{\nu}_x + \nu_x$ and photoannihilation by $\gamma + e^+ \Rightarrow \bar{\nu}_x + \nu_x$ contribute to neutrino-pair production as well. Finally, the aforementioned electron-capture reactions, in addition to positron capture on nuclei or free neutrons as $e^+ + (A,Z) \Rightarrow p + \bar{\nu}_e$ and $e^+ + n \Rightarrow p + \bar{\nu}_e$, produce electron-neutrino pairs. Between 100 km and 300 km from the center of the neutron star, the outward-propagating shock wave generated by the core bounce loses kinetic energy to the thermal energy of the shocked iron-rich matter which, in turn, heats up and photo-disintegrates under the action of thermally-produced photons.
An abundance of nucleons builds up and, in addition to \( \approx 8.8 \text{ MeV/nucleon} \) of energy lost via these photo-disintegrations, the shock wave loses energy as neutrinos produced in nucleon-capture reactions behind the shock wave and above the neutrino sphere free-stream out of the core. Such energy losses are too much and the shock wave halts.

### H.1.3 Shock Re-vitalization by Neutrino-Driven Wind and Hot Bubbles

Neutrinos diffusing out from the core are able to revive the shock wave by restoring its kinetic energy via capture of the aforementioned abundant nucleons. Because the charged-current cross-section for capture of nucleons by electron neutrinos and anti-neutrinos is greater than the corresponding cross-section for the neutral-current capture reactions of all neutrino types, these particles deposit the largest amount of energy behind the shock wave. The reactions responsible for transferring energy to the matter behind the shock wave include the following: \( \nu_e + n \Rightarrow e^- + p \) and \( \bar{\nu}_e + p \Rightarrow e^+ + n \), the nucleons being free or embedded within nuclei, and scattering via \( \nu_x + e^- \Rightarrow \nu_x + e^- \) and \( \nu_x + N \Rightarrow \nu_x + N \). The neutrino heating rate per nucleon decreases with increasing distance from the core center, as \( 1/r^2 \). Meanwhile, the neutrino cooling rate per nucleon increases with the 6th power of the temperature. Because the temperature of the core falls off as \( 1/r \), the neutrino cooling rate per nucleon must suffer an even steeper drop with increasing distance from the core center, as \( 1/r^6 \). Only above a sphere defined by the gain radius, then, will the neutrino-capture reactions result in a net heating of the matter. At the gain radius, the neutrino-heating reactions are in equilibrium with the reverse cooling reactions that remove kinetic energy from the system in the form of escaping neutrinos.

Behind the shock wave, the matter is characterized by negative radial gradients of entropy and \( Y_e \) (number of electrons per nucleon). Deep in the interior of the core, the neutrinos remain trapped and their degeneracy prevents the capture of electrons by nuclei and free protons. The neutrinos produced in such reactions would be unable to fill an energy state, as all available neutrino energy states below the Fermi energy are occupied. However, as the radial distance from the core increases and extends beyond the neutrino sphere, the neutrinos are no longer trapped and begin to random-walk out of the core and, within one mean free path from the surface, can free-stream out. As more and more neutrinos escape with increasing distance from the core, the rate of electron-capture reactions increases as well, thus diminishing \( Y_e \) and establishing a negative radial gradient of \( Y_e \).
As infalling matter crosses the shock wave, it decelerates and compresses, the density increasing as a consequence. The matter encounters increasing neutrino fluxes as it plunges toward the core and thereby heats, via the above reactions, to increasingly-high temperatures. The aforementioned neutronization severely decreases the opacity of the electron anti-neutrinos relative to that of the neutrinos and, in turn, increases their mean free path. Characterized by its extreme hot temperatures, many anti-neutrinos deeper in the core may then more easily escape. Although capture of electron neutrinos by neutrons produces the slightly less massive and, in turn, more stable proton, such increased temperatures favor the capture of these anti-neutrinos by protons in further enhancing the neutron excess of the material. The anti-neutrinos as the catalyst, this convective flow of high-temperature, neutron-rich matter from deep in the core is commonly referred to as the "neutrino-driven wind".

By means of the neutrino-heating reactions, the kinetic energy of the neutrinos in the wind is transferred to the thermal and kinetic energies of the newly-created nucleons, electrons, and positrons. The matter adiabatically expands to form low-density yet high-temperature bubbles, the entropy inside of which is now dominated by radiation and approximately valued at \( \frac{4}{3} a T^3 \). Electron-positron pairs also contribute to the entropy at such high temperatures with a value given by \( \frac{7}{3} a T^3 \).

A surplus of bubbles form and grow as infalling matter continues to be impeded while crossing the shock wave, downdrafts of high-density, low-temperature, and low-entropy matter approaching the deep interior of the core as the high-entropy bubbles swell against the stalled shock wave. The pressure of the gas inside these bubbles increases and the shock wave propels outward once again in response.

Large neutron densities characteristic of the r-process, in excess of \( 10^{20} \text{ cm}^{-3} \), result in the rapid capture of neutrons by various heavy nuclei. Concurrent with the efficient production of photons, these extreme neutron densities are achieved in high-temperature (on the order of or greater than \( 10^9 \text{ K} \)) environments. The timescales for the neutron-capture and photo-disintegration reactions are comparable and much shorter than the corresponding \( \beta \)-decay timescales of the nuclei, on the order of \( \approx 1 \text{ s} \). All above conditions are satisfied in the formation and propagation of the hot bubbles by the neutrino-driven wind. Also, to account for the \( 3 \times 10^4 M_\odot \) of r-process material in the Galaxy, each core-collapse supernova would need to eject \( 10^{-4} M_\odot \) of such matter. Given a mass-loss rate of the neutrino-driven wind of \( 10^{-5} M_\odot \text{ s}^{-1} \) in some models, it is possible to extract the right amount of r-process nuclei during the explosions.
For a given Z along an isotopic chain, the forward \((n,\gamma)\) and reverse \((\gamma,n)\) reactions remain in equilibrium until the temperature and neutron flux diminish and the unstable neutron-rich nuclei begin to \(\beta\)-decay back to the most stable isobar of that corresponding mass. For \(A = 129\), that isobar is \(^{129}\text{Xe}\) while for \(A = 182\), it is \(^{182}\text{W}\). However, due to the long lifetimes, the mass of \(A = 129\) will be contained within explosive yields of \(^{129}\text{I}\) while that of \(A = 182\) will be contained within yields of \(^{182}\text{Hf}\) until sufficient time has passed for the complete decay back to \(^{129}\text{Xe}\) and \(^{182}\text{W}\), respectively.

H.2 Uniqueness of the r-Process

On the basis of additional investigations and recent discoveries, however, I now wish to retract the above discussion. Before delving into my newfound insight, I will first consider why the models aim to match the Solar r-process abundance distribution. Observations of many early Galactic metal-poor halo stars enriched (relative to iron) in isotopes from generations of previous r-process events show remarkable similarity from star to star, as well as with respect to the corresponding Solar values, in the heavy (i.e., \(Z \geq 56\)) r-process abundances. The correlations are highlighted in Figs. (H.1) and (H.2) \[72\], and Fig. (H.3) \[237\] for the most r-process-rich halo stars. A likewise correlation exists in Figs. (H.4) \[214\] and (H.5) \[215\] for the tellurium (\(Z = 52\)) abundances in other old halo stars, designating those isotopes as the lightest to predominantly be produced by the r-process in the early Galaxy. The bottom panels of Fig. (H.5), in particular, emphasize the slight differences in r-process abundances between the Sun and halo stars for \(Z \geq 52\). Although their relative r-process abundances are comparable, the primitive halo stars of Fig. (H.6) \[53\] exhibit a large scatter in overall abundances of various isotopes that only widens as the metallicity decreases.

What is the implication of these correlations? The event responsible for producing and injecting the heavy r-process nuclides into the nascent halo-star material must be near identical to that for the heavy r-process abundance distribution of the Solar System at the time of its creation. The heavy Solar r-process abundances are not the result of Galactic averages over stellar events or generations of events. The large scatter in overall abundances of the halo stars accentuates this point. Such scatter is the product of local inhomogeneities of the ISM caused by random nucleosynthetic (r-process, s-process, or some combination) events as the Galaxy was just beginning to form. For
Cowan et al. (2011)

Figure H.1: Abundance determinations in five r-process-rich halo stars, based on new atomic lab data, compared with two Solar-System r-process-only predictions.

Cowan et al. (2011)

Figure H.2: Abundance comparisons between 10 r-process-rich halo stars and Solar-System r-process values.
Figure H.3: r-Process abundance comparisons between ultra-metal-poor halo star, CS 22892-052, and Sun.

Figure H.4: Logarithmic abundances in r-process-rich halo stars. Filled squares indicate detections while curves represent Solar-System s-, r-, and s- + r-process abundance distributions.
Roederer et al. (2014)

Figure H.5: Logarithmic abundances and abundance differences in r-process-rich halo stars. Filled squares indicate detections while curves represent Solar-System s-, r-, and s- + r-process abundance distributions.

Burris et al. (2000)

Figure H.6: Abundances relative to iron for various isotopes of metal-poor Bond giants.
example, matter that happened to undergo star formation near the location of an r-process event would be enriched in that material while star-forming matter farther away would not [53]. If the heavy r-process abundances of the oldest metal-poor halo stars originated from arbitrary and distinct nucleosynthetic events, the fresh material lacking sufficient time to mix prior to being locked up in stars, then it stands to reason that so, too, did the heavy Solar r-process abundances. As more than 8 billion years separate the formation of the Galaxy and Solar System, the conditions narrowly constraining the production of the heavy r-process isotopes in such events must therefore be unique across time [72][6][171].

H.3 Evolving the Origin of the r-Process Isotopes

Much work has been done over the years in attempting to unravel the conditions conducive to r-process nucleosynthesis and where exactly said conditions manifest. In my own search to understand the complexities of the process, I came across the relatively (considering the long history) recent review of Ref. [25]. The first section of Chapter 3 provides an excellent overview, dating back to 1957, of the analytical and numerical work by various groups to extract the necessary parameters in replicating the Solar r-process abundance distribution. The first hydrodynamical nucleosynthesis studies of the r-process came in the late '70s when the prompt mechanism for the Type II supernova explosion yielded encouraging results. Although approximating the Solar r-process abundances well, too much material would have been ejected by the many Type II explosions throughout Galactic history to account for its r-process content. Considering estimates for the Galactic age and supernova rate, Hillebrandt et al. (1978) concluded a rare category of supernova must be responsible for the Galactic r-process content. Or, perhaps, the r-process occurs in only a small region of each Type II explosion or most of the ejected r-process material falls back onto the remnant neutron star [110][164]. Of course, today’s simulations demonstrate the prompt mechanism is not nearly as efficient and likely as the delayed neutrino-driven explosions, thereby ruling it out as the dominant source of Galactic r-process isotopes.

H.3.1 Neutrino-Driven Wind

The discovery of and nucleosynthesis within these delayed explosions began in the mid '80s. Woosley & Hoffman (1992) succeeded in generating the r-process for high entropy and low electron
fractions during the late-time evolution of Type II supernova explosions. Meyer et al. (1992) prevailed in acquiring excellent agreement between its and the Solar System’s r-process abundances utilizing a superposition of trajectories defined by distinct neutron excesses within the neutrino-driven hot bubble. In addition, their assessment of the r-process mass expelled per Type II explosion of $\approx 10^{-4} \, M_{\odot}$ was ideal for producing the right amount of such mass in the early Solar System. Woosley et al. (1994) achieved this optimal r-process mass per supernova occurrence as well as consistency with the Solar r-process abundance distribution in a spherically-symmetric hydrodynamical model that tracked the evolution beyond 10 s. Witti et al. (1994), however, found opposing entropies and electron fractions in similar simulations that culminated in too many seed nuclei, too few neutrons, and an overproduction of nuclei about $A = 90$. But increasing the entropy by a factor of 5.5 removed said overproduction and gave the Solar r-process abundances. Conflicting parameters notwithstanding, the neutrino-driven hot bubble was becoming a formidable candidate for the site of dominant r-process production.

Other groups also failed to replicate the conditions of Woosley et al. (1994) or induce the r-process altogether. The entropy in the analytic investigation by Qian & Woosley (1996) was low by at least a factor of 2 to accommodate a strong r-process. The work of Hofmann et al. (1997) confirmed no such activation yet produced isotope clusters corresponding to mass numbers of individual Solar r-process peaks when contraining the electron fraction, dynamic timescale, and entropy through various combinations. In particular, like Witti et al. (1994), Hofmann et al. (1997) found the high entropy favoring the r-process in the work of Woosley et al. (1994) elusive when inputting the latter’s dynamic timescales and electron fractions into the wind model of Qian & Woosley (1996). A general relativistic treatment of the neutrino-driven wind by Cardall & Fuller (1997) boosted the entropy, Otsuki et al. (2000) and Thompson et al. (2001) corroborating the increase. However, while successful in synthesizing many of the Solar r-process abundances, the parameters in the model of Otsuki et al. (2000) were incompatible with those of Woosley et al. (1994). The chaotic early environment of the long-time hydrodynamical simulations by Arcones et al. (2007) did not convince them of the plausibility for heavy Solar r-process production there. Due to low entropies, the follow-up two-dimensional simulations by Arcones & Janka (2011) were deficient in high neutron-to-seed ratios necessary for a robust r-process. A study by Wanajo (2013) [267] incorporating a time evolution of the electron fraction equivalent to that of Roberts et al. (2012) [213] accomplished the r-process only for neutron-star masses near the causality limit and thereby concluded the neutrino-
driven wind as unlikely for the site of major r-process nucleosynthesis. Finally, the recent works of Refs. [112], [213], [163], [25], and [91] all portray the neutrino-driven wind as slightly neutron-rich or proton-rich and thus detrimental to the r-process. Collectively, progress toward understanding the catalyst for the r-process has only highlighted the discrepancies between multiple groups in the exact conditions to achieve it.

H.3.2 Decompression and Cooling of Neutron-Star Matter

The controversy surrounding the hot bubbles produced within the neutrino-driven wind as the backdrop for r-process nucleosynthesis facilitated the emergence of another setting: the disruption of a neutron star and subsequent decompression and cooling of its matter. Collisions of a black hole and neutron star or of two neutron stars are processes that may effect such relaxation of a companion neutron star and ripen conditions for the r-process. Meyer (1989) extended the studies of Lattimer et al. (1977) (and others referenced therein), one of the first groups to analyze the nucleosynthesis during these violent events, by including a more realistic network of nuclei at the onset of system evolution as opposed to the single nuclear species of Lattimer et al. (1977). In the latter’s work, heavy neutron-rich nuclei accumulated and then underwent substantial $\beta$-decays in increasing the temperature, density, and neutron-to-proton ratio to values suitable for the r-process. Establishing similar conditions, Meyer (1989) amassed nuclei in the range, $Z \approx 40 - 70$, as input seeds for future continuation r-process calculations [176][145].

Flash forward to within the last five years and the merger of two neutron stars has only strengthened its hold as a feasible site for r-process nucleosynthesis. Previous arguments against this approach cited the rarity of such occurrences and long timescale to coalesence, as well as the enormity of abundances released in the ejecta. The first binary NSM (neutron-star merger) would arrive too late to explain the scatter among the early Galactic halo stars described in § H.2. Relative to observations, stars forming after the initial NSM would have too high of a metallicity alongside the scatter since the r-process isotopes were already present in older halo stars with measured lower metallicities. Also, the bulk abundances ejected in and sizable delay between the events would result in a scatter of the r-process/Fe ratios attributable to local inhomogeneities more significant than what is observed [164][26].

To alleviate these discrepancies, Tsujimoto & Shigeyama (2014) developed a model for the formation of early Galactic halo stars aligned with the accepted scheme of hierarchical galaxy
Figure H.7: Early Galactic enrichment history of the r-process element, europium, in chemical evolution models identifying binary neutron-star mergers as the sole birthplace of r-process isotopes.

formation. Binary NSMs and Type II SNs (supernova) occur in proto-galactic fragments of varying masses, the r-process isotopes of each merger permeating the entirety of the host fragment’s volume while each supernova explosion dilutes, with heavy isotopes, only that part of the fragment taken up by the dense ejecta shell. Considering the interplay between the fragments and rates of NSMs and Type II SNs within them, Fig. (H.7) features the predicted enrichment of the r-process element, europium, in halo stars as a function of metallicity. Said stars form in small (green), moderate (red), and massive (blue) proto-galactic fragments in the vicinity of NSMs and Type II SNs, the black crosses denoting the observational data. Having certainly accounted for the observed scatter in the metal-poor halo stars, the authors proclaimed the collisions as the main site of r-process nucleosynthesis [253].

Utilizing relativistic, hydrodynamical simulations, Bauswein et al. (2013) examined the impact of 40 different nuclear equations of state representative of neutron-star matter on the masses of and nucleosynthesis within binary NSM ejecta. The resemblance of the final abundances to the Solar r-process composition for $A \gtrsim 130$ in Figs. (H.8) and (H.9), the indistinguishability of the models and data about $A = 195$ in particular, in conjunction with agreements between model and data merger rates for arriving at the current Galactic r-process content, lends credence to binary
Figure H.8: Nuclear abundance pattern for the 1.35-1.35 M$_\odot$ (left) and 1.2-1.5 M$_\odot$ (right) mergers with 3 equations of state as compared to the Solar r-process abundance distribution.

Figure H.9: Nuclear abundance pattern for the 1.35-1.35 M$_\odot$ mergers with two other equations of state as compared to the Solar r-process abundance distribution.
NSMs as the major source of r-process isotopes. Wanajo et al. (2014) improved upon the work of Bauswein et al. (2013) with a fully general-relativistic, 3-dimensional, hydrodynamical simulation of a binary NSM embodying neutrino interactions and transport. The harvested nucleosynthetic products are displayed in Fig. (H.10) for individual trajectories at the top and their weighted average at the bottom. The agreement with the Solar r-process abundance distribution is superior to that of Bauswein et al. (2013) in encompassing a wider range of $A$ from $\approx 90$ to 240. Likewise reconciling the current r-process mass in the Galaxy per the estimated merger rate, Wanajo et al. (2014), too, proclaimed binary NSMs as the principle origin of such matter [36][268][28].

H.4 First Direct Detection of a Binary NSM

H.4.1 Pre-Merger System Properties

The detection of the gravitational-wave event, GW170817, on 2017-08-17 at 12:41:04 UTC signaled the beginning of a new era in astronomy, as the ripple in space-time appeared to emanate
from a binary NSM. Previous detections having included gravity waves from binary black-hole mergers, this was the first to be consistent with the inspiral of two neutron stars. The top and middle panels of Figure (H.11) [18], from LIGO-Hanford and LIGO-Livingston, respectively, reveal just how incredibly fast the stars were moving about each other right up until coalescence, the massive, compact objects completing roughly 500 orbits every second (more clearly visible in the combined signal of Fig. (H.12) [19])! The event occurred \(\approx 40 \, Mpc\) away within the host galaxy, NGC 4993, or, roughly 130 million years ago early in the Cretaceous period as flowering plants first began to appear [97] and future South America started its break from Gondwana. The determined masses of the neutron stars, residing to within error between 0.86 and 2.26 M\(_{\odot}\) individually and between 2.73 and 3.29 M\(_{\odot}\) totally, are in accord with those of component stars in observed binary NS systems [246][282] and thereby imply such a system as the source of GW170817.
H.4.2 Electromagnetic Counterpart as Evidence for the r-Process

Within 12 hours of its discovery, several groups independently detected an optical and infrared counterpart to GW170817. Designated SSS17a and also known as a "kilonova" due to the maximum luminosity exceeding that of a nova by a factor of $10^3$, the transient of Fig. (H.13) [82] dimmed and reddened significantly between 0.5 and 4.5 days post merger. Binary NSMs have long been theorized to emit short $\gamma$-ray bursts beamed along a particular direction possibly not intersecting our line of sight. If NSMs are indeed prominent producers of r-process isotopes, many of which are radioactive, then a more-isotropic signature could be powered by their decay and have a much higher probability of reaching us. Once acquired, analysis of said radiation may finally expose the true machinery behind r-process nucleosynthesis.

That analysis launched the night of 08/17/17, the essence of the work of Chornock et al. (2017) captured in Figs. (H.14) and (H.16) [59]. As part of the coalition in pursuit of the transient and its properties, they loaded their follow-up spectroscopy program using the Gemini-South telescope and collected the spectral sequence of Fig. (H.14). At 1.5 days post merger, the flux is smooth (save for interference from $\text{H}_2\text{O}$ absorption outlined by gray box) and visible as blue light (left panel of Fig. (H.13). A peak in the flux materialized at 2.5 days post merger near 1.05 $\mu$m and shifted redward over the next several nights. A second peak about 1.55 $\mu$m emerged at 4.5 days post merger, the redness of the light indistinguishable by this point (right panel of Fig. (H.13). The change in flux shape and transient color betray a corresponding transition in opacity sources.
H.4.2.1 Dynamical vs. Wind Ejecta

Matter in a binary NSM may be ejected as a result of hydrodynamic effects within the hot interaction region between the stars or tidal stripping from gravitational torques (both outflows referred to as "dynamical ejecta"), or, as the accretion disk evolves, by various "winds" attributable to neutrino emission, viscous and magnetic stresses, and nuclear recombination. Figure (H.15) [217] provides a schematic of such discharges. The dynamical ejecta are composed of low-$Y_e$, neutron-rich matter containing mostly heavy lanthanide isotopes ($A \gtrsim 140$) moving at speeds between 0.1-0.3$c$ while the wind ejecta comprise larger-$Y_e$ ($\gtrsim 0.3$) matter of Fe-group and light r-process isotopes ($A \lesssim 140$) moving at slower speeds between 0.01-0.15$c$. The higher speeds and, therefore, kinetic energies, of the dynamical ejecta cause a faster rise to greater peak luminosities of the associated transient that then decline more rapidly on a timescale of $\approx 1$ day. The dimmer luminosities of the lower-energy wind ejecta, on the other hand, gradually decline within a week. The peak luminosities of the dynamical and wind ejecta radiation manifest at blue-optical and red-optical to near-infrared wavelengths, respectively, the separate emissions thereby dubbed the "blue" and "red" kilonova.
H.4.2.2 Red vs. Blue Kilonovae

Why the distinction between the blue and red kilonovae? The difference in opacity of the dynamical and wind ejecta demarcates the characteristics of the two resulting emissions. Lanthanide isotopes have their outer valence electrons in the \( f \)-shell, thus permitting a far greater number of transitions within a few eV of the ground state. The absorbed photons are re-emitted with lower energies as the excited electrons fall back through the multiple available states, rather than a single large transition, to the ground state. In forcing most of the photons to be re-emitted in the infrared, the lanthanides, in effect, "blanket" the whole UV/optical region of the spectrum. As the r-process produces a diverse mixture of many high-Z isotopes, each contributing their own series of lines, the opacity to UV/optical photons is much more enhanced relative to that of the wind ejecta. Specifically, the opacity of the heavy r-process isotopes is on the order of 10-100 times larger. The photons, hence, take much longer to diffuse through such opaque material, the week-long duration of the infrared signal a consequence. As the photons undergo extended expansion due to the longer
Figure H.15: Sketch of the various mass-loss mechanisms from the remnant of a binary NS or NSBH (neutron-star-black-hole) merger.

diffusion time, more energy is lost before it can be radiated in the escaping photons, the reduced luminosities another consequence.

**H.4.2.3 What It All Means: Interpreting the Spectral Sequence**

The smooth continuum of the spectrum at 1.5 days post merger in Fig. (H.14) is indicative of a blue kilonova and all successive spectra correlate with a red kilonova. Chornock et al. (2017) consulted the kilonova spectral models of Kasen et al. (2017), the free parameters being ejecta mass, mean velocity, and fractional lanthanide abundance. Figure (H.16) represents their best fit to the data at 4.5 days post merger, this spectrum clearly depicting the features that develop as soon as 2.5 days post merger with little interference from noise and long after the blue kilonova has faded. Although the height and wavelength of the 1.07-µm peak in the data are replicated well by the model, the data peak at 1.55 µm is somewhat bluer and higher in the model. The two shelves of emission bounded by 1.1 and 1.25 µm are present in both the model and data. Overall, the agreement is promising in describing the ejecta as embodying 0.04 M⊙ of lanthanide-rich (X_{lanthanide} = 10^{-2}) material moving at a tenth of the speed of light.

Much work has yet to be done in unraveling the information embedded within these signals.
But, so far, the evidence offers the first glimpses into r-process nucleosynthesis courtesy of binary NSMs. Given the uncertainties in neutrino-driven wind models and recently-revived interest in NSM models, the detection and analysis of GW170817 and its electromagnetic counterpart instills confidence in further constraining the conditions of the r-process and finally pinpointing its exact location in the near future [59][82][128][275][33][127][175][74][195].
Appendix I

A Special Scenario for Aluminum-26: Summary of University of Chicago Collaboration

I.1 A Contradiction of Discrepancies

The discrepancy between the high isotopic abundance ratio of $\approx 5 \times 10^{-5}$ for $^{26}\text{Al}/^{27}\text{Al}$ inferred from most meteorites and that acquired for the mean Galactic background from $\gamma$-ray observations or GCE models (including ours) contradicts the corresponding discrepancy between the favorable low (on the order of $10^{-9}$ as in our models) $^{60}\text{Fe}/^{56}\text{Fe}$ meteoritic abundance ratios and mean Galactic background values. Late incorporation of stellar material or other special scenario is then necessary to account for these discrepancies by allowing a significant injection of $^{26}\text{Al}$ in the absence of a similar deluge of $^{60}\text{Fe}$ into the forming Solar System. One such scenario was conceived through the collaboration of myself and Bradley Meyer with Vikram Dwarkadas, Nicolas Dauphas, and Peter Boyajian of the University of Chicago. Our results are included in the published manuscript of Ref. [84]. As the full details are visible there, I will provide a summary here for how
the Solar System could have been born inside the shell of a Wolf-Rayet wind bubble.

I.2 Wolf-Rayet Wind Bubbles

For stars initially massive enough to evolve through the Wolf-Rayet phase of stellar evolution, mass loss includes a fraction of the helium core prior to formation of the helium convective shell, thus preserving much $^{26}$Al in the winds and preventing significant stellar production of $^{60}$Fe. As dominant producers of $^{26}$Al (without an analogous $^{60}$Fe component) in the ISM, Wolf-Rayet stars may therefore prove a natural origin for the excess $^{26}$Al and inadequate $^{60}$Fe present at the time of Solar-System formation. Figure (I.1) illustrates the evolution of a windblown bubble around an initially-40-$M_\odot$ Wolf-Rayet star at four different epochs, beginning clockwise from top left.

The freely-expanding, super-sonic wind moves outward in radius before eventually encountering a shock due to the abrupt stoppage of material from interactions with the surrounding ISM. The wind itself, internal to the blue shocked region of Fig. (I.1), is characterized by low density and
high velocity (1000-2000 km s$^{-1}$). The golden photo-ionized region beyond the shocked material is created by the large number of ionizing photons with a UV flux on the order of $10^{49}$ s$^{-1}$ emanating from the hot (T > 30,000 K) stellar surface. The thin, dense shell shaded yellow in Fig. (I.1) designates the swept-up material and is susceptible to hydrodynamical instabilities that fragment the otherwise smooth spherical symmetry and, in turn, corrugate the boundary between this and the photo-ionized region. The resulting dense filaments and clumps define the inhomogeneous density of the shell.

The amount of swept-up mass depends on the bubble size and surrounding density. Taking the age of the bubble as the mean lifetime of our initially-40-$M_{\odot}$ star of 4.8 Myr (assuming a Solar metallicity) and adopting the corresponding mechanical wind luminosity during the main sequence on the order of $10^{35}$ g cm$^2$ s$^{-3}$, along with a maximum ISM density of $10^{-3}$ cm, gives a bubble radius of 27.5 pc. Although a theoretical estimate for the swept-up mass, provided the aforementioned parameters, yields a value of $\approx 23,500$ $M_{\odot}$, we instead chose a value of 1000 $M_{\odot}$ in agreement with a (mostly) maximum value from observations.

I.3 Comparison of Massive-Star and Early-Solar-Nebula $^{26}$Al Abundances

Utilizing the recommended elemental abundances of the proto-Sun (as measured relative to a silicon abundance of $10^6$ atoms) in conjunction with the canonical meteoritic aluminum abundance ratio, we determine $3.25 \times 10^{-9}$ Solar masses of $^{26}$Al per total number of Solar masses of the forming Solar System to be present 4.5 billion years ago. Are the amounts of $^{26}$Al ejected by massive stars sufficient to explain this concentration? As, per our scenario, the Solar System is formed by the collapse of material within the dense shell swept up by the Wolf-Rayet wind bubble, the fraction of the star’s ejected $^{26}$Al that mixes in must enrich said shell to at least the above concentration in order to correlate with the meteoritic ratio. During the transfer in the Wolf-Rayet phase, we allow the $^{26}$Al nuclei to decay with a half-life of $7.16 \times 10^5$ yr for up to 300,000 yr given that decay for smaller intervals will not significantly reduce their abundance prior to mixing.

As discussed in chapter 1, the aluminum abundance ratios inferred from chondrules are anywhere from slightly less to more than an order of magnitude greater than those ratios inferred from CAIs while FUN CAIs show negligible ratios. One explanation I gave there was the heterogeneous
distribution of $^{26}$Al in the early Solar nebula. Assuming, then, the CAI and chondrule compositions are representative of the proto-planetary disk around the Sun and not of the star itself, since the Sun’s initial $^{26}$Al content is uncertain, perhaps the inferred $^{26}$Al abundances were embedded within a minimum-mass Solar nebula. To satisfy the requirements for agreement with meteoritic compositions, the minimum concentration of $^{26}$Al within the dense shell must be the following:

$$C_{^{26}Al,bub} = 0.01 \frac{\eta M_{^{26}Al}}{M_{shell}} e^{-t_d \ln(2)/t_{1/2}},$$  \hspace{1cm} (I.1)

where the exponential term takes into account the decay during transfer and the factor of 0.01 in front reduces the concentration of the entire proto-Solar nebula to only that included within the 0.01 Solar masses of the minimum-mass disk. Another factor, $\eta$, is the fraction of $^{26}$Al that mixes into the shell.

Figure (I.2) highlights the Solar masses of $^{26}$Al ejected for various stellar models as a function of initial stellar mass. The intersection of the dashed purple lines with the y-axis denotes the values
of $\eta$ satisfying the minimum constraint of $C_{26^{\text{Al}}, \text{bub}} = C_{26^{\text{Al}}, \text{pss}}$ for $t_d = 300,000$ yr. Because not all of the stellar $^{26}\text{Al}$ will mix in, we consider a range of fractions between 0.005 (below which no solutions exist) and 0.1. If only 10% of the ejected $^{26}\text{Al}$ coalesces with the dense shell, we find many stellar models above an initial mass of $25 \, M_\odot$ yield more than enough $^{26}\text{Al}$ to satisfy our constraint.

### I.4 Mechanism of Transport

From sources cited in our manuscript of Ref. [84], there is indeed precedent, both observationally and theoretically, for conditions appropriate in triggering star formation at the boundaries of windblown bubbles. The question, now, becomes: What mechanism is responsible for the transport of $^{26}\text{Al}$ nuclei from the the hot wind to the cold, dense shell? Researchers have previously accredited it to turbulent mixing or only assumed such mixing occurred from winds to molecular clouds but all failed to provide relevant details of the processes. Others have suggested dust grains as the means by which $^{26}\text{Al}$ nuclei are delivered to the cloud from the Wolf-Rayet winds. However, the grains are too small to endure passage to the dense shell and eventually come to a halt, while the ejected $^{26}\text{Al}$ nuclei move too slow to survive sputtering at the reverse shock once incorporated onto grains, these invalidations per competing theorists.

Regarding the more general problem of mixing between fast, hot material and slower, cold material, still others have investigated the interactions of a supernova shock wave with the resulting cold collapsing clouds yet found the mixing to be inefficient. Wolf-Rayet wind speeds far exceed those of supernova shocks to essentially tear apart clouds instead of collapsing them and their density is much less than that of supernova ejecta for the material to have adequate momentum in generating collapse, both deviations further diminishing the efficiency (relative to supernova shock waves) with which Wolf-Rayet winds may mix into molecular clouds. For fully-formed cloud cores, Wolf-Rayet winds sweeping past will shear their edges and induce instabilities that strip away the cloud material though allow a miniscule fraction of the wind to mix in. These considerations thereby convey hydrodynamical mixing of the Wolf-Rayet winds with molecular clouds as implausible. Rather, we return to the above proposition of dust grains as injection vectors for $^{26}\text{Al}$ nuclei into the dense shell of the Wolf-Rayet wind bubble and provide many supporting details.

Implications from earlier modeling and spectroscopy have suggested grain radii on the order of 1 $\mu$m for dust formed in Wolf-Rayet wind bubbles, about one to two orders of magnitude larger.
than the grains in the preceding refutation. Moreover, the measured mean bulk velocity of the $\gamma$-emitting $^{26}$Al nuclei is actually dominated by the $^{26}$Al nuclei that have already slowed considerably upon reaching the dense shells after $\approx 20,000$ yr, the Doppler broadening thus proving inconsequential to reverse-shock sputtering of the grains. In fact, for a grain radius of 1 $\mu$m and typical bubble densities on the order of $10^{-2}$ cm$^{-3}$, the lifetime against thermal sputtering in the hot gas is 100,000 yr, nearly two orders of magnitude greater than the lifetime of our initially-40-$M_\odot$ star. And calculations of the destruction of C-rich dust grains (like that produced by Wolf-Rayet stars) in supernova ejecta have elucidated their particular resilience to sputtering. Accordingly, thermal sputtering may be considered negligible for the large-size dust grains of Wolf-Rayet wind bubbles.

### I.5 Injection into Dense Shell

Consequent to condensing onto dust grains, the $^{26}$Al nuclei must traverse the bubble interior to access the dense shell. For $\mu$m-size grains with a mass density of 2 g cm$^{-3}$ traveling through a bubble of internal number density of $10^{-2}$ cm$^{-3}$, the computed stopping distance of $\approx 3000$ pc extends well beyond the radius of the bubble in a high-density molecular cloud. Given a larger bubble density of 1 cm$^{-3}$, the stopping distance of 30 pc achieved by the grains is comparable to the bubble radius. In light of possible overestimation, we find most logical parameters of the formula affirm survival of the grains across the bubble interior. Impact with the dense shell substantially reduces the speed of the wind as the grains detach and continue en route though their stopping distance now drops to 10s to 100s of AU due to the extreme shell densities. These high densities notwithstanding, the corresponding low temperatures invoke a grain lifetime against sputtering of several tens of millions of years, still not short enough to remove many of the grains antecedent to star formation.

On the other hand, collisional processes become important once the grains impact and/or enter the shell. Relative velocities in excess of several hundred kilometers per second at the bubble/shell boundary cause a fraction of the grains to heat up above dust-condensation temperatures and eventually vaporize. The lifetime against non-thermal sputtering inside the shell is on the order of 1000-10000 yr, culminating in a fraction of the grains being expelled. To assess the fraction of grains that survive all processes before and after shell impingement requires numerical simulations beyond the scope of our work. Others have carried out said simulations for similar conditions and
concluded a large fraction of 1-µm-size grains successfully breach a dense disk and inject 40-80% of the short-lived radioactivities into the dense shell. We therefore expect at least half of the $^{26}$Al nuclei that survive bubble passage to be injected from the grains into the shell. Several dynamic and radiative instabilities that distort the surface of the shell (as visible in Fig. 1.1) and disrupt the density distribution, combined with the range of stopping distances attributable to a diversity in grain sizes about the mean of 1 µm, establish a degree of heterogeneity for the injection of $^{26}$Al nuclei into the anticipated cloud cores.

### I.6 What about $^{60}$Fe?

Regarding the issue of minimal $^{60}$Fe injection accompanying that of $^{26}$Al into the forming Solar System, our initially-40-$M_\odot$ star (and others more massive to satisfy the constraints of our model) may either die violently in a supernova explosion or quietly in falling back onto a black hole. Lack of a supernova explosion implies lack of explosive nucleosynthesis of $^{60}$Fe. And any $^{60}$Fe nuclei synthesized and later ejected during the star’s evolution do not possess the necessary ample thrust to reach the dense shell. Fallback supernovae and events prior thereby introduce a miniscule fraction of $^{60}$Fe into the proto-Solar nebula.

Rayleigh-Taylor instabilities in the aftermath of interaction between a supernova shock wave and the dense shell could allow explosively-produced $^{60}$Fe and other nuclei of the ejecta to infiltrate said shell. If, however, the forward shock surges over 1000 km s$^{-1}$, the gas may become too hot and no nuclei, including $^{60}$Fe, will be able to dilute the shell. Also, observations support a general asphericity of the ejecta from Wolf-Rayet supernova explosions, and that of the supernova ejecta from any stripped-envelope stars, the highest associated with ejecta coupled to γ-ray bursts. As the dense shell dwarfs the size of the future Solar nebula, such asphericity portends at least a 50% probability that no supernova debris permeate the fledgling Solar System. It is highly likely, then, that $^{60}$Fe contamination of the early Solar nebula is limited to the $^{60}$Fe concentration of the swept-up dense shell. That amount reflects steady-state Galactic evolution up until the beginning of the Solar System while accounting for differences between the stellar and $^{60}$Fe-decay lifetimes. Hence, following the death of our initially-40-$M_\odot$ Wolf-Rayet star, we expect the abundance of $^{60}$Fe to decrease in yielding a value of $1.157 \times 10^{-8}$ for the isotopic abundance ratio of $^{60}$Fe/$^{56}$Fe as inferred from chondrites.
I.7 Shell Collapse and Molecular Core Formation

The stellar wind arrives at the dense shell between several and ten thousand years after the onset of the Wolf-Rayet phase in our model, its immediate deceleration causing the subsequent detachment and injection of the dust grains. The total time for the $^{26}$Al nuclei to mix into the shell post-ejection is no more than $10^5$ years, contingent on uncertainties in dust-formation and aluminum dust-condensation time scales. As the distribution and ages of CAIs are indicative of an interval of $10^5$ years for the consolidation of $^{26}$Al nuclei with the proto-Solar nebula, our results are promising.

The mean time until onset of fragmentation of the dense shell into molecular cores is on the order of 0.9 $M yr$. Because the injection of $^{26}$Al nuclei into the dense shell occurs late in the Wolf-Rayet phase of stellar evolution, core formation begins almost contemporaneous to the mixing. The aforementioned heterogeneity of the $^{26}$Al distribution embedded within the dust grains is well preserved as the shell collapses. Some regions of the shell will contain much $^{26}$Al and some will contain little to none, a range of abundances dispersed inbetween. Such a diverse distribution is in agreement with the corresponding variable aluminum abundance ratios inferred from meteorites.

I.8 Review and Results

To summarize, we propose the Solar System was born at the periphery of a Wolf-Rayet wind bubble by triggered star formation. The $^{26}$Al nuclei synthesized during the evolution of our initially-40-$M_\odot$ Wolf-Rayet star are discharged in the Wolf-Rayet phase via supersonic winds that carve out a bubble around the star (Fig. (I.3a) where blue is bubble, yellow is dense shell, and white is ionized region separating them). The bubble is distinguished by a low-density cavity surrounded by a high-density shell of swept-up material. The ejected $^{26}$Al nuclei condense onto dust grains (Fig. (I.3b) that persist on the wind trajectory in (mostly uninterrupted) transit to the dense shell (Fig. (I.3c)). Grain size and shell density determine the depths to which the grains penetrate the shell following detachment from the wind (Fig. (I.3d)). By this time, triggered star formation has begun and various regions collapse to form molecular cores (Fig. (I.3e) as the wombs of future stellar systems not unlike our own. Ultimately, a supernova shock wave from the death of the Wolf-Rayet star will decimate the bubble or, in the event of a quiet fallback death, the bubble will dissipate. Regardless, ours and other stellar systems will no longer be confined. On the basis of a few assumptions, we conservatively estimate that between 1% and 16% of Solar-mass stars could be
formed by triggered star formation per the above description.

Our work suggests a single central star as the culprit for the anomalous aluminum isotopic abundance ratios of the early Solar nebula. Yet observations of dust around Wolf-Rayet stars corroborate the assistance of a companion for its creation while most massive stars of the Galaxy (as low as 50% or as high as 90%) are paired in binary systems. If that bubble out of which formed the Solar System was the consequence of a Wolf-Rayet star with a companion, the probability of having a sufficient abundance of $^{26}$Al nuclei to pollute the dense shell increases with the greater expectation of dust formation and, in turn, amount of dust in binary systems. Furthermore, the enhanced mass transfer and mass-loss rates of a binary system lower the initial mass required for one of the stars to evolve to the Wolf-Rayet stage of stellar evolution, thereby ensuring a larger fraction of Wolf-Rayet stars and the Solar-mass stars they give rise to. Our previous conservative estimates grow and we are therefore more assured of our results.
Appendix J

Alpha-Capture Reactions on $^{38}\text{Ar}$ and Production of $^{41}\text{Ca}$

Summary: This section summarizes work I completed with Rashi Talwar at Argonne National Laboratory. She and her colleagues measured alpha-capture cross sections on $^{38}\text{Ar}$, namely, the $(\alpha,p)$ and $(\alpha,n)$ reactions. In this chapter, I analyze the influence these new cross sections have on the production of the SLR, $^{41}\text{Ca}$, in a massive star utilizing the simple Type II supernova model I developed for my Master’s thesis [44]. This code uses detailed pre-supernova stellar models calculated by others [212] and applies the Rankine-Hugoniot conditions [185] to compute the jump in temperature and density by the passing supernova shock wave. To do this, the model uses the simplifying assumption, motivated by the observation of Ref. [276], that all energy behind the shock is uniformly distributed and in the form of relativistic particles. This, plus the equation of state, allows one to compute the post-shock conditions from the pre-shock conditions in the input stellar model. From my Master’s work, we found good agreement between the results of our calculations and those of more detailed hydrodynamical calculations [212], which gives us confidence in the general applicability of the model to the work of Talwar et al. (2018) [244] and, perhaps, many others in the future.
Figure J.1: Final $^{41}$Ca mass fraction as a function of interior mass coordinate 1 year after the 1.0 B explosion of s25a28 for the indicated reaction networks. Also shown for comparison is the pre-supernova value from Ref. [212].

J.1 Zone 284 Evolution

To study the effect of explosive nucleosynthesis on the production of $^{41}$Ca in an initially 25-Solar-mass star, we first ran our open-source simple_snII.cpp explosion code [44] on the xml file for the pre-supernova stellar model s25a28, constructed using the structure and composition data text files from Rauscher et al. [212] at http://nucastro.org/nucleosynthesis and the nuclear and reaction data xml files at www.jinaweb.org. The star is evolved to the point of core-collapse in this model and the energy of our explosion is 1.0 B, or $10^{51}$ erg. Next, we ran our open-source run_multiple_zone_omp.cpp code on the explosion output file for a duration of 1 year to probe the consequences of the extreme temperatures and densities associated with shock propagation. Figure (J.1) shows the resulting $^{41}$Ca mass fraction in the ejecta of the initially 25-Solar-mass star for the $^{38}$Ar($\alpha$,n)$^{41}$Ca and $^{38}$Ar($\alpha$,p)$^{41}$K reaction rates of Sevior et al. [229] and the updated rates measured in this work. The peak in the $^{41}$Ca mass fraction from the pre-supernova star appears to shift to the
right after the explosion, residing in zone 284 of our networks. Noticeable production also occurs farther out in the ejecta at interior masses of $7 \ M_\odot$ and $7.75 \ M_\odot$.

At an interior mass of about $2.7439 \ M_\odot$, zone 284 resides just inside of a convective carbon-burning shell within the 25-Solar-mass star, as evidenced by the uniform mass fractions across the range of interior mass coordinates from $3.1 \ M_\odot$ to $5.7 \ M_\odot$ in Fig. (J.2). The large mass fractions of $^{12}\text{C}$ and $^{16}\text{O}$ in this shell are attributable to the previous competition between core helium-burning reactions, $^4\text{He}(\alpha\alpha,\gamma)^{12}\text{C}$ and $^{12}\text{C}(\alpha,\gamma)^{16}\text{O}$, for the available $\alpha$ particles. A portion of the $^{14}\text{N}$ mass fraction leftover from CNO-cycle processing during hydrogen-core burning was subsequently destroyed as $^{14}\text{N}(\alpha,\gamma)^{18}\text{F}(\beta^+\nu)^{18}\text{O}$ to create $^{18}\text{O}$, which then suffered $\alpha$-capture in the transmutation to either $^{21}\text{Ne}$ with the emission of a neutron or $^{22}\text{Ne}$ with the emission of a $\gamma$-ray. The high output of $^{20}\text{Ne}$ and ample $^{23}\text{Na}$ yield infer the operation of the ensuing carbon burning by $^{12}\text{C}(^{12}\text{C},\alpha)^{20}\text{Ne}$ and $^{12}\text{C}(^{12}\text{C},p)^{23}\text{Na}$. The increase in the $^{20}\text{Ne}$ mass fraction facilitated the onset of neon-burning reactions, $^{20}\text{Ne}(^{20}\text{Ne},^{16}\text{O})^{24}\text{Mg}$ and $^{20}\text{Ne}(\gamma,\alpha)^{16}\text{O}$, the liberated $\alpha$ particles of the latter reaction and aforementioned carbon burning aiding in the further production of $^{24}\text{Mg}$ via

![Figure J.2: Pre-supernova mass fractions of relevant species as a function of interior mass coordinate for stellar model s25a28 of Ref. [212].](image-url)
$^{20}\text{Ne}(\alpha,\gamma)^{24}\text{Mg}$. Per $^{21}\text{Ne}(\alpha,n)^{24}\text{Mg}$, $^{22}\text{Ne}(\alpha,n)^{25}\text{Mg}$, and $^{23}\text{Na}(\alpha,p)^{26}\text{Mg}$, this release of $\alpha$ particles also caused the incomplete destruction of $^{21}\text{Ne}$, $^{22}\text{Ne}$, and $^{23}\text{Na}$, respectively, the mix of significant mass fractions of $^{21}\text{Ne}$, $^{22}\text{Ne}$, $^{23}\text{Na}$, $^{24}\text{Mg}$, $^{25}\text{Mg}$ throughout the shell betraying such inefficiency. The neon-burning reactions having proved detrimental to the $^{20}\text{Ne}$ mass fraction, proton-captures on the growing $^{23}\text{Na}$ mass fraction quickly restored balance.

Through the use of our diverse computational and visual tools, we can explore the evolution of relevant nuclear species in zone 284 as the shock wave approaches, compresses and heats up matter, and then dissipates, allowing the matter to expand while reactions freeze out. We ran our open-source run_single_zone.cpp code on the explosion output file in zone 284 for a duration of 1 year to analyze the ongoing nucleosynthesis. The mass fractions for the updated reaction rates of this work are presented in Fig. (J.3). Prior to shock arrival, the dominant net reaction flow (in number of nuclei per total number of nucleons per second) is the production of $^{39}\text{K}$ via $^{38}\text{Ar}(p,\gamma)^{39}\text{K}$. Whereas the product of the total number of nucleons per volume and thermally-averaged cross section ($\rho N_A < \sigma \nu$) for the reactions, $^{38}\text{Ar}(n,\gamma)^{39}\text{Ar}$, $^{40}\text{Ca}(n,\gamma)^{41}\text{Ca}$, $^{41}\text{Ca}(n,\alpha)^{38}\text{Ar}$, and $^{39}\text{K}(n,\gamma)^{40}\text{K}$, are all larger than that for $^{38}\text{Ar}(p,\gamma)^{39}\text{K}$ at these temperatures, the overwhelming pre-supernova mass fraction of $^{38}\text{Ar}$, concurrent with a difference on the order of $10^2$-$10^3$ of protons relative to neutrons (see Fig. (J.4), establishes the initial prevailing flow of $^{38}\text{Ar}$ to $^{39}\text{K}$. As the shock wave nears, the net production of neutrons courtesy of the rapid $\alpha$-capture reactions on the abundant $^{25}\text{Mg}$ and $^{26}\text{Mg}$ in the pre-supernova star causes marginal destruction of the likewise bountiful $^{40}\text{Ca}$, visible upon close inspection of Fig. (J.3). There is negligible flow into $^{40}\text{Ca}$ to offset such destruction, and the mass fraction of $^{41}\text{Ca}$ benefits by building up as $^{40}\text{Ca}(n,\gamma)^{41}\text{Ca}$. Although $\rho N_A < \sigma \nu$ for this flow is more than an order of magnitude less than that for the major outflow, $^{41}\text{Ca}(n,\alpha)^{38}\text{Ar}$, the $^{41}\text{Ca}$ pre-supernova mass fraction is more than two orders of magnitude less than that of $^{40}\text{Ca}$ and hence the rise in its mass fraction with time. The increase in temperature and density from shock passage escalates all reaction flows, the mass fraction of $^{39}\text{K}$ upsurging by more than an order of magnitude as the temperature and density peak at $2.7263 \times 10^9$ K and $9.663 \times 10^5$ g/cc, respectively, consequent to the arrival of the shock wave at $t = 0.71866$ s post core bounce. In addition to neutron captures in proliferation of the $^{39}\text{Ar}$ mass fraction, $^{38}\text{Ar}$ accordingly depletes. The burgeoning neutron mass fraction propels production of $^{40}\text{K}$, a meager pre-supernova presence expediting its growth at modest consumption of $^{39}\text{K}$.

Opposing the production of $^{39}\text{Ar}$ is the reverse flow of $^{39}\text{K}(n,p)^{39}\text{Ar}$ in supplying an ad-
Figure J.3: Time evolution of the mass fractions of relevant species in zone 284 during the $E = 1.0$ B explosion of s25a28.

Figure J.4: Time evolution of the proton and neutron mass fractions in zone 284 during the $E = 1.0$ B explosion of s25a28.
ditional channel to $^{39}$K. Within the pre-supernova star, these flows are negligible. Once the shock wave forms and begins hurtling toward zone 284, though, the reverse flow more hastily inflates with respect to the forward flow. The value of $\rho N_A < \sigma \nu$ for the forward flow is roughly 6 times larger than that for the reverse flow for $T_9$ in the range from 1.5 to 2.5 and the pre-supernova and pre-shock mass fractions of $^{39}$K are more than an order of magnitude greater than those of $^{39}$Ar. But the aforementioned difference between the mass fractions of protons and neutrons and the slightly higher net rate of increase of protons against that of neutrons is what triggers the amplified reverse flow. At $t = 0.717725$, just before shock arrival, this net destruction of $^{39}$Ar comes to balance its neutron-capture production. Yet to attain a maximum value across the next several time steps, the proton mass fraction continues growing in corresponding proportion to the reverse $^{39}$K($n,p$)$^{39}$Ar flow and the $^{39}$Ar mass fraction appropriately deteriorates. Amidst this interval and beyond, the proton-capture flow to $^{40}$K also becomes relevant in destroying $^{39}$Ar.

An intriguing facet of Fig. (J.3) is the location of the peak in the $^{39}$Ar mass fraction, as it is antecedent to all other peaks. Of the species that peak in Fig. (J.3), $^{39}$Ar is the only one in which proton-capture interactions are the main culprit in lessening its mass fraction. The other peak species suffer destruction primarily by neutron-capture interactions. Because the proton mass fraction is significantly larger and more steeply ascending than the neutron mass fraction, the net destruction of $^{39}$Ar via these proton captures will execute earlier and, in turn, shift the peak.

Alternatively, the $^{40}$Ar mass fraction prospers after all other mass fractions of peak species have begun to climb. At the applicable temperatures, $\rho N_A < \sigma \nu$ for the major production flows of $^{40}$Ar, $^{39}$Ar($n,\gamma$)$^{40}$Ar and $^{40}$K($n,p$)$^{40}$Ar, are $\sim 8 \times 10^5$ s$^{-1}$ and $3-4 \times 10^6$ s$^{-1}$, respectively. Leading the destruction are the $^{40}$Ar($p,\alpha$)$^{37}$Cl and $^{40}$Ar($p,\gamma$)$^{41}$K flows, the rates proportional to $10^3$-$10^4$. Since the $^{40}$Ar pre-supernova and pre-shock mass fractions are almost an order of magnitude less than those of $^{39}$Ar, destruction of $^{40}$Ar nominally lags its production, the net flow to $^{40}$Ar on the order of $10^{-5}$ and far less than other peak flows in Fig. (J.3). The peak in its mass fraction therefore endures a delay and does not extend much before a build-up of protons, as the shock wave converges on zone 284, bolsters the proton-capture flows in toppling the $^{40}$Ar mass fraction.

For temperatures less than 2.0, in units of $10^9$ K ($T_9$), the value of $\rho N_A < \sigma \nu$ for the reverse flow of $^{38}$Ar($p,\gamma$)$^{39}$K is negligible. However, above 2.0 for $T_9$, that quantity increases by at least a couple of orders of magnitude for every half-integer increment of $T_9$. The analogous ascent for the forward flow is minimal, essentially remaining on the same order of magnitude. For a
considerable number of time steps post shock departure, the temperature holds steady at a $T_9$ of $\sim 2.72$, during which the forward flow of $^{38}\text{Ar}(p,\gamma)^{39}\text{K}$, having earlier peaked, is in monotonic decline while the reverse flow, owing to the high $T_9$ as well as a peak in the $^{39}\text{K}$ mass fraction, continues to advance before settling at $\sim 5 \times 10^{-2}$ s$^{-1}$. Soon after, as both flows contract, the reverse flow exceeds the forward flow and $^{39}\text{K}$ transmutates back to $^{38}\text{Ar}$, its mass fraction rebounding in the absence of the shock wave. As the proton mass fraction also culminated on the order of $10^{-8}$ at shock arrival, the disintegration of $^{39}\text{K}$ further transpires as $^{39}\text{K}(p,\gamma)^{40}\text{Ca}$. The proton inflation and preceding swell in the $^{40}\text{K}$ mass fraction drive an additional flow to $^{40}\text{Ca}$ by $^{40}\text{K}(p,n)^{40}\text{Ca}$. The inflow to $^{40}\text{Ca}$ now exceeds the major outflow to $^{41}\text{Ca}$ and the $^{40}\text{Ca}$ mass fraction rises slightly in Fig. (J.3).

Simultaneous to the growth of the $^{40}\text{Ca}$ mass fraction is an aggregation of other destructive interactions for $^{40}\text{K}$:

- $^{40}\text{K}(p,\gamma)^{41}\text{Ca}$
- $^{40}\text{K}(p,\alpha)^{37}\text{Ar}$
- $^{40}\text{K}(p,n)^{40}\text{Ca}$
- $^{40}\text{K}(n,p)^{40}\text{Ar}$
- $^{40}\text{K}(n,\alpha)^{37}\text{Cl}$
- $^{40}\text{K}(n,\gamma)^{41}\text{K}$

The sum of these flows is the accelerated drop-off in the $^{40}\text{K}$ mass fraction relative to the other species in Fig. (J.3).

Supporting the turnover of the $^{38}\text{Ar}$ mass fraction are $\alpha$-capture interactions on the substantial $^{41}\text{Ca}$ mass fraction. A dearth of these flows in the pre-supernova star, enhancement followed shock propagation with the burst of neutrons and $^{41}\text{Ca}$ production. The magnitude of this flow is now comparable to the dominant flow into $^{41}\text{Ca}$, $^{40}\text{Ca}(n,\gamma)^{41}\text{Ca}$. Yet, neutron captures on $^{41}\text{Ca}$ augment its destruction by an order of magnitude less than the flow to $^{38}\text{Ar}$. The $^{41}\text{Ca}$ mass fraction thereby experiences a miniscule net decline in Fig. (J.3) before leveling off due to the expansion of the matter and reaction freeze-out.

One of the above neutron-capture flows, destructive to $^{41}\text{Ca}$ and the reverse of $^{41}\text{K}(p,n)^{41}\text{Ca}$, provides the central channel for $^{41}\text{K}$ production early in the evolution. Other minor routes in bearing $^{41}\text{K}$ are the proton-capture flow from $^{40}\text{Ar}$ and neutron-capture flow from $^{40}\text{K}$. As the value of $\rho N_A < \sigma \nu$ for the flow from, and pre-supernova and pre-shock mass fractions of, $^{41}\text{Ca}$
overshadow the corresponding quantities in the principal destructive flow of $^{41}$K($p,\alpha$)$^{38}$Ar by 1 to 2 orders of magnitude, the $^{41}$K mass fraction elevates. With the shock wave inbound, the forward and reverse flows of $^{41}$K($p,n$)$^{41}$Ca strengthen while competing with each other. Such engagement between the flows begets a reduced net reverse flow and, synchronous with the proton bombardment accompanying the imminent shock wave, the proton-capture demolition of $^{41}$K promptly surpasses this reverse flow. Previously unimportant as a pathway to destruction, the $^{41}$K($p,\gamma$)$^{42}$Ca flow also participates in sapping the $^{41}$K mass fraction. The deluge of neutrons and heightened $^{40}$K mass fraction in the wake of shock contact accelerates production via $^{40}$K($n,\gamma$)$^{41}$K. The value of $\rho N_A < \sigma_\nu >$ for this flow, however, is an order of magnitude less than the flow of $^{41}$K to $^{38}$Ar for $T_9$ on the order of 2.0 and it duly cannot compensate. In the void left by the shock wave, the $^{41}$K mass fraction eventually stabilizes due to the expansion of the matter and reaction freeze-out.

Why does the $^{41}$Ca 25-Solar-mass star after the explosion? What prevents the peak from appearing in zones to the left or right of zone 284? To better understand the peak behavior, we ran our open-source run_single_zone.cpp code on the explosion output file in zone 268 (at an interior mass of 2.5830 $M_\odot$) and zone 308 (at an interior mass of 2.9850 $M_\odot$) for a duration of 1 year. As illustrated in Fig. (J.1), explosive nucleosynthesis yields terminal values of $4.7618 \times 10^{-5}$ and $5.82333 \times 10^{-5}$ for the $^{41}$Ca mass fraction in zones 268 and 308, respectively.

Immediately prior to contact of the shock wave with zone 268, the $^{40}$Ca($n,\gamma$)$^{41}$Ca reaction has the following flow magnitudes for $T_9 = 2.849$ and $\rho = 1.111 \times 10^6$ g / cc:

- Forward - $5.264 \times 10^{-3}$ s$^{-1}$
- Reverse - $1.186 \times 10^{-4}$ s$^{-1}$
- Net - $1.186 \times 10^{-4}$ s$^{-1}$

The neutron mass fraction has peaked at this time and, hereupon, the forward flow begins a monotonic decline. However, the reverse flow continues to increase until holding steady at a value of $\sim 4.5 \times 10^{-4}$ s$^{-1}$ for 6 time steps while the temperature is near constant (between $T_9 = 2.9461$ and $T_9 = 2.9427$) and the forward flow succumbs to the order of $10^{-4}$. As the temperature remains $\sim 2.9$ for $T_9$, thus favoring the reverse flow, the neutrons are quickly consumed and the forward flow drops off more dramatically and approaches the reverse flow, with the net flow descending an order of magnitude to $10^{-5}$. The net $^{41}$Ca($n,\alpha$)$^{38}$Ar flow, meanwhile, is $\sim 3 \times 10^{-4}$ s$^{-1}$, more dominant and thereby allowing for the net destruction that we see in the $^{41}$Ca mass fraction in Fig. (J.5) posterior to the peak.
The impending shock collision imparts the $^{40}\text{Ca}(n,\gamma)^{41}\text{Ca}$ reaction with the following flow magnitudes for $T_9 = 2.704$ and $\rho = 9.418 \times 10^5 \text{ g/cc}$ in zone 284:

- **Forward**: $6.217 \times 10^{-3} \text{ s}^{-1}$
- **Reverse**: $1.288 \times 10^{-5} \text{ s}^{-1}$
- **Net**: $6.204 \times 10^{-3} \text{ s}^{-1}$

As in zone 268, the neutron mass fraction has peaked at this time and the forward flow begins a monotonic decline. For the next 8 time steps, the reverse flow remains steady near $2 \times 10^{-5} \text{ s}^{-1}$ as $T_9$ ranges from 2.7261 to 2.7119 and the forward flow plummets to $\sim 2 \times 10^{-4} \text{ s}^{-1}$. The net flow is $2.509 \times 10^{-4} \text{ s}^{-1}$ while the net flow for the $^{41}\text{Ca}(n,\alpha)^{38}\text{Ar}$ flow is $2.611 \times 10^{-4} \text{ s}^{-1}$. Both net flows continue to fall as the matter expands and neutrons are consumed, with the destruction marginally ahead of the production. Figure (J.5) suggests the $^{41}\text{Ca}$ mass fraction levels off, but zooming in confirms an ever slight waning first.

Consider the magnitudes of the rate factor, $\rho N_A < \sigma \nu >$ for the following reactions in zone 284 at $T_9 = 2.72$:

- $^{40}\text{Ca}(n,\gamma)^{41}\text{Ca}$
  - **Forward**: $1.3568 \times 10^6 \text{ s}^{-1}$
  - **Reverse**: $4.6867 \text{ s}^{-1}$
- $^{41}\text{Ca}(n,\alpha)^{38}\text{Ar}$
  - **Forward**: $3.2194 \times 10^7 \text{ s}^{-1}$
  - **Reverse**: $1.5336 \times 10^{-2} \text{ s}^{-1}$

And in zone 268 at $T_9 = 2.94$:

- $^{40}\text{Ca}(n,\gamma)^{41}\text{Ca}$
  - **Forward**: $1.3885 \times 10^6 \text{ s}^{-1}$
  - **Reverse**: $77.821 \text{ s}^{-1}$
- $^{41}\text{Ca}(n,\alpha)^{38}\text{Ar}$
  - **Forward**: $3.3273 \times 10^7 \text{ s}^{-1}$
  - **Reverse**: $8.3988 \times 10^{-2} \text{ s}^{-1}$

There is little change in the forward $^{40}\text{Ca}(n,\gamma)^{41}\text{Ca}$ rate factor as the temperature increases from a $T_9$ of 2.72 to 2.94 while the reverse factor rises by more than an order of magnitude. In both zones, the neutron mass fraction peaks at a value on the order of $10^{-11}$, at $2.10929 \times 10^{-11}$ in zone 268 and $4.69186 \times 10^{-11}$ in zone 284, and the $^{41}\text{Ca}$ pre-supernova mass fractions are alike at 3.1842.
Figure J.5: Time evolution of the $^{41}$Ca mass fraction in zones 268, 284, and 308 during the $E = 1.0$ B explosion of s25a28.

$x \times 10^{-5}$ and $2.0706 \times 10^{-5}$, respectively. Accounting for these discrepancies as well as the almost indistinguishable trajectories followed by the $^{41}$Ca mass fraction in each zone, we can further clarify the similar magnitudes of the forward flows and difference (by an order of magnitude) in the reverse flows of this reaction in zones 284 and 268. The reverse flow catches up to the forward flow in zone 268, the detracted net flow slowing the production of $^{41}$Ca via this channel. The rate factor for the forward $^{41}(n,\alpha)^{38}$Ar flow undergoes limited change within the said range of $T_9$ values. Although there is more of a change in the reverse rate factor, the magnitudes are negligible when contrasted against the corresponding rate factors for the forward flow. The chief catalyst in depleting the $^{41}$Ca mass fraction in zone 268 prior to freeze-out in Fig. (J.5), then, must be the increase in the rate factor of the reverse $^{40}$Ca($n,\gamma$)$^{41}$Ca flow with increasing $T_9$.

Referring once more to Fig. (J.5), the $^{41}$Ca mass fraction in zone 308 levels off at approximately the same value as that in zone 268. Upon shock arrival, the $T_9$ and density in zone 308 peak at 2.4732 and 7.0777 g/cc, respectively, values appreciably less than the peak values in zones 268 and 284. The $^{40}$Ca and $^{41}$Ca mass fractions also begin evolving from a lower starting point.
in zone 308 in the pre-supernova star, anywhere from 3 to 6 times less than in zones 268 and 284. Despite the neutron mass fraction reaching the largest peak value of $5.5921 \times 10^{-11}$ in the 3 zones, the temperature and density do not soar high enough to elevate the neutron-capture production of $^{41}\text{Ca}$ commensurate with that in zones 268 and 284, for the $^{41}\text{Ca}$ mass fraction can not grow as much with more of an altitude to climb and less of the $^{40}\text{Ca}$ seed nuclei present.

Figure (J.6) represents the distinction in the rates of this work and those of Sevior et al. [229] by displaying the correlated evolution of the $^{41}\text{Ca}$ mass fraction in zone 284. The green and orange curves serve the evolution stemming from the uncertainty limits in the rates of this work, which achieve a 34% increase of the final $^{41}\text{Ca}$ mass fraction over the gain from the Sevior et. al [229] rates. A small increase nonetheless, we can deduce its origin by first contemplating a useful analytic concept described as the net integrated current for various reaction flows of a given network. Consider the reaction, $^{41}\text{Ca}(n,\alpha)^{38}\text{Ar}$, in discussing such a concept. To refresh, the abundance, $Y$, of a nuclear species or type of particle is the number of nuclei or particles per total number of nucleons. The change in the abundance, $Y_{^{41}\text{Ca}}$, of $^{41}\text{Ca}$ via the reaction, $^{41}\text{Ca} + n \leftrightarrow \alpha + ^{38}\text{Ar}$, is governed by:

$$
\text{Initial Mass} = 25 \, \text{M}_\odot
$$

**Zone 284**

![Figure J.6: Time evolution of the $^{41}\text{Ca}$ mass fraction in zone 284 during the E = 1.0 B explosion of s25a28 for the indicated reaction networks.](image)

219
by the following equation:

\[ \frac{dY_{41\text{Ca}}}{dt} = -\rho N_A <\sigma v>_{41\text{Ca},n} Y_{41\text{Ca}} Y_n + \rho N_A <\sigma v>_{38\text{Ar},\alpha} Y_{38\text{Ar}} Y_\alpha, \]

where \( Y_{41\text{Ca}}, Y_n, Y_\alpha, \) and \( Y_{38\text{Ar}} \) denote the abundances of \( ^{41}\text{Ca}, \) neutrons, \( \alpha \) particles, and \( ^{38}\text{Ar}, \) respectively. In integrating both sides of the equation across the duration of the calculation, we obtain the following:

\[ \int_i^f \frac{dY_{41\text{Ca}}}{dt} \, dt = \int_i^f (-\rho N_A <\sigma v>_ {41\text{Ca},n} Y_{41\text{Ca}} Y_n + \rho N_A <\sigma v>_ {38\text{Ar},\alpha} Y_{38\text{Ar}} Y_\alpha) \, dt \]

\[ \Rightarrow \Delta Y_{41\text{Ca}} = -\int_i^f \rho N_A <\sigma v>_ {41\text{Ca},n} Y_{41\text{Ca}} Y_n \, dt + \int_i^f \rho N_A <\sigma v>_ {38\text{Ar},\alpha} Y_{38\text{Ar}} Y_\alpha \, dt, \]

where \( \int_i^f \rho N_A <\sigma v>_ {41\text{Ca},n} Y_{41\text{Ca}} Y_n \, dt \) is the integrated current flowing out of \( ^{41}\text{Ca} \) and \( \int_i^f \rho N_A <\sigma v>_ {38\text{Ar},\alpha} Y_{38\text{Ar}} Y_\alpha \, dt \) is the integrated current flowing into \( ^{41}\text{Ca}. \) Their difference, or net integrated current, denoted as \( I[^{41}\text{Ca}(n,\alpha)^{38}\text{Ar}](t,t_0) \), is the change in abundance of \( ^{41}\text{Ca} \) and provides the number of nuclei per total number of nucleons that flow from \( ^{41}\text{Ca} \) to \( ^{38}\text{Ar} \) in the interval between the initial and final times of the calculation. Although our code computes the integrated currents as abundance changes, the mass fraction (of which I plotted many times in my analysis) is easily extracted as the product of the abundance of a nuclear species and the relative atomic mass in atomic mass units (numerically close to the mass number).

Figure J.7: Net integrated currents of interest for the rates of this work in zone 284 for the 1-year interval after the 1.0 B explosion of s25a28.

Figs. (J.7) and (J.8) exhibit the net integrated currents of interest in zone 284 for the
rates of this work and those of Sevior et al. [229], respectively. The differences are difficult to distinguish when examining the calculations separately. If, instead, we subtract the Sevior et al. [229] net integrated currents from the corresponding currents acquired in this work, Fig. (J.9) results. The thickness of the arrow from $^{38}\text{Ar}$ to $^{41}\text{Ca}$ tells us that the net flow from $^{41}\text{Ca}$ to $^{38}\text{Ar}$ via $^{41}\text{Ca}(\alpha,n)^{38}\text{Ar}$ is more pronounced when evolving the stellar explosion with the rates of Sevior et al. [229]. In adopting the rates of this work, however, the destruction of $^{41}\text{Ca}$ by $\alpha$-captures is not as rapid and, thus, more of it is free to circulate through other channels, apropos the arrows from $^{41}\text{K}$ to $^{41}\text{Ca}$, $^{41}\text{Ca}$ to $^{40}\text{Ca}$, and $^{41}\text{Ca}$ to $^{42}\text{Ca}$ in Fig. (J.9). The reverse flow of $^{41}\text{K}(p,n)^{41}\text{Ca}$ is larger than the forward flow and yet the arrow is pointing from $^{41}\text{K}$ to $^{41}\text{Ca}$, emphasizing the smaller abundance change of $^{41}\text{Ca}$ by this route when applying the rates of $^{41}\text{Ca}(n,\alpha)^{38}\text{Ar}$ and $^{41}\text{K}(p,\alpha)^{38}\text{Ar}$ from this work.

How do these distinctions in the abundances changes of $^{41}\text{Ca}$ originate with the updated cross-section measurements of the indicated reactions? To begin unraveling the answers to such a question, we again ran our open-source run_single_zone.cpp code on the explosion output file in zone 284 for a duration of 1 year for the cases in which we 1) modified only the $^{41}\text{K}(p,\alpha)^{38}\text{Ar}$ rate and 2) modified only the $^{41}\text{Ca}(n,\alpha)^{38}\text{Ar}$ rate. The forthcoming analysis demonstrates the contributions of each reaction to the abundance changes of $^{41}\text{Ca}$ and $^{41}\text{K}$.

First, contemplate the net integrated current differences displayed in Fig. (J.10). These differences arise when subtracting the Sevior et al. [229] net integrated currents from the corresponding currents acquired after employing only the updated rate measurement for the $^{41}\text{K}(p,\alpha)^{38}\text{Ar}$ reaction in our network. The disparity between flows becomes apparent when reflecting on the destruction
of $^{41}\text{K}$ in the flow to $^{38}\text{Ar}$, as such destruction has slowed considerably upon updating its rate from this work. In the network utilizing the Sevior et al. [229] rates, the $^{41}\text{K}$ abundance change attributable to this channel is $-1.7509 \times 10^{-6}$ nuclei per nucleon. The ensuing abundance change with rate adjustment is $-1.0802 \times 10^{-6}$ nuclei per nucleon, the sluggish destruction enabling $6.7112 \times 10^{-7}$ \((1.7509 \times 10^{-6} - 1.0802 \times 10^{-6})\) more $^{41}\text{K}$ nuclei per nucleon to survive. Because the reverse flow of $^{41}\text{K}(p,n)^{41}\text{Ca}$ dominates the forward flow, $5.5869 \times 10^{-7}$ less $^{41}\text{Ca}$ nuclei per nucleon are destroyed as the excess $^{41}\text{K}$ nuclei permit an enhanced forward flow to $^{41}\text{Ca}$ in the network with the updated $^{41}\text{K}(p,\alpha)^{38}\text{Ar}$ rate.

Having described the difference in the main productive route for $^{41}\text{Ca}$ between the networks, what can we say about the changes in destructive flows? The arrow from $^{41}\text{Ca}$ to $^{40}\text{Ca}$ in Fig. (J.10) illustrates the strengthening of the reverse $^{40}\text{Ca}(n,\gamma)^{41}\text{Ca}$ flow as does the arrow from $^{41}\text{Ca}$ to $^{42}\text{Ca}$ exemplify a greater flow along the $^{41}\text{Ca}(n,\gamma)^{42}\text{Ca}$ channel, both increases the outcome of the lowered reverse $^{41}\text{K}(p,n)^{41}\text{Ca}$ flow since the $^{41}\text{Ca}$ nuclei not destroyed by this route are redistributed across other channels. In the updated network, $1.880 \times 10^{-8}$ less $^{41}\text{Ca}$ nuclei per nucleon are produced in the flow from $^{40}\text{Ca}$ and $3.1608 \times 10^{-8}$ more $^{41}\text{Ca}$ nuclei per nucleon are destroyed in the flow to $^{42}\text{Ca}$. Similarly, the abundance change of $^{41}\text{Ca}$ in the original network through the $^{41}\text{Ca}(n,\alpha)^{38}\text{Ar}$ channel is $-1.6294 \times 10^{-5}$ nuclei per nucleon while the change that develops in altering the $^{41}\text{K}(p,\alpha)^{38}\text{Ar}$ rate

Figure J.9: Difference in the net integrated currents of interest for the rates of this work and those of Ref. [229] in zone 284 for the 1-year interval after the 1.0 B explosion of s25a28.
Figure J.10: Difference in the net integrated currents of interest for the updated $^{41}$K($p,\alpha$)$^{38}$Ar rate of this work and that of Ref. [229] in zone 284 for the 1-year interval after the 1.0 B explosion of s25a28.

is $-1.6708 \times 10^{-5}$ nuclei per nucleon. In the network utilizing the updated $^{41}$K($p,\alpha$)$^{38}$Ar rate, then, $4.1432 \times 10^{-7} \times (1.6708 \times 10^{-5} - 1.6294 \times 10^{-5})$ more $^{41}$Ca nuclei per nucleon are destroyed courtesy of the flow to $^{38}$Ar.

As evident in Fig. (J.11), the $^{41}$Ca mass fraction peaks at a value marginally above that produced by the network with no rate modifications, the deviation $\sim 3.1\%$. The decreased $^{41}$K($p,\alpha$)$^{38}$Ar rate measured in this work promotes less fall-off of the $^{41}$K mass fraction (i.e., Fig. (J.12) in the updated network. That surplus of $^{41}$K nuclei then counteracts the destruction of $^{41}$Ca by capturing protons in opposition to the reverse $^{41}$K($p,n$)$^{41}$Ca flow. Remnants of this leftover $^{41}$Ca mass fraction are destroyed in the flows to $^{38}$Ar, $^{40}$Ca, and $^{42}$Ca, the magnitudes of which are on the order of $10^{-4}$-$10^{-3}$ s$^{-1}$ and essentially identical in both networks in the lead-up to shock impact. The resultant diminutive differences of order $10^{-8}$-$10^{-7}$ in the networks’ $^{41}$Ca abundance changes attributable to these flows, and the modest proton-capture production relative to the original network, favor the minute net growth seen in Fig. (J.11) in the updated network.

From Fig. (J.11), $^{41}$Ca sustains net production for the duration of each calculation, with more positive change in the modified network. As the production of $^{41}$Ca surpasses destruction in both networks, the major pathways for each being the $^{41}$K($p,n$)$^{41}$Ca, $^{41}$Ca($n,\alpha$)$^{38}$Ar, $^{40}$Ca($n,\gamma$)$^{41}$Ca, and $^{41}$Ca($n,\gamma$)$^{42}$Ca flows, the difference of $9.3962 \times 10^{-8} (5.5869 \times 10^{-7} - 4.1432 \times 10^{-7} - 1.880 x$
Figure J.11: Time evolution of the $^{41}\text{Ca}$ mass fraction in zone 284 during the E = 1.0 B explosion of s25a28 for the indicated reaction networks.

$10^{-8} - 3.1608 \times 10^{-8}$ provides the net supplemental $^{41}\text{Ca}$ nuclei per nucleon produced in the updated network across these channels. The value being $\sim 98\%$ of the difference in $^{41}\text{Ca}$ abundance changes between the networks is thus demonstrative of the flows’ effect in enhancing the $^{41}\text{Ca}$ mass fraction relative to the original network.

From Fig. (J.12), $^{41}\text{K}$ suffers net destruction in both networks for the duration of the calculations, the negative mass fraction change less in the network with the modified $^{41}\text{K}(p,\alpha)^{38}\text{Ar}$ rate. As the destruction of $^{41}\text{K}$ surpasses production in both networks, the major pathway for each being the $^{41}\text{K}(p,\alpha)^{38}\text{Ar}$ flow and reverse $^{41}\text{K}(p,\alpha)^{41}\text{Ca}$ flow, the difference of $1.1243 \times 10^{-7}$ ($6.7112 \times 10^{-7} - 5.5869 \times 10^{-7}$) provides the net fewer $^{41}\text{K}$ nuclei per nucleon destroyed in the updated network across these channels. The arrows from $^{41}\text{K} - {\rightarrow}^{42}\text{Ca}$ and from $^{41}\text{K} - {\rightarrow}^{42}\text{K}$ in Fig. (J.10) indicate other minor differences between the networks in the $^{41}\text{K}$ abundance changes due to those channels. In the updated network, $9.1746 \times 10^{-8}$ and $1.0330 \times 10^{-8}$ more $^{41}\text{K}$ nuclei per nucleon are destroyed in the flows to $^{42}\text{Ca}$ and $^{42}\text{K}$, respectively. Further subtracting these differences from $1.1243 \times 10^{-7}$ returns $1.0354 \times 10^{-8}$ nuclei per nucleon, a value representative of about 78% of the
Figure J.12: Time evolution of the $^{41}$K mass fraction in zone 284 during the E = 1.0 B explosion of s25a28 for the indicated reaction networks.

difference in $^{41}$K abundance changes between the networks.

Next, we turn our attention to interpreting the net integrated current differences of Fig. (J.13), obtained by subtracting the Sevior et al. [229] net integrated currents from those derived in the network with only the updated rate measurement for the $^{41}$Ca($n,\alpha$)$^{38}$Ar reaction. The 3 arrows linking $^{38}$Ar, $^{41}$K, and $^{41}$Ca all now point in the opposite direction. How does the modification of the $^{41}$Ca($n,\alpha$)$^{38}$Ar rate affect this change? From Fig. (J.11), the peak $^{41}$Ca mass fraction (1.9293 x $10^{-4}$) diverges by almost 25% in comparison to the peak achieved in the original network. As the difference in abundance changes of $^{41}$Ca in the flow to $^{38}$Ar between the networks is -1.7354 x $10^{-6}$, the abated destruction results in 1.7354 x $10^{-6}$ more $^{41}$Ca nuclei per nucleon withstanding the nucleosynthesis of this channel after updating its rate, just over 3 times as much as the amount remaining in the wake of the enhanced flow from $^{41}$K following reduction of the $^{41}$K($p,\alpha$)$^{38}$Ar rate. The arrow from $^{38}$Ar to $^{41}$Ca in Fig. (J.13) highlights this decreased destruction.

The value of $\rho N_A < \sigma \nu >$ for the $^{41}$Ca($n,\alpha$)$^{38}$Ar reaction is on the order of $10^7$ for the peak $T_9$ of 2.7263 in both networks and the corresponding value for the flow from $^{41}$K to $^{38}$Ar is on the
order of 10^{-4}-10^{-5}, significantly less than that responsible for the destruction of $^{41}$Ca. As the $^{41}$Ca pre-supernova and pre-shock mass fractions exceed that of $^{41}$K by about an order of magnitude, and given the vast gap in the said rate factors, we therefore expect a greater direct loss of $^{41}$Ca in the flow to $^{38}$Ar than the gain that emerges indirectly via proton captures on $^{41}$K. Such loss is on the order of 10^{-5}, thus explaining the difference between networks being on the order of 10^{-6} (i.e., 1.7354 x 10^{-6} nuclei per nucleon) and whereby the diminished $^{41}$Ca($n,\alpha$)$^{38}$Ar rate can exhibit a superior contribution to the net production of $^{41}$Ca.

The build-up of the $^{41}$K mass fraction, on the other hand, benefits more from the diminished $^{41}$K($p,\alpha$)$^{38}$Ar rate. The peak in the $^{41}$K mass fraction follows from the interplay between the $^{41}$K($p,\alpha$)$^{38}$Ar and reverse $^{41}$K($p,\alpha$)$^{38}$Ar flows, the network with the slower $^{41}$K($p,\alpha$)$^{38}$Ar rate generating 1.1243 x 10^{-7} more $^{41}$K nuclei per nucleon (see above) across these channels. When updating the $^{41}$Ca($n,\alpha$)$^{38}$Ar rate, meanwhile, only 2.969 x 10^{-8} more $^{41}$K nuclei per nucleon result from this interplay. Whereas production of $^{41}$K occurs predominantly as the reverse of the $^{41}$K($p,n$)$^{41}$Ca flow, destruction of $^{41}$Ca transpires as the many flows already discussed. Had the reverse flow to $^{41}$K been the primary mode of destruction, perhaps more of the $^{41}$Ca not destroyed in the reduced flow to $^{38}$Ar would have traversed this route in a larger contribution to the $^{41}$K mass fraction, a conclusion accentuated in Fig. (J.12) by the blue curve reaching a higher peak antecedent to a more gradual
With less $^{41}$Ca nuclei destroyed in the flow to $^{38}$Ar in the updated network, the reverse of the $^{41}$K($p,n$)$^{41}$Ca flow quickens and 3.4318 $\times 10^{-7}$ more $^{41}$Ca nuclei per nucleon are destroyed by this route. The arrow from $^{41}$Ca to $^{41}$K in Fig. (J.13) depicts the improved destruction but its thickness betrays the small magnitude relative to that of the arrow from $^{38}$Ar to $^{41}$Ca. The destruction of $^{41}$Ca correlates with production of $^{41}$K, as the flow from $^{41}$Ca to $^{41}$K yields 3.4318 $\times 10^{-7}$ more $^{41}$Ca nuclei per nucleon in the network with the rate modification. Of these additional $^{41}$K nuclei, almost all of the abundance proceeds in the flow to $^{38}$Ar, the arrow from $^{41}$K to $^{38}$Ar signifying the accelerated destruction and its thickness proportional to 3.1349 $\times 10^{-7}$. Minor flows to $^{42}$Ca and $^{42}$K destroy 2.3774 $\times 10^{-8}$ and 2.4030 $\times 10^{-9}$ more $^{41}$K nuclei per nucleon, respectively, in the updated network.

Like the preceding case of limiting the destruction of $^{41}$K in the flow to $^{38}$Ar, the accumulation of $^{41}$Ca nuclei upon weakening the $^{41}$Ca($n,\alpha$)$^{38}$Ar rate allows even larger flows to $^{42}$Ca and $^{40}$Ca via the $^{41}$Ca($n,\gamma$)$^{42}$Ca and reverse $^{40}$Ca($n,\gamma$)$^{41}$Ca channels, respectively, the updated network destroying 2.9460 $\times 10^{-7}$ more $^{41}$Ca nuclei per nucleon en route to $^{42}$Ca and producing 1.6337 $\times 10^{-7}$ less $^{41}$Ca nuclei per nucleon in the flow from $^{40}$Ca. These abundance changes, however, reside about an order of magnitude below the change emanating from the subsided $^{41}$Ca($n,\alpha$)$^{38}$Ar destruction and so the $^{41}$Ca mass fraction ascends accordingly in Fig. (J.11).

In contrast to the above discussion, in which the $^{41}$K nuclei mostly cycled from $^{38}$Ar to $^{41}$K, here the bulk of the flow is from $^{41}$Ca to $^{38}$Ar. The difference of 3.513 $\times 10^{-9}$ (3.4318 $\times 10^{-7}$ - 3.1349 $\times 10^{-7}$ - 2.3774 $\times 10^{-8}$ - 2.4030 $\times 10^{-9}$), though, still provides the net fewer $^{41}$K nuclei per nucleon destroyed in the updated network across the major productive and destructive channels, these pathways responsible for $\sim$ 92% of the difference in $^{41}$K abundance changes between the networks. Similarly, the contribution of the former $^{41}$Ca channels to the difference in its abundance change between the networks of 9.3425 $\times 10^{-7}$ nuclei per nucleon (1.7354 $\times 10^{-6}$ - 3.4318 $\times 10^{-7}$ - 2.946 $\times 10^{-7}$ - 1.6337 $\times 10^{-7}$) is near 99%. The relevance of such routes in influencing the $^{41}$K and $^{41}$Ca mass fractions relative to the network containing the rates of Sevior et al. [229] for the $^{41}$Ca($n,\alpha$)$^{38}$Ar and $^{41}$K($p,\alpha$)$^{38}$Ar reactions cannot be overstated.

When evolving the network with both of the $^{41}$K($p,\alpha$)$^{38}$Ar and $^{41}$Ca($n,\alpha$)$^{38}$Ar rates from this work, the $^{41}$Ca mass fraction in Fig. (J.11) appears to grow as the sum of the mass fractions in each of the singly-updated networks. The combined effect of lessening both rates yields residual decline.
$^{41}$Ca nuclei via the $^{41}$Ca($n,\alpha$)$^{38}$Ar and $^{41}$K($p,n$)$^{41}$Ca channels, while increased destruction with the extra nuclei remains minimal. Similarly, in Fig. (J.12), the $^{41}$K mass fraction peaks at a value the culmination of the dual $^{41}$K($p,\alpha$)$^{38}$Ar and reverse $^{41}$K($p,n$)$^{41}$Ca routes for surviving and newly-produced $^{41}$K nuclei, respectively.

### J.2 Evolution in Other Zones and Resulting Publication

The analysis of this chapter is in contribution to the work spear-headed by Rashi Talwar of Argonne National Laboratory in measuring the cross sections of the $^{38}$Ar($\alpha,n$)$^{41}$Ca and $^{38}$Ar($\alpha,p$)$^{41}$K reactions. The publication of Ref. [244] is the result of a significant collaboration among many. Please refer to it for the context within which to place our contribution. Near the end, there is a brief mention of the slight production of $^{41}$Ca in zones 530 and 560 at interior masses of 7.1064 $M_\odot$ and 7.7013 $M_\odot$, respectively.
Appendix K

Considerations of Reservoir Mixing with Radioactive Species

Summary: This section discusses mixing between two reservoirs (e.g., molecular cloud and supernova ejecta). It is necessary for understanding the computational results.

Task: Find a non-linear relationship for $\delta_{ji}$ as a function of the variable $f$ and the parameters $f_0$, $X_i^{(1)}$, $X_i^{(2)}$, $X_j^{(1)}$, and $X_j^{(2)}$. Find expressions for $\delta_{ji}^{(1)}$ and $\delta_{ji}^{(2)}$, each as a function of the parameters $f_0$, $X_i^{(1)}$, $X_i^{(2)}$, $X_j^{(1)}$, and $X_j^{(2)}$.

Reservoir 1 has a mass of $M_1$ and reservoir 2 has a mass of $M_2$. The two reservoirs undergo instantaneous mixing to produce reservoir 3, having a mass of $M_1 + M_2$. As the mixing is instantaneous and thereby allows no time for decay in the interim, we consider only stable isotopes in this analysis. $X_i^{(1)}$ and $X_j^{(1)}$ are the mass fractions of isotopes $i$ and $j$ in reservoir 1, respectively, while $X_i^{(2)}$ and $X_j^{(2)}$ are the mass fractions of $i$ and $j$ in reservoir 2, respectively. These are the mass fractions in each reservoir at the time of mixing. All mass fractions are assumed uniform throughout each reservoir, as are the mass fractions of the resultant mixture. As an example, reservoir 1 represents the proto-Solar nebula while reservoir 2 represents winds from a massive star or ejecta from the supernova explosion of such a star. Or, reservoir 1 represents a gas component of particular chemical composition within the proto-Solar nebula while reservoir 2 represents a dust component of
separate and distinct composition. Alternatively, reservoirs 1 and 2 represent some portion of these gas and dust components. Instead of the entirety of both components undergoing instantaneous mixing, then, only the portions do so. Similarly, only portions of the stellar winds or supernova ejecta may mix into the proto-Solar nebula rather than the whole of each.

The masses of isotopes \( i \) and \( j \) in reservoirs 1 and 2 at the time of mixing are given by the following:

\[
\begin{align*}
\text{mass of isotope } i \text{ in reservoir 1} & \quad \text{mass of isotope } i \text{ in reservoir 2} \\
M_i^{(1)} &= M_1 X_i^{(1)} & M_i^{(2)} &= M_2 X_i^{(2)} \\
\text{mass of isotope } j \text{ in reservoir 1} & \quad \text{mass of isotope } j \text{ in reservoir 2} \\
M_j^{(1)} &= M_1 X_j^{(1)} & M_j^{(2)} &= M_2 X_j^{(2)}
\end{align*}
\]

The masses of isotopes \( i \) and \( j \) in reservoir 3 at the time of mixing are

\[
\begin{align*}
M_i^{(3)} &= M_i^{(1)} + M_i^{(2)} \\
M_j^{(3)} &= M_j^{(1)} + M_j^{(2)}.
\end{align*}
\]

In terms of the mass fractions, we can rewrite the above equations correspondingly:

\[
\begin{align*}
M_3 X_i^{(3)} &= M_1 X_i^{(1)} + M_2 X_i^{(2)} \\
M_3 X_j^{(3)} &= M_1 X_j^{(1)} + M_2 X_j^{(2)},
\end{align*}
\]

where \( M_3 \) is the mass of reservoir 3 at the time of mixing (given by \( M_1 + M_2 \), as stated in the opening paragraph), \( X_i^{(1)} \), \( X_i^{(2)} \), and \( X_i^{(3)} \) are the mass fractions of isotope \( i \) in reservoirs 1, 2, and 3, respectively, and \( X_j^{(1)} \), \( X_j^{(2)} \), and \( X_j^{(3)} \) are the mass fractions of isotope \( j \) in reservoirs 1, 2, and 3, respectively. In solving the above equations for the mass fractions of \( i \) and \( j \) in reservoir 3 at the time of mixing, we find

\[
\begin{align*}
X_i^{(3)} &= \frac{M_1 X_i^{(1)} + M_2 X_i^{(2)}}{M_1 + M_2} \quad \text{(K.1)} \\
X_j^{(3)} &= \frac{M_1 X_j^{(1)} + M_2 X_j^{(2)}}{M_1 + M_2}. \quad \text{(K.2)}
\end{align*}
\]
Let $f$ be defined as the fraction of total mass of the two-reservoir system embedded in reservoir 1:

$$f = \frac{M_1}{M_1 + M_2} \quad \text{(K.3)}$$

$$\Rightarrow X_i^{(3)} = fX_i^{(1)} + (1 - f)X_i^{(2)}$$

$$\Rightarrow X_j^{(3)} = fX_j^{(1)} + (1 - f)X_j^{(2)},$$

where $1 - f$ is the fraction of total mass embedded in reservoir 2. For isotopes $i$ and $j$, the ratio of mass fractions in reservoir 3 at the time of mixing is determined by

$$\frac{X_j^{(3)} - X_i^{(3)}}{X_j^{(3)} - X_i^{(3)}} = \frac{fX_j^{(1)} + (1 - f)X_j^{(2)}}{fX_i^{(1)} + (1 - f)X_i^{(2)}}. \quad \text{(K.4)}$$

Similarly, the ratio of mass fractions in the atmosphere of the Sun can be expressed as

$$\frac{X_{j0}^{(3)} - X_{i0}^{(3)}}{X_{j0}^{(3)} - X_{i0}^{(3)}} = \frac{f_0X_j^{(1)} + (1 - f_0)X_j^{(2)}}{f_0X_i^{(1)} + (1 - f_0)X_i^{(2)}}. \quad \text{(K.5)}$$

As the outer layers of the Sun have not been modified over the lifetime of the Solar System, these mass fractions preserve the composition of the material from which the Sun formed. Hence, $f_0$ is the value for $f$ that produces such mass fractions at the time of mixing. For ease of reading, we’ll hide the (3) superscript in Eqs. (K.4) and (K.5) for the remainder of this analysis. The delta value for reservoir 1 is defined as

$$\frac{\delta^{(1)}_{j}}{1000} = \frac{X_j^{(1)}/X_i^{(1)}}{X_{j0}/X_{i0}} - 1. \quad \text{(K.6)}$$

Replace the denominator of the first term on the right side of Eq. (K.6) with the right side of Eq.
\[ \frac{\delta_{ji}^{(1)}}{1000} = \frac{X_j^{(1)} / X_i^{(1)}}{f_0 X_i^{(1)} + (1 - f_0) X_j^{(2)}} - 1 \]

\[ \Rightarrow \frac{\delta_{ji}^{(1)}}{1000} = \frac{X_j^{(1)} (f_0 X_i^{(1)} + X_j^{(2)}) - f_0 X_i^{(1)} X_j^{(2)}}{X_i^{(1)} (f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)})} - 1. \]

Combine both terms on the right side of the equation into a single fraction and multiply out the terms of the numerator:

\[ \frac{\delta_{ji}^{(1)}}{1000} = \frac{X_j^{(1)} (f_0 X_i^{(1)} + X_j^{(2)}) - f_0 X_i^{(1)} X_j^{(2)}}{X_i^{(1)} (f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)})}. \]

Factor \( f_0 \) from the terms of the numerator:

\[ \frac{\delta_{ji}^{(1)}}{1000} = \frac{X_i^{(2)} X_j^{(1)} - f_0 X_i^{(2)} X_j^{(1)} - X_i^{(1)} X_j^{(2)} + f_0 X_i^{(1)} X_j^{(2)}}{X_i^{(1)} (f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)})}. \]

In factoring \( (X_j^{(2)} X_j^{(1)} - X_i^{(1)} X_j^{(2)}) \) from the terms of the numerator, we arrive at our expression for the delta value for reservoir 1 as a function of the parameters \( f_0 \), \( X_i^{(1)} \), \( X_i^{(2)} \), \( X_j^{(1)} \), and \( X_j^{(2)} \):

\[ \frac{\delta_{ji}^{(1)}}{1000} = \frac{(1 - f_0)(X_i^{(2)} X_j^{(1)} - X_i^{(1)} X_j^{(2)})}{X_i^{(1)} (f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)})}. \]

\[ \Rightarrow \delta_{ji}^{(1)} = \frac{1000(1 - f_0)(X_i^{(2)} X_j^{(1)} - X_i^{(1)} X_j^{(2)})}{X_i^{(1)} (f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)})}. \] (K.7)

The delta value for reservoir 2 is defined as

\[ \frac{\delta_{ji}^{(2)}}{1000} = \frac{X_j^{(2)} / X_i^{(2)}}{X_j / X_i} - 1. \]
Similarly, it can be shown that our expression for the delta value for reservoir 2 as a function of the parameters \( f_0, X_i^{(1)}, X_i^{(2)}, X_j^{(1)}, \) and \( X_j^{(2)} \) is given by

\[
\delta_{ji}^{(2)} = -\frac{1000 f_0 (X_i^{(2)} - X_i^{(1)} X_j^{(2)})}{X_i^{(2)} [f_0 X_i^{(1)} + (1 - f_0) X_j^{(2)}]}.
\] (K.8)

The delta value for reservoir 3 is defined as

\[
\frac{\delta_{ji}}{1000} = \frac{X_j/X_i}{X_{j0}/X_{i0}} - 1.
\] (K.9)

Replace the numerator of the first term on the right side of Eq. (K.9) with the right side of Eq. (K.4) and the denominator with the right side of Eq. (K.5) and then simplify the fraction on the right side of the equation:

\[
\frac{\delta_{ji}}{1000} = \frac{\left[ fX_i^{(1)} + (1 - f)X_j^{(2)} \right] \left[ f_0 X_i^{(1)} + (1 - f_0) X_j^{(2)} \right]}{f_0 X_i^{(1)} [fX_i^{(1)} + (1 - f)X_j^{(2)}]} - 1
\]

\[
\Rightarrow \frac{\delta_{ji}}{1000} = \frac{\left[ fX_i^{(1)} + (1 - f)X_j^{(2)} \right] \left[ f_0 X_i^{(1)} + (1 - f_0) X_j^{(2)} \right]}{f_0 X_i^{(1)} [fX_i^{(1)} + (1 - f)X_j^{(2)}]} - 1.
\]

Combine both terms on the right side of the equation into a single fraction and multiply out the terms of the numerator:

\[
\frac{\delta_{ji}}{1000} = \frac{fX_i^{(1)} X_j^{(1)} - f_0 fX_i^{(1)} X_j^{(1)} + fX_i^{(2)} X_j^{(1)} - f_0 fX_i^{(2)} X_j^{(1)} + fX_i^{(1)} X_j^{(2)} - f_0 fX_i^{(1)} X_j^{(2)} + fX_i^{(2)} X_j^{(2)} - f_0 fX_i^{(2)} X_j^{(2)} - fX_i^{(1)} X_j^{(2)} - f_0 X_i^{(1)} X_j^{(2)} + X_i^{(2)} X_j^{(2)} - f_0 X_i^{(2)} X_j^{(2)} + X_i^{(2)} X_j^{(2)}}{fX_i^{(1)} + (1 - f)X_j^{(2)}} \frac{fX_j^{(1)} + (1 - f_0) X_j^{(2)}}{fX_j^{(1)} + (1 - f)X_j^{(2)}}
\]

\[
\Rightarrow \frac{\delta_{ji}}{1000} = \frac{fX_i^{(2)} X_j^{(1)} + f_0 X_i^{(1)} X_j^{(2)} - fX_i^{(1)} X_j^{(2)} - f_0 X_i^{(2)} X_j^{(1)}}{fX_i^{(1)} + (1 - f)X_j^{(2)}} \frac{fX_j^{(1)} + (1 - f_0) X_j^{(2)}}{fX_j^{(1)} + (1 - f)X_j^{(2)}}
\]

Factor \( f \) and \( f_0 \) from the terms of the numerator:

\[
\frac{\delta_{ji}}{1000} = \frac{f \left[ X_i^{(2)} X_j^{(1)} - X_i^{(1)} X_j^{(2)} \right] - f_0 \left[ X_i^{(2)} X_j^{(1)} - X_i^{(1)} X_j^{(2)} \right]}{fX_i^{(1)} + (1 - f)X_j^{(2)}} \frac{fX_j^{(1)} + (1 - f_0) X_j^{(2)}}{fX_j^{(1)} + (1 - f)X_j^{(2)}}.
\]
In factoring \((X_i^{(2)}X_j^{(1)} - X_i^{(1)}X_j^{(2)})\) from the terms of the numerator, we arrive at our non-linear relationship for the delta value for reservoir 3 as a function of the variable \(f\) and the parameters \(f_0\), \(X_i^{(1)}\), \(X_i^{(2)}\), \(X_j^{(1)}\), and \(X_j^{(2)}\):

\[
\frac{\delta_{ji}}{1000} = \frac{(f - f_0)(X_i^{(2)}X_j^{(1)} - X_i^{(1)}X_j^{(2)})}{[fX_i^{(1)} + (1 - f)X_i^{(2)}][f_0X_j^{(1)} + (1 - f_0)X_j^{(2)}]}
\]

\[\Rightarrow \delta_{ji} = \frac{1000(f - f_0)(X_i^{(2)}X_j^{(1)} - X_i^{(1)}X_j^{(2)})}{[fX_i^{(1)} + (1 - f)X_i^{(2)}][f_0X_j^{(1)} + (1 - f_0)X_j^{(2)}]},\]  

(K.10)

As a check, if \(f = 0\) (i.e., \(M_1 = 0\)), then Eq. (K.10) reduces to

\[
\delta_{ji} = \frac{-1000f_0(X_i^{(2)}X_j^{(1)} - X_i^{(1)}X_j^{(2)})}{X_i^{(2)}[f_0X_j^{(1)} + (1 - f_0)X_j^{(2)}]},
\]

the same expression as that of Eq. (K.8). In other words, with no mass in reservoir 1, mixing does not occur. Reservoir 2 becomes reservoir 3 and the corresponding delta value for reservoir 3 is that for reservoir 2. As another check, if \(f = 1\) (i.e., \(M_2 = 0\)), then Eq. (K.10) reduces to

\[
\delta_{ji} = \frac{1000(1 - f_0)(X_i^{(2)}X_j^{(1)} - X_i^{(1)}X_j^{(2)})}{X_i^{(1)}[f_0X_j^{(1)} + (1 - f_0)X_j^{(2)}]},
\]

the same expression as that of Eq. (K.7). In other words, with no mass in reservoir 2, mixing does not occur. Reservoir 1 becomes reservoir 3 and the corresponding delta value for reservoir 3 is that for reservoir 1.

**Task:** Find a linear relationship for \(X_{ki}\) as a function of the variable \(X_{ji}\) and the parameters \(X_i^{(1)}, X_i^{(2)}, X_j^{(1)}, X_j^{(2)}, X_k^{(1)},\) and \(X_k^{(2)}\). Find a linear relationship for \(\delta_{ki}\) as a function of the variable \(\delta_{ji}\) and the parameters \(f_0, X_i^{(1)}, X_i^{(2)}, X_j^{(1)}, X_j^{(2)}, X_k^{(1)},\) and \(X_k^{(2)}\).

As before, reservoir 1 has a mass of \(M_1\) and reservoir 2 has a mass of \(M_2\). The two reservoirs undergo instantaneous mixing to produce reservoir 3, having a mass of \(M_1 + M_2\). Now, we consider the presence of a third isotope, \(k\), in the mixing. \(X_i^{(1)}, X_j^{(1)},\) and \(X_k^{(1)}\) are the mass fractions of isotopes \(i, j,\) and \(k\) in reservoir 1, respectively, while \(X_i^{(2)}, X_j^{(2)},\) and \(X_k^{(2)}\) are the mass fractions of
i, j, and k in reservoir 2, respectively. These are the mass fractions in each reservoir at the time of mixing. All mass fractions are assumed uniform throughout each reservoir.

From Eq. (K.4),

$$\frac{X_j}{X_i} = \frac{fX_j(1) + (1 - f)X_j(2)}{fX_i(1) + (1 - f)X_i(2)}. \quad (K.11)$$

Similarly,

$$\frac{X_k}{X_i} = \frac{fX_k(1) + (1 - f)X_k(2)}{fX_i(1) + (1 - f)X_i(2)}. \quad (K.12)$$

In multiplying both sides of Eq. (K.11) by the denominator on the right side, we obtain the following:

$$\frac{X_j}{X_i} [fX_i(1) + (1 - f)X_i(2)] = fX_j(1) + (1 - f)X_j(2)$$

$$\Rightarrow fX_i(1)X_jX_i + X_i(2)X_jX_i - fX_i(2)X_jX_i = fX_j(1) + X_j(2) - fX_j(2).$$

Rearrange the terms of the equation and factor f:

$$f [(X_i(1) - X_i(2))X_jX_i - X_j(1) + X_j(2)] = X_j(2) - X_j(1)X_i.$$  

Divide both sides of the equation by \([(X_i(1) - X_i(2))X_jX_i - X_j(1) + X_j(2)] to solve for f:

$$f = \frac{X_j(2) - X_j(1)X_i}{(X_i(1) - X_i(2))X_jX_i - X_j(1) + X_j(2)}. \quad (K.13)$$

Subtract f from 1 and simplify:

$$1 - f = 1 - \frac{X_j(2) - X_j(1)X_i}{(X_i(1) - X_i(2))X_jX_i - X_j(1) + X_j(2)}$$

$$= \frac{(X_i(1) - X_i(2))X_jX_i - X_j(1) + X_j(2) - (X_i(2) - X_i(1)X_i)}{(X_i(1) - X_i(2))X_jX_i - X_j(1) + X_j(2)}$$

$$\Rightarrow 1 - f = \frac{X_i(1)X_jX_i - X_j(1)}{(X_i(1) - X_i(2))X_jX_i - X_j(1) + X_j(2)}. \quad (K.14)$$
Replace $f$ of Eq. (K.12) with the right side of Eq. (K.13) and $1 - f$ of Eq. (K.12) with the right side of Eq. (K.14):

$$X_k \over X_i = \left[ \frac{X_k^{(2)} - X_k^{(2)} X_j}{(X_i^{(1)} - X_i^{(2)} X_j X_i^{(1)} + X_j^{(2)})} \right] X_k^{(1)} + \left[ \frac{X_i^{(1)} X_j - X_i^{(1)} X_j^{(2)}}{(X_i^{(1)} - X_i^{(2)} X_j X_i^{(1)} + X_j^{(2)})} \right] X_i^{(1)}.$$  

Factoring the common denominator from the terms of the numerator and denominator on the right side of Eq. (K.14):

$$X_k \over X_i = \left[ \frac{X_k^{(2)} - X_k^{(2)} X_j}{(X_i^{(1)} - X_i^{(2)} X_j X_i^{(1)} + X_j^{(2)})} \right] \left[ (X_j^{(2)} - X_j^{(2)} X_k) X_k^{(1)} + (X_i^{(1)} X_j - X_j^{(1)} X_k^{(2)}) \right] \left[ (X_j^{(2)} - X_j^{(2)} X_k) X_k^{(1)} + (X_i^{(1)} X_j - X_j^{(1)} X_k^{(2)}) \right]$$

$$= \frac{(X_j^{(2)} - X_j^{(2)} X_k) X_k^{(1)} + (X_i^{(1)} X_j - X_j^{(1)} X_k^{(2)})}{(X_j^{(2)} - X_j^{(2)} X_k) X_k^{(1)} + (X_i^{(1)} X_j - X_j^{(1)} X_k^{(2)})} X_j^{(2)} - X_j^{(2)} X_k^{(1)}.$$  

Multiply out the terms of the numerator and denominator and simplify:

$$X_k \over X_i = \frac{X_i^{(1)} X_j^{(2)} X_k^{(2)} - X_i^{(1)} X_j^{(2)} X_k^{(1)} X_j^{(2)} + X_i^{(1)} X_j^{(2)} X_k^{(2)} - X_i^{(1)} X_j^{(2)} X_k^{(1)}}{X_i^{(1)} X_j^{(2)} - X_i^{(2)} X_j^{(1)}}$$

$$\Rightarrow X_k \over X_i = \frac{(X_i^{(1)} X_j^{(2)} - X_i^{(1)} X_j^{(2)} X_k^{(1)} X_j^{(2)} + X_i^{(1)} X_j^{(2)} X_k^{(2)} - X_i^{(1)} X_j^{(2)} X_k^{(1)})}{X_i^{(1)} X_j^{(2)} - X_i^{(2)} X_j^{(1)}}.$$  

Rewriting the equation in the form of a line (i.e., $y = mx + b$) leads to

$$X_k \over X_i = \left( \frac{X_i^{(1)} X_j^{(2)} - X_i^{(1)} X_j^{(2)} X_k^{(1)} X_j^{(2)} + X_i^{(1)} X_j^{(2)} X_k^{(2)} - X_i^{(1)} X_j^{(2)} X_k^{(1)}}{X_i^{(1)} X_j^{(2)} - X_i^{(2)} X_j^{(1)}} \right) X_i^{(1)} X_j^{(2)} - X_i^{(2)} X_j^{(1)}.$$  

Changing the notation of the equation such that $\frac{X_k}{X_i} \equiv X_{ki}$ and $\frac{X_j}{X_i} \equiv X_{ji}$ allows us to write

$$X_{ki} = \left( \frac{X_i^{(1)} X_j^{(2)} - X_i^{(1)} X_j^{(2)} X_k^{(1)} X_j^{(2)} + X_i^{(1)} X_j^{(2)} X_k^{(2)} - X_i^{(1)} X_j^{(2)} X_k^{(1)}}{X_i^{(1)} X_j^{(2)} - X_i^{(2)} X_j^{(1)}} \right) X_{ji} + \frac{X_j^{(2)} X_k^{(1)} - X_j^{(1)} X_k^{(2)}}{X_i^{(1)} X_j^{(2)} - X_i^{(2)} X_j^{(1)}}$$

for our linear relationship for $X_{ki}$ as a function of the variable $X_{ji}$ and the parameters $X_i^{(1)}, X_i^{(2)}$,
\(X_j^{(1)}, X_j^{(2)}, X_k^{(1)}, \) and \(X_k^{(2)}\). Eq. (K.16) can be rewritten in terms of \(\delta_{ji}\) and \(\delta_{ki}\). From Eq. (K.9),

\[
\frac{\delta_{ji}}{1000} = \frac{X_j/X_i}{X_{j0}/X_{i0}} - 1.
\]

Similarly,

\[
\frac{\delta_{ki}}{1000} = \frac{X_k/X_i}{X_{k0}/X_{i0}} - 1.
\]

Or, with the new notation,

\[
\frac{\delta_{ji}}{1000} = \frac{X_{ji}}{X_{ji0}} - 1
\]

\[
\frac{\delta_{ki}}{1000} = \frac{X_{ki}}{X_{ki0}} - 1.
\]

In solving the above equations for \(X_{ji}\) and \(X_{ki}\), respectively, we obtain the following:

\[
X_{ji} = \left(\frac{\delta_{ji}}{1000} + 1\right) X_{ji0}
\]  \hspace{1cm} (K.17)

\[
X_{ki} = \left(\frac{\delta_{ki}}{1000} + 1\right) X_{ki0}.
\]  \hspace{1cm} (K.18)

Replace \(X_{ji}\) of Eq. (K.16) with the right side of Eq. (K.17) and \(X_{ki}\) of Eq. (K.16) with the right side of Eq. (K.18):

\[
\left(\frac{\delta_{ki}}{1000} + 1\right) X_{ki0} = \left(\frac{X_{i}^{(1)} X_{k}^{(2)} - X_{i}^{(2)} X_{k}^{(1)}}{X_{i}^{(1)} X_{j}^{(2)} - X_{i}^{(2)} X_{j}^{(1)}}\right) \left(\frac{\delta_{ji}}{1000} + 1\right) X_{ji0} + \frac{X_{j}^{(2)} X_{k}^{(1)} - X_{j}^{(1)} X_{k}^{(2)}}{X_{i}^{(1)} X_{j}^{(2)} - X_{i}^{(2)} X_{j}^{(1)}}.
\]

Multiply out the terms on both sides of the equation and rearrange and group:

\[
\frac{\delta_{ki}}{1000} X_{ki0} + X_{ki0} = \frac{X_{i}^{(1)} X_{k}^{(2)} - X_{i}^{(2)} X_{k}^{(1)}}{X_{i}^{(1)} X_{j}^{(2)} - X_{i}^{(2)} X_{j}^{(1)}} \frac{\delta_{ji}}{1000} X_{ji0} + \frac{X_{j}^{(2)} X_{k}^{(1)} - X_{j}^{(1)} X_{k}^{(2)}}{X_{i}^{(1)} X_{j}^{(2)} - X_{i}^{(2)} X_{j}^{(1)}} X_{ji0} + \frac{X_{j}^{(1)} X_{k}^{(2)} - X_{j}^{(2)} X_{k}^{(1)}}{X_{i}^{(1)} X_{j}^{(2)} - X_{i}^{(2)} X_{j}^{(1)}} X_{ji0} + \frac{X_{j}^{(1)} X_{k}^{(2)} - X_{j}^{(2)} X_{k}^{(1)}}{X_{i}^{(1)} X_{j}^{(2)} - X_{i}^{(2)} X_{j}^{(1)}} X_{ji0}.
\]

Multiply both sides of the equation by \(\frac{1000}{X_{ki0}}\):

\[
\delta_{ki} = \frac{X_{i}^{(1)} X_{k}^{(2)} - X_{i}^{(2)} X_{k}^{(1)}}{X_{i}^{(1)} X_{j}^{(2)} - X_{i}^{(2)} X_{j}^{(1)}} X_{ki0} + \left[\frac{X_{j}^{(1)} X_{k}^{(2)} - X_{j}^{(2)} X_{k}^{(1)}}{X_{i}^{(1)} X_{j}^{(2)} - X_{i}^{(2)} X_{j}^{(1)}} X_{ji0} - \frac{X_{j}^{(1)} X_{k}^{(2)} - X_{j}^{(2)} X_{k}^{(1)}}{X_{i}^{(1)} X_{j}^{(2)} - X_{i}^{(2)} X_{j}^{(1)}} X_{ji0}\right] \frac{1000}{X_{ki0}}.
\]
Distribute \( \frac{1}{X_{ki0}} \) to the terms inside the square brackets on the right side of the equation:

\[
\delta_{ki} = \frac{X_i^{(1)} X_j^{(2)} - X_i^{(2)} X_k^{(1)}}{X_i^{(1)} X_j^{(2)} - X_i^{(2)} X_j^{(1)}} X_{ki0} \delta_{ji} + \left[ \frac{(X_i^{(1)} X_k^{(2)} - X_i^{(2)} X_k^{(1)}) X_{ki0} - X_i^{(1)} X_j^{(2)} + X_j^{(2)} X_i^{(1)}}{(X_i^{(1)} X_j^{(2)} - X_i^{(2)} X_j^{(1)}) X_{ki0}} - 1 \right] \times 1000.
\] (K.19)

From Eq. (K.5),

\[
X_{ji0} = \frac{f_0 X_j^{(1)}}{f_0 X_i^{(1)}} + (1 - f_0) X_j^{(2)}.
\] (K.20)

Similarly,

\[
X_{ki0} = \frac{f_0 X_k^{(1)}}{f_0 X_i^{(1)}} + (1 - f_0) X_k^{(2)}.
\] (K.21)

Replace \( X_{ji0} \) of Eq. (K.19) with the right side of Eq. (K.20) and \( X_{ki0} \) of Eq. (K.19) with the right side of Eq. (K.21):

\[
\delta_{ki} = \left( \frac{X_i^{(1)} X_j^{(2)} - X_i^{(2)} X_j^{(1)}}{X_i^{(1)} X_j^{(2)} - X_i^{(2)} X_j^{(1)}} \right) \left[ \frac{f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)}}{f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)}} \right] \delta_{ji} + \left[ \frac{(X_i^{(1)} X_k^{(2)} - X_i^{(2)} X_k^{(1)}) \left[ \frac{f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)}}{f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)}} \right] - X_i^{(1)} X_j^{(2)} + X_j^{(2)} X_i^{(1)}}{(X_i^{(1)} X_j^{(2)} - X_i^{(2)} X_j^{(1)}) \left[ \frac{f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)}}{f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)}} \right]} - 1 \right] \times 1000.
\]

Factor \[ \frac{1}{f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)}} \] from the numerator and denominator of the fractions inside parentheses on the right side of the equation and simplify:

\[
\delta_{ki} = \left( \frac{X_i^{(1)} X_k^{(2)} - X_i^{(2)} X_k^{(1)}}{X_i^{(1)} X_k^{(2)} - X_i^{(2)} X_k^{(1)}} \right) \left[ \frac{f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)}}{f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)}} \right] \delta_{ji} + \left[ \frac{(X_i^{(1)} X_k^{(2)} - X_i^{(2)} X_k^{(1)}) \left[ \frac{f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)}}{f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)}} \right] - (X_i^{(1)} X_j^{(2)} - X_j^{(2)} X_i^{(1)}) \left[ \frac{f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)}}{f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)}} \right]}{(X_i^{(1)} X_j^{(2)} - X_i^{(2)} X_j^{(1)}) \left[ \frac{f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)}}{f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)}} \right]} - 1 \right] \times 1000
\]

\[
\Rightarrow \delta_{ki} = \left( \frac{X_i^{(1)} X_k^{(2)} - X_i^{(2)} X_k^{(1)}}{X_i^{(1)} X_k^{(2)} - X_i^{(2)} X_k^{(1)}} \right) \left[ \frac{f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)}}{f_0 X_j^{(1)} + (1 - f_0) X_j^{(2)}} \right] \delta_{ji}.
\] (K.22)

Eq. (K.22) represents our linear relationship for \( \delta_{ki} \) as a function of the variable \( \delta_{ji} \) and the parameters \( f_0, X_i^{(1)}, X_i^{(2)}, X_j^{(1)}, X_j^{(2)}, X_k^{(1)}, \) and \( X_k^{(2)} \).

**Task:** Find a non-linear relationship for \( X_{ik} \) as a function of the variable \( X_{ji} \), and the parameters \( X_i^{(1)}, X_i^{(2)}, X_j^{(1)}, X_j^{(2)}, X_k^{(1)}, X_k^{(2)}, X_l^{(1)}, \) and \( X_l^{(2)} \).
Similarly, the presence of a fourth isotope, \( l \), in the mixing. \( X_i^{(1)}, X_j^{(1)}, X_k^{(1)}, \) and \( X_l^{(1)} \) are the mass fractions of isotopes \( i, j, k, \) and \( l \) in reservoir 1, respectively, while \( X_i^{(2)}, X_j^{(2)}, X_k^{(2)}, \) and \( X_l^{(2)} \) are the mass fractions of \( i, j, k, \) and \( l \) in reservoir 2, respectively. These are the mass fractions in each reservoir at the time of mixing. All mass fractions are assumed uniform throughout each reservoir.

From Eq. (K.4),
\[
\frac{X_j}{X_i} = \frac{f X_j^{(1)} + (1-f) X_j^{(2)}}{f X_i^{(1)} + (1-f) X_i^{(2)}} .
\]

Similarly,
\[
\frac{X_l}{X_k} = \frac{f X_l^{(1)} + (1-f) X_l^{(2)}}{f X_k^{(1)} + (1-f) X_k^{(2)}} .
\]

Also, from Eq. (K.15),
\[
\frac{X_k}{X_i} = \frac{X_j^{(2)} X_k^{(1)} - X_i^{(2)} X_k^{(1)} X_j + X_i^{(1)} X_k^{(2)} X_j - X_j^{(1)} X_k^{(2)}}{X_k^{(1)} X_j^{(2)} - X_i^{(2)} X_k^{(1)} X_j + X_i^{(1)} X_k^{(2)} X_j - X_j^{(1)} X_k^{(2)}} .
\]

\[
\Rightarrow \frac{X_l}{X_k} = \frac{X_j^{(2)} X_l^{(1)} - X_i^{(2)} X_l^{(1)} X_j + X_i^{(1)} X_l^{(2)} X_j - X_j^{(1)} X_l^{(2)}}{X_l^{(2)} X_k^{(1)} - X_i^{(2)} X_l^{(1)} X_j + X_i^{(1)} X_l^{(2)} X_j - X_j^{(1)} X_l^{(2)}} .
\]

Factor \( \frac{X_l}{X_i} \) from the terms of the numerator and denominator:
\[
\frac{X_l}{X_k} = \frac{(X_l^{(1)} X_i^{(2)} - X_i^{(2)} X_l^{(1)}) \frac{X_l}{X_i} + X_l^{(2)} X_i^{(1)} - X_l^{(1)} X_i^{(2)}}{(X_l^{(1)} X_k^{(2)} - X_i^{(2)} X_l^{(1)}) \frac{X_l}{X_i} + X_l^{(2)} X_k^{(1)} - X_l^{(1)} X_l^{(2)}} .
\]

Changing the notation of the equation such that \( \frac{X_l}{X_i} \equiv X_{ik} \) and \( \frac{X_j}{X_i} \equiv X_{ji} \) allows us to write
\[
X_{ik} = \frac{(X_i^{(1)} X_j^{(2)} - X_i^{(2)} X_i^{(1)}) X_{ji} + X_j^{(2)} X_i^{(1)} - X_j^{(1)} X_i^{(2)}}{(X_i^{(1)} X_k^{(2)} - X_i^{(2)} X_i^{(1)}) X_{ji} + X_j^{(2)} X_k^{(1)} - X_j^{(1)} X_k^{(2)}} .
\]

(K.23)

for our non-linear relationship for \( X_{ik} \) as a function of the variable \( X_{ji} \) and the parameters \( X_i^{(1)}, X_i^{(2)}, X_j^{(1)}, X_j^{(2)}, X_k^{(1)}, X_k^{(2)}, X_l^{(1)}, \) and \( X_l^{(2)} \).
As a check, if $k = i$, then the above equation becomes

\[ X_{li} = \frac{(X_i^{(1)}X_i^{(2)} - X_i^{(2)}X_i^{(1)})X_{ji} + X_j^{(2)}X_i^{(1)} - X_j^{(1)}X_i^{(2)}}{(X_i^{(1)}X_i^{(2)} - X_i^{(2)}X_i^{(1)})X_{ji} + X_j^{(2)}X_i^{(1)} - X_j^{(1)}X_i^{(2)}} \]

\[ \Rightarrow X_{li} = \frac{(X_i^{(1)}X_i^{(2)} - X_i^{(2)}X_i^{(1)})X_{ji} + X_j^{(2)}X_i^{(1)} - X_j^{(1)}X_i^{(2)}}{X_j^{(2)}X_i^{(1)} - X_j^{(1)}X_i^{(2)}} \].

Rewriting the equation in the form of a line (i.e., $y = mx + b$) leads to

\[ X_{li} = \left( \frac{X_i^{(1)}X_i^{(2)} - X_i^{(2)}X_i^{(1)}}{X_j^{(2)}X_i^{(1)} - X_j^{(1)}X_i^{(2)}} \right) X_{ji} + \frac{X_j^{(2)}X_i^{(1)} - X_j^{(1)}X_i^{(2)}}{X_j^{(2)}X_i^{(1)} - X_j^{(1)}X_i^{(2)}} \]

the linear relationship for $X_{li}$ as a function of the variable $X_{ji}$ and the parameters $X_i^{(1)}$, $X_i^{(2)}$, $X_j^{(1)}$, $X_j^{(2)}$, $X_i^{(1)}$, and $X_i^{(2)}$ previously deduced for the three-isotope system.

Eqs. (K.16) and (K.23) each represent an instantaneous mixture between two reservoirs characterized by distinct compositions. If we take two new reservoirs identical in composition but dissimilar in mass to the previous reservoirs and instantaneously mix them, the mass fractions of this resulting mixture will vary from those of the previous mixture yet both compositions now define a mixing curve (Eq. (K.16) for three isotopes or Eq. (K.23) for four) that highlights the correlation between these mass fractions. As we mix more and more pairs of reservoirs of the same composition but different mass (and thus different $f$ value), we acquire additional points on this curve.

Or, instead of the entirety of both reservoirs mixing, as their mass fractions are uniform throughout, Eqs. (K.16) and (K.23) each represent an instantaneous mixture between portions of the two reservoirs. As we remove and instantaneously mix pairs of sub-reservoirs of varying masses (i.e., $f$ values), the resulting compositions correlate via the mixing curve as defined by Eq. (K.16) or Eq. (K.23). Multiple pairs are mixed together, corresponding to multiple points on the curve, until none of the original reservoirs remain.

**Task:** Find a non-linear relationship for $X_i^{(1)}$ as a function of the variable $M_j^{(2)}$ and the parameters $M_0^{(1)}$, $M_0^{(2)}$, $X_{i0}^{(1)}$, and $X_{i0}^{(2)}$. Find a non-linear relationship for $X_i^{(1)}(t)$ as a function of time and the parameters $M_0^{(1)}$, $M_0^{(2)}$, $X_{i0}^{(1)}$, $X_{i0}^{(2)}$, $\tau_{\text{decay}}$, and $\tau_{\text{mix}}$. For the case of a stable isotope $i$, show that the two relationships are identical.
We can return to the example in which reservoir 1 represents the proto-Solar nebula while reservoir 2 represents winds from a massive star or ejecta from the supernova explosion of such a star. If portions of the winds/ejecta mix into the proto-Solar nebula, how does the composition of the proto-Solar nebula evolve? Consider, first, successive instantaneous mixings. The initial mass of the proto-Solar nebula is $M_0^{(1)}$ and the initial mass of the winds/ejecta is $M_0^{(2)}$. After the first instantaneous mixing, the mass of the winds/ejecta decreases to $M_1^{(2)}$ and the mass of the proto-Solar nebula increases to $M_1^{(1)}$ as an amount of mass, $M_0^{(2)} - M_1^{(2)}$, mixes into the proto-Solar nebula. From Eq. (K.1), after the first instantaneous mixing, the mass fraction of isotope $i$ in the proto-Solar nebula becomes

$$X_{i1}^{(1)} = \frac{M_0^{(1)} X_{i0}^{(1)} + (M_0^{(2)} - M_1^{(2)}) X_{i0}^{(2)}}{M_0^{(1)} + M_0^{(2)} - M_1^{(2)}}, \quad (K.24)$$

where the (1) superscript denotes the proto-Solar nebula and the (2) superscript denotes the winds/ejecta and the 0 and 1 subscripts denote quantities before and after the first mixing, respectively. In forming the winds/ejecta portions by the removal of parcels of mass from reservoir 2, we do not disrupt the uniformity of its mass fractions, as there is no addition of mass and consequent mixing. Hence, $X_{i0}^{(2)}$ remains constant and we can remove the subscript of 0 for future reference.

After the second instantaneous mixing, the mass of the winds/ejecta decreases to $M_2^{(2)}$ and the mass of the proto-Solar nebula increases to $M_2^{(1)}$ as an amount of mass, $M_1^{(2)} - M_2^{(2)}$, mixes into the proto-Solar nebula. The mass fraction of $i$ in the proto-Solar nebula subsequently transitions into

$$X_{i2}^{(1)} = \frac{M_1^{(1)} X_{i1}^{(1)} + (M_1^{(2)} - M_2^{(2)}) X_{i1}^{(2)}}{M_1^{(1)} + M_1^{(2)} - M_2^{(2)}}, \quad (K.25)$$

where the 1 and 2 subscripts denote quantities before and after the second mixing, respectively. Replace $X_{i1}^{(1)}$ of Eq. (K.25) with the right side of Eq. (K.24):

$$X_{i2}^{(1)} = \frac{M_1^{(1)} M_0^{(1)} X_{i0}^{(1)} + (M_1^{(2)} - M_2^{(2)}) M_0^{(2)} X_{i0}^{(2)}}{M_1^{(1)} + M_1^{(2)} - M_2^{(2)}} + (M_1^{(2)} - M_2^{(2)}) X_{i1}^{(2)}.$$
As \( M_1^{(1)} = M_0^{(1)} + M_0^{(2)} - M_1^{(2)} \), simplify the numerator and denominator accordingly:

\[
X_{12}^{(1)} = \frac{M_0^{(1)} X_{i0}^{(1)} + (M_0^{(2)} - M_1^{(2)})X_i^{(2)}}{M_0^{(1)} + M_0^{(2)} - M_1^{(2)}}
\]

\[
\Rightarrow X_{12}^{(1)} = \frac{M_0^{(1)} X_{i0}^{(1)} + (M_0^{(2)} - M_1^{(2)})X_i^{(2)}}{M_0^{(1)} + M_0^{(2)} - M_1^{(2)}}.
\]

(K.26)

After the third instantaneous mixing, the mass of the winds/ejecta decreases to \( M_3^{(2)} \) and the mass of the proto-Solar nebula increases to \( M_3^{(3)} \) as an amount of mass, \( M_2^{(2)} - M_3^{(2)} \), mixes into the proto-Solar nebula. The mass fraction of \( i \) in the proto-Solar nebula further enriches to

\[
X_{i3}^{(1)} = \frac{M_0^{(1)} X_{i0}^{(1)} + (M_0^{(2)} - M_3^{(2)})X_i^{(2)}}{M_0^{(1)} + M_0^{(2)} - M_3^{(2)}}.
\]

(K.27)

where the 2 and 3 subscripts denote quantities before and after the third mixing, respectively. Replace \( X_{12}^{(1)} \) of Eq. (K.27) with the right side of Eq. (K.26):

\[
X_{i3}^{(1)} = \frac{M_0^{(1)} X_{i0}^{(1)} + (M_0^{(2)} - M_3^{(2)})X_i^{(2)}}{M_0^{(1)} + M_0^{(2)} - M_3^{(2)}}.
\]

(K.28)

As \( M_1^{(1)} = M_0^{(1)} + M_0^{(2)} - M_1^{(2)} \) and \( M_2^{(1)} = M_1^{(1)} + M_1^{(2)} - M_2^{(2)} \), rewrite \( M_2^{(1)} \) as \( M_0^{(1)} + M_0^{(2)} - M_2^{(2)} \) so that Eq. (K.28) reduces to

\[
X_{i3}^{(1)} = \frac{M_0^{(1)} X_{i0}^{(1)} + (M_0^{(2)} - M_3^{(2)})X_i^{(2)}}{M_0^{(1)} + M_0^{(2)} - M_3^{(2)}}.
\]

(K.29)

We find the mass fraction of \( i \) in the proto-Solar nebula after the \( j \)th instantaneous mixing to be a function of the mass of the winds/ejecta after that mixing. Because Eq. (K.29) exemplifies...
the format of Eq. (K.1), rather than carry out \( j \) instantaneous mixings to obtain the updated composition of the proto-Solar nebula, only one suffices as we mix a portion of the winds/ejecta having mass, \( M_0^{(2)} - M_j^{(2)} \), into the original pre-mixed nebula. Moreover, similar derivations that produced Eqs. (K.16) and (K.23) result in the following mass-fraction correlations between isotopes \( i, k \), and \( l \) and between \( i, k, l \), and \( m \) in the proto-Solar nebula after the \( j \)th instantaneous mixing:

\[
X_{ki,j} = \frac{X_0^{(1)} X_k^{(2)} - X_0^{(2)} X_k^{(1)}}{X_0^{(1)} X_i^{(2)} - X_0^{(2)} X_i^{(1)}} \times \frac{X_i^{(2)} X_k^{(1)} - X_i^{(1)} X_k^{(2)}}{X_i^{(2)} X_l^{(1)} - X_i^{(1)} X_l^{(2)}} \times \frac{X_i^{(2)} X_l^{(1)} - X_i^{(1)} X_l^{(2)}}{X_i^{(2)} X_k^{(1)} - X_i^{(1)} X_k^{(2)}}.
\]

Like the points defining the mixing curves of Eqs. (K.16) and (K.23), these correlations also define mixing curves.

In contrast to the above instantaneous evolution of the proto-Solar nebula, we now consider the evolution of the mass of a stable or radioactive isotope \( i \) as a function of time via delayed mixing on a timescale \( \tau_{mix} \) and spontaneous decay (if radioactive) on a timescale \( \tau_{decay} \). Once more, reservoir 1 represents the proto-Solar nebula while reservoir 2 represents winds from a massive star or ejecta from the supernova explosion of such a star. If portions of the winds/ejecta mix into the proto-Solar nebula, how does the composition of the proto-Solar nebula evolve? The equation governing the net time rate of change of the mass of a radioactive isotope \( i \) in the winds/ejecta can be expressed as the sum of two destructive terms, one causing decay and the other responsible for mixing:

\[
\frac{dM_i^{(2)}(t)}{dt} = D_{\text{decay}} + D_{\text{mix}} = \left( \frac{dM_i^{(2)}(t)}{dt} \right)_{\text{decay}} + \left( \frac{dM_i^{(2)}(t)}{dt} \right)_{\text{mix}}.
\]

For any given moment in time, more mass of \( i \) will undergo decay and mix out for a larger sample size of the winds/ejecta. Likewise, not as much mass loss ensues if less of the winds/ejecta is present.
Because both reductions in the mass of \( i \) must then be proportional to said mass,

\[
\left( \frac{dM^{(2)}_i(t)}{dt} \right)_{\text{decay}} = -\lambda_{\text{decay}} M^{(2)}_i(t) \quad (K.30)
\]

\[
\left( \frac{dM^{(2)}_i(t)}{dt} \right)_{\text{mix}} = -\lambda_{\text{mix}} M^{(2)}_i(t) \quad (K.31)
\]

\[\Rightarrow \frac{dM^{(2)}_i(t)}{dt} = -\lambda_{\text{decay}} M^{(2)}_i(t) - \lambda_{\text{mix}} M^{(2)}_i(t), \quad (K.32)\]

where \( M^{(2)}_i(t) \) is the mass of \( i \) at time \( t \), \( \lambda_{\text{decay}} \) is the probability of decay per unit of mass of \( i \) per unit of time, and \( \lambda_{\text{mix}} \) is the probability of mixing per mass per time. The first term on the right side of Eq. (K.32) describes the decrease in the mass of \( i \) attributable to the decay while the second term describes the decrease due to the mixing. The evolution of the mass of \( i \) in the winds/ejecta thus manifests as

\[M^{(2)}_i(t) = M^{(2)}_{i0} e^{-\left(\lambda_{\text{decay}} + \lambda_{\text{mix}}\right)t}, \quad (K.33)\]

where \( M^{(2)}_{i0} \) is the initial mass of \( i \).

For a small time step, Eq. (K.30) can be rewritten as

\[
\frac{\left( \frac{dM^{(2)}_i(t)}{dt} \right)_{\text{decay}}}{M^{(2)}_i(t)} \approx -\lambda_{\text{decay}}.
\]

The fractional change in \( M^{(2)}_i(t) \) per unit of time from decay, during that time step, is approximately \(-\lambda_{\text{decay}}\). In inverting this equation, we find the time per that fractional change is given by \( \frac{1}{\lambda_{\text{decay}}} \), or, \( \frac{1}{\tau_{\text{decay}}} \). We denote this timescale as \( \tau_{\text{decay}} \). For instance, if 10% of the mass of \( i \) decays in 20 s, then \( \tau_{\text{decay}} \) is 2 s. In other words, during that time step, it would take about 2 s for the mass of \( i \) to decay by 100%. Similarly, the fractional change in \( M^{(2)}_i(t) \) per unit of time from mixing is approximately \(-\lambda_{\text{mix}}\). Analogous to \( \tau_{\text{decay}} \), the mixing timescale \( \tau_{\text{mix}} \) is gauged through the reciprocal of \( \lambda_{\text{mix}} \). In terms of these timescales, Eq. (K.33) becomes

\[M^{(2)}_i(t) = M^{(2)}_{i0} e^{-\left(\frac{1}{\tau_{\text{decay}}} + \frac{1}{\tau_{\text{mix}}}\right)t}.
\]
As the evolution of the mass of $i$ in the proto-Solar nebula is dictated by the decay of $i$ in reservoir 1 and the flow of $i$ from reservoir 2, we can express its time rate of change as the sum of a destructive and productive term:

$$\frac{dM^{(1)}_i(t)}{dt} = D_{\text{decay}} + P_{\text{mix}}$$

$$= -\frac{M^{(1)}_i(t)}{\tau_{\text{decay}}} + \frac{M^{(2)}_i(t)}{\tau_{\text{mix}}}$$

$$= -\frac{M^{(1)}_i(t)}{\tau_{\text{decay}}} + \frac{M^{(2)}_i(t_0)}{\tau_{\text{mix}}} e^{-\left(\frac{1}{\tau_{\text{decay}}} + \frac{1}{\tau_{\text{mix}}}\right)t}. \quad (K.34)$$

Rearrange Eq. (K.34) in the format of a first-order linear differential equation:

$$\frac{dM^{(1)}_i(t)}{dt} + \frac{M^{(1)}_i(t)}{\tau_{\text{decay}}} = \frac{M^{(2)}_i(t)}{\tau_{\text{mix}}} e^{-\left(\frac{1}{\tau_{\text{decay}}} + \frac{1}{\tau_{\text{mix}}}\right)t}. \quad (K.35)$$

The solution of Eq. (K.35) and, in turn, the mass of $i$ as a function of time in the proto-Solar nebula is

$$M^{(1)}_i(t) = e^{-\frac{t}{\tau_{\text{decay}}}} \left[ M^{(1)}_i(t_0) + M^{(2)}_i(t_0) \left(1 - e^{-\frac{t}{\tau_{\text{mix}}}}\right) \right].$$

Since loss occurs only through mixing, the equation governing the net time rate of change of the mass of the winds/ejecta can be expressed as the following:

$$\frac{dM^{(2)}(t)}{dt} = -\frac{M^{(2)}(t)}{\tau_{\text{mix}}}. \quad (K.36)$$

To compute the change in its mass, rearrange Eq. (K.36) and integrate from $t = 0$ to some later time $t$:

$$\int_0^t \frac{1}{M^{(2)}(t')} \frac{dM^{(2)}(t')}{dt'} = \int_0^t \frac{1}{\tau_{\text{mix}}} dt'$$

$$\Rightarrow M^{(2)}(t) = M^{(2)}_0 e^{-\frac{t}{\tau_{\text{mix}}}}. \quad (K.37)$$
This loss of the winds/ejecta is the gain of the proto-Solar nebula:

\[
\frac{dM^{(1)}(t)}{dt} = -\frac{dM^{(2)}(t)}{dt}
\]

\[
= \frac{M^{(2)}(t)}{\tau_{\text{mix}}}
\]

\[
= \frac{M_0^{(2)}}{\tau_{\text{mix}}} e^{-\frac{t}{\tau_{\text{mix}}}}
\]

\[
\Rightarrow M^{(1)}(t) = M_0^{(1)} + M_0^{(2)} \left(1 - e^{-\frac{t}{\tau_{\text{mix}}}}\right).
\]

The mass fraction of \(i\) in the proto-Solar nebula as a function of time, then, is simply the ratio of the mass of \(i\) to the mass of its reservoir, which grows in time as material mixes in from the winds/ejecta:

\[
X_i^{(1)}(t) = \frac{M_i^{(1)}(t)}{M^{(1)}(t)}
\]

\[
= e^{-\frac{t}{\tau_{\text{decay}}}} \left[\frac{M_0^{(1)} + M_0^{(2)} (1 - e^{-\frac{t}{\tau_{\text{mix}}}})}{M_0^{(1)} + M_0^{(2)} (1 - e^{-\frac{t}{\tau_{\text{mix}}}})}\right]
\]

\[
= e^{-\frac{t}{\tau_{\text{decay}}}} \left[\frac{M_0^{(1)} X_0^{(1)} + M_0^{(2)} X_0^{(2)} (1 - e^{-\frac{t}{\tau_{\text{mix}}}})}{M_0^{(1)} + M_0^{(2)} (1 - e^{-\frac{t}{\tau_{\text{mix}}}})}\right],
\]  \text{(K.38)}

the initial masses of \(i\) in reservoirs 1 and 2 being conveyed in terms of the associated reservoir masses and mass fractions. As acknowledged in the discussion of instantaneous mixing, the mass fraction of \(i\) in the winds/ejecta remains constant and we can therefore remove the subscript of 0 for future reference. Long after the conclusion of mixing, the reservoir is devoid of \(i\) courtesy of its decay. As \(t \to \infty\), \(e^{-\frac{t}{\tau_{\text{decay}}}}\) becomes negligible and \(X_i^{(1)}(t)\) certainly vanishes.
To compare the above equation with Eq. (K.29), rewrite it as the following:

\[ X_i^{(1)}(t) = \frac{M_0^{(1)} X_{i0}^{(1)} e^{-\frac{t}{\tau_{\text{decay}}}} + (M_0^{(2)} - M_0^{(2)} e^{-\frac{t}{\tau_{\text{mix}}}}) X_i^{(2)} e^{-\frac{t}{\tau_{\text{decay}}}}}{M_0^{(1)} + M_0^{(2)} - M_0^{(2)} e^{-\frac{t}{\tau_{\text{mix}}}}} . \]  \( \text{(K.39)} \)

As Eq. (K.29) depicts the mixture of a portion of the winds/ejecta and the original pre-mixed nebula, so, too, does Eq. (K.39) allow us to imagine a displaced allocation of the winds/ejecta pouring into the pre-mixed nebula across the duration from \( t = 0 \) to some later time \( t \). From Eq. (K.37), \( M_0^{(2)} e^{-\frac{t}{\tau_{\text{mix}}}} \) is the remaining mass of the winds/ejecta at time \( t \), \( X_{i0}^{(1)} e^{-\frac{t}{\tau_{\text{decay}}}} \) is the remaining mass fraction of \( i \) in the proto-Solar nebula from decay had no mixing occurred, and \( X_i^{(2)} e^{-\frac{t}{\tau_{\text{decay}}}} \) is the remaining mass fraction of \( i \) in the winds/ejecta transit from decay. Similarly, from Eq. (K.29), \( M_j^{(2)} e^{-\frac{t}{\tau_{\text{mix}}}} \) is the remaining mass of the winds/ejecta after the \( j \)th instantaneous mixing, \( X_{i0}^{(1)} \) is the mass fraction of \( i \) in the proto-Solar nebula had no mixing occurred (nor decay since only stable isotopes were considered in that analysis), and \( X_i^{(2)} \) is the mass fraction of \( i \) in the winds/ejecta transit (again neglecting decay). Eqs. (K.29) and (K.39) thus correlate in calculating the evolving mass fraction of \( i \) in the proto-Solar nebula as the winds/ejecta mix in. By analogy to Eq. (K.3), then, we may define \( f(t) \), the fraction of total mass embedded in reservoir 1 at time \( t \), as

\[ f(t) = \frac{M_0^{(1)}}{M_0^{(1)} + M_0^{(2)} - M_0^{(2)} e^{-\frac{t}{\tau_{\text{mix}}}}} , \]

the fraction decreasing over time as more and more of the winds/ejecta coalesce with the proto-Solar nebula.

\[ \Rightarrow 1 - f(t) = \frac{M_0^{(2)} - M_0^{(2)} e^{-\frac{t}{\tau_{\text{mix}}}}}{M_0^{(1)} + M_0^{(2)} - M_0^{(2)} e^{-\frac{t}{\tau_{\text{mix}}}}} \]

for the fraction of total mass having accumulated in the winds/ejecta allocation by time \( t \).

\[ \Rightarrow X_i^{(1)}(t) = f(t) X_{i0}^{(1)} e^{-\frac{t}{\tau_{\text{decay}}}} + [1 - f(t)] X_i^{(2)} e^{-\frac{t}{\tau_{\text{decay}}}} . \]

In the limit of a stable isotope \( i \), as \( \tau_{\text{decay}} \to \infty \), \( \frac{1}{\tau_{\text{decay}}} \) becomes negligible and Eq. (K.38) thereby reduces to

\[ X_i^{(1)}(t) = \frac{M_0^{(1)} X_{i0}^{(1)} + M_0^{(2)} X_i^{(2)} (1 - e^{-\frac{t}{\tau_{\text{mix}}}})}{M_0^{(1)} + M_0^{(2)} (1 - e^{-\frac{t}{\tau_{\text{mix}}}})} . \]
At the start of mixing (i.e., $t = 0$), when $i$ has yet to mix in from the winds/ejecta, $1 - e^{-\tau_{mix}}$ vanishes and the initial mass fraction of $i$ is that of the pre-mixed nebula, as expected. Also, $f(0) = 1$ because reservoir 1 initially contains all of the mass of the two-reservoir (proto-Solar nebula plus winds/ejecta allocation) system. As $t \rightarrow \infty$, $e^{-\frac{t}{\tau_{mix}}}$ becomes negligible and the mass fraction of $i$ reflects the culmination of both reservoirs having fully merged, once more expected. Accordingly, $f(t) \rightarrow \frac{M_0^{(1)}}{M_0^{(1)} + M_0^{(2)}}$.

In the limit of instantaneous mixing, as $\tau_{mix} \rightarrow 0$ and, thus, $\frac{1}{\tau_{mix}} \rightarrow \infty$, $e^{-\frac{t}{\tau_{mix}}}$ becomes negligible and Eq. (K.38) thereby reduces to

$$X_i^{(1)}(t) = M_0^{(1)} X_i^{(1)}_0 + M_0^{(2)} X_i^{(2)}_0$$

Initially, at $t = 0$, the mass fraction of $i$ in the proto-Solar nebula is that of the consolidation of the pre-mixed nebula and winds/ejecta. Such a mass fraction then decreases exponentially as $i$ undergoes decay. $f(t)$ remains constant by virtue of the absence of any mixing delay for the winds/ejecta. In the limit of a stable isotope $i$ and instantaneous mixing, Eq. (K.38) reduces to

$$X_i^{(1)}(t) = \frac{M_0^{(1)} X_i^{(1)}_0 + M_0^{(2)} X_i^{(2)}_0}{M_0^{(1)} + M_0^{(2)}} e^{-\frac{t}{\tau_{decay}}}$$

as deduced in the lead-up to Eq. (K.1).
Bibliography


268


