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CHEMICAL EVOLUTION OF THE NEUTRON-RICH IRON-GROUP ISOTOPES AND IMPLICATIONS FOR THE FORMATION OF FUN CAIS

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CHEMICAL EVOLUTION OF THE NEUTRON-RICH IRON-GROUP ISOTOPES AND IMPLICATIONS FOR THE FORMATION OF FUN CAIS

A Dissertation
Presented to
the Graduate School of
Clemson University

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

by
Tianhong Yu
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Accepted by:
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ABSTRACT

Calcium-aluminum-rich inclusions (CAIs) are millimeter-sized refractory objects found in primitive meteorites. CAIs are considered as some of the first solids to form in the solar system, because they are refractory. FUN CAIs, those with Fractionated and Unknown Nuclear effects, are a small subset of CAIs. These FUN CAIs show correlated excesses and deficits in the neutron-rich iron-group isotopes such as $^{48}\text{Ca}$ and $^{50}\text{Ti}$ which regular CAIs do not. Interestingly, these isotopes are most likely produced infrequently but in huge quantities in a rare class of thermonuclear (Type Ia) supernovae. I propose that the isotopic effects in the neutron-rich iron-group nuclei in FUN CAIs arise from the rarity ($\sim 2\%$) of the Type Ia supernovae that produce them. To quantitatively test this hypothesis we built a simple Ia model to get the yields and trajectories, and then estimated the chemical forms and sizes of dust grains into which those isotopes condense. Our results show that these rare dense Type Ia supernovae can produce a large quantity of neutron-rich iron-group isotopes; with unburned carbon and oxygen added the chemical perovskite (CaTiO$_3$) would form and may count for more than 5% of total atoms in the outflow; the size of dust grains can grow up to the order of 0.1 micron. All these findings suggest the rare dense Type Ia supernovae may be the source of these isotopes and the outflows may form Ca-Ti carriers which will bring the heterogeneity of these isotopes to the early solar system. The future Galactic Chemical Evolution simulation with these inputs would help constrain the Solar System formation in the nucleosynthetic and dust formation aspects.
DEDICATION

To my parents,
Finally about to finish my PhD, after so many years. Now I am ready to move on.

To Su Meng,
You kind of influenced me into astrophysics. I hope you find it interesting.
ACKNOWLEDGEMENTS

I would like to thank my advisor Dr. Brad Meyer, for teaching me so much knowledge and skills, for telling me so much history and funny stories, for helping me with research and life. He masters math, physics and programming. And he is still learning new stuff everyday, with interest and passion. He is a real scientist. I will never forget his charming personality in my life.

I also would like to thank my committee members, Dr. Brittain, Dr. Hartmann and Dr. Sosolik, for giving me good suggestion on my research. Dr. Lih-sin The helped me with computational physics and the usage of IDL and I appreciate it. I thank Dr. Sasha Krot and Dr. Gary Huss for hosting me in Hawaii and showing real meteorites. I thank Dr. Zhang Junjun for letting me see CAIs for the first time. I thank Dr. Tang Haolan and Liu Nan for teaching me basic cosmochemistry. All the three ladies above are from University of Chicago. Also I’d like to thank Ginger Bryngelson and other friends here in PandA Clemson. I’ll remember our good times.

Dr. Donald D. Clayton is still doing research at almost his 80’s. It’s a great honor to work with him. His mind is sharp, his idea is clear, and his words are humorous. I wish him all the best.

I also thank NASA for an Earth and Space Science Fellowship.
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CHAPTER 1
INTRODUCTION

Millions of stars over the course of the Galaxy’s history contributed material to the cloud of gas and dust that became the Solar System (SS). The cumulative ejecta from these stars mixed together to form our Sun, the planets, and us, and this mixing was quite efficient, both elementally and (at least) isotopically (See Appendix A for more information about mixing). When the materials experience various physical and chemical processes during the formation of the Solar System there are certain fractionated effects, again both elementally and isotopically. That means the compositions of different objects in the Solar System are different (See Appendix B for more information about fractionation.). Studying these elemental and isotopic anomalies of various samples would give information about early Solar System and then help us to understand its formation.

1.1 FUN CAIs

Calcium-aluminum-rich Inclusions (CAIs) are sub-millimeter to centimeter-sized refractory objects found in carbonaceous chondrite meteorites (see Fig. 1.1). Lead-lead dating (see Appendix C for a brief description of chronology) shows that they are among the oldest solid condensates in the early solar system, if in fact not the oldest (e.g., Amelin et al. 2002; Connelly et al. 2008). This is mainly because they are refractory and condensed relatively early during the solar system formation at a high temperature (e.g. Al with a condensation temperature of 1650 Kelvin).

CAIs contain evidence of now extinct short-lived radioisotopes (e.g. $^{26}$Al, $^{41}$Ca, and $^{182}$Hf) synthesized in one or multiple stars and then added to the protosolar molecular cloud before or during its collapse. Let’s take $^{26}$Al (halflife $t_{1/2} \sim 0.7$ Ma) as an example. The majority of CAIs contain high abundance of radiogenic $^{26}$Mg, the decay product of $^{26}$Al, corresponding to an inferred initial $^{26}$Al/$^{27}$Al ratio of $(4.5 - 5.5) \times 10^{-5}$ (see Fig. C.2 in Appendix C). This means these CAIs must have formed within a few million years after the fresh $^{26}$Al was
Figure 1.1 Calcium-aluminum rich inclusions (CAIs) are found in carbonaceous chondrites, like the Allende meteorite pictured here (53 mm-long sample). The CAIs are the oldest materials to have formed in the Solar System, beating the Earth by 50 to 100 million years. Caption from Jeffrey Taylor.

produced and injected into protosolar system. Fig. 1.2 shows a demonstration of the formation timeline for different objects.

However there is a rare subset of refractory minerals (e.g. hibonite) and inclusions (FUN CAIs) that have low initial $^{26}\text{Al}/^{27}\text{Al}$ ratios ($< 5 \times 10^{-6}$) [Holst et al. 2013]. FUN CAIs are a small subset of CAIs with Fractionated and Unknown Nuclear effects. Hibonite ((Ca,Ce)Al$_{12}$O$_{19}$) is a common mineral in the CAIs found in some chondritic meteorites. Besides the feature of low $^{26}\text{Al}$, both FUN CAIs and Hibonite grains carry isotopic anomalies in neutron-rich isotopes (see Fig. 1.3). This is the “UN” part of FUN CAIs. In the meanwhile, both FUN CAIs and regular CAIs show $^{16}\text{O}$-rich in the three-isotope oxygen diagram (Fig. 1.4). But FUN CAIs are distributed on a slope $1/2$ fractionation line. This is the “F” part of the FUN CAIs. So the puzzling question is: when did these objects form?

From $^{26}\text{Al}$ point of view, it may be either before regular CAIs formed when few fresh $^{26}\text{Al}$ has been injected into the proto solar system, or after regular CAIs formed when a large portion of $^{26}\text{Al}$ has decayed. Both possibilities cannot be confirmed or ruled out so far, although
the presence of once-live $^{182}$Hf in a FUN CAI suggests the former interpretation [Holst et al. 2013].

So studying the correlation of neutron-rich iron-group isotopes such as $^{48}$Ca and $^{50}$Ti in FUN CAIs and Hibonite is another and important way to explore the early history of the solar system. The notation in Fig. [1.3] is defined as:

Studying the isotopic correlations will help constrain the Solar System formation in the nucleosynthetic aspect.

### 1.2 Neutron-Rich Iron-Group Isotopes

The most neutron-rich stable iron-group isotopes (namely, $^{48}$Ca, $^{50}$Ti, $^{54}$Cr, $^{58}$Fe, and $^{62,64}$Ni) present an important challenge for nucleosynthesis theory, Galactic chemical evolution studies, and for our understanding of the birth of the Solar System. With the exception of
Figure 1.3 Isotopic anomalies in the neutron-rich isotopes \(^{48}\text{Ca}\) and \(^{50}\text{Ti}\) measured in FUN and hibonite-bearing inclusions. The isotopic ratios are expressed as \(\delta\) values: deviations from the normal ratios are in permil: 

\[
\delta^{48}\text{Ca}/^{40}\text{Ca} \equiv \left( \frac{^{48}\text{Ca} / ^{40}\text{Ca}}{^{\text{sample}}^{48}\text{Ca} / ^{40}\text{Ca}} \right)_{\text{standard}} - 1 \right] \times 1000.
\]

Isotopic anomalies are qualitatively correlated in that most inclusions with \(^{48}\text{Ca}\) excesses have \(^{50}\text{Ti}\) excesses and vice versa. Figure and caption from [Meyer and Zinner 2006a].

\(^{48}\text{Ca}\), they are significantly produced by slow neutron capture in massive stars (the weak \(s\)-process) (e.g., [The et al. 2007]). Such processing occurs primarily in the large helium-burning convective core that follows core hydrogen burning.

The short beta-decay half life of \(^{45}\text{Ca}\) (162.2 days) and even shorter half life of \(^{47}\text{Ca}\) (4.536 days) prevent \(^{48}\text{Ca}\) from being produced in the same environment. The site of \(^{48}\text{Ca}\) synthesis is suspected to be a subset of thermonuclear supernovae (type Ia supernovae) that achieve high enough densities to have significant electron capture during the explosion (e.g., [Meyer et al. 1996; Woosley 1997]) (See Appendix D for more information about the formation of \(^{48}\text{Ca}\).) Because the matter in these explosions has low entropy per nucleon (typically less than 0.1 \(k_B\), where \(k_B\) is Boltzmann’s constant, per nucleon), the nuclear abundances are
Figure 1.4  Three-isotope oxygen diagram of oxygenisotope compositions of individual minerals in the Allende STP-1 FUN CAI. Similarly to the majority of FUN CAIs, the oxygenisotope compositions of anorthite, spinel, hibonite, and most Al,Ti-diopside grains in STP-1 plot along a mass-dependent fractionation line defining an initial $\Delta^{17}$O value of $\sim 24\%_\circ$ that is, similar to the oxygenisotope composition of canonical CAIs and that of the Sun. Oxygenisotope compositions of melilite and some of the Al,Ti-diopside grains plot along a line with a slope of $\sim 1$, suggesting subsequent isotope exchange with a $^{16}$O-depleted gaseous reservoir. In contrast with most FUN CAIs from CV chondrites characterized by $^{16}$O-poor compositions of melilite and anorthite, melilite in STP-1 shows a range of $\Delta^{17}$O values, whereas anorthite is uniformly $^{16}$O-rich. These observations indicate that STP-1 is more pristine than all previously known FUN CAIs. Figure and caption from Holst et al. 2013
characterized by an overabundance of heavy nuclei relative to nuclear statistical equilibrium. This permits production of abundant $^{48}\text{Ca}$ when nuclear statistical equilibrium would require even larger production of $^{66}\text{Ni}$, an isotope with nearly the same degree of neutron richness [Hartmann et al. 1985].

The type Ia supernovae that make $^{48}\text{Ca}$ also make $^{50}\text{Ti}$, $^{54}\text{Cr}$, and the other neutron-rich iron-group isotopes. The yields depend in large measure on the degree of neutron-richness achieved during the explosion. This, in turn, depends on the weak interaction rates on the nuclei. The interesting challenge for nucleosynthesis theory, then, is to understand the complex dynamics of the nuclear abundances as they shift due to both weak interactions and changing temperature and density.

Because the neutron-rich iron-group isotopes are made in at least two different sites, they also present a challenge to Galactic chemical evolution studies. Massive stars live and die quickly on astronomical timescales. For example, a star 25 times as massive as the Sun may be born, live, and die in a core-collapse supernova event over a time span of only 7 million years (e.g., The et al. 2007). A type Ia supernova is thought to be the explosion of a white dwarf star that has accreted enough mass to trigger a thermonuclear runaway that disrupts the entire star. The white dwarf formed from a lower mass star (less than roughly eight times the mass of the Sun) and then had to accrete matter from a companion star (see Appendix ?? for more discussion about white dwarf). The timescale for this to happen is hundreds of millions of years. The build up of abundance of an isotope like $^{50}\text{Ti}$ in the Galaxy is coming from two different sources operating on two different timescales while the build up of the $^{48}\text{Ca}$ abundance is apparently happening only on the longer timescale. The interesting challenge for Galactic chemical evolution is, then, to follow the relative build up of these isotopes over time, especially $^{48}\text{Ca}$ compared to its sister neutron-rich iron-group species.

These differing formation scenarios and different production timescales for the neutron-rich isotopes may have significant implications for the very early history of the Solar System. FUN CAIs (and smaller grain hibonites) show roughly correlated anomalies in $^{48}\text{Ca}$ and $^{50}\text{Ti}$ (see Fig. 1.3 and Lee et al. 1978; Niederer et al. 1980). The anomalies are roughly correlated in the sense that CAIs or hibonites that show excesses (relative to average Solar composition) of $^{48}\text{Ca}$ tend also to show excesses of $^{50}\text{Ti}$ while those that show deficits of $^{48}\text{Ca}$ also show
deficits of $^{50}$Ti. A possible explanation for this is that the precursor dust of the Solar System had a heterogeneous (but correlated) distribution of these isotopes. As this precursor dust gathered to form the FUN CAIs, some sampled an excess of the dust with large quantities of the neutron-rich iron-group isotopes while others sampled a deficit of that dust. The challenge for Solar System studies is to characterize the precursor dust and mixing in the early Solar nebula to understand the origin of the FUN CAIs.

1.3 Rare Ia Supernovae and Galactic Chemical Evolution

The neutron-rich iron group isotopes are thought to be made in low entropy QSE (quasi statistical equilibrium). In the QSE’s, the isotopes like $^{48}$Ca are the dominantly produced ones. That the solar-system abundance of these isotopes is low, then, tells us that their production must be rare. And that environment happens during a thermonuclear supernovae explosion (Type Ia). Of interest for the present work is the question of the chemical form in which these nuclei are ejected from type Ia supernova.

My thesis is that the rarity of the $^{48}$Ca-producing Ia’s is reflected in the FUN CAIs. Rare type Ia supernovae produce a large amount of dust with correlated anomalies in $^{48}$Ca and $^{50}$Ti, and the interstellar medium is then heterogeneous in its distribution of $^{48}$Ca and $^{50}$Ti in its dust. These dust grains are incorporated into the solar nebula and give rise to the isotopic anomalies seen in the FUN CAIs.

These elements may all be related. The rareness of the type Ia supernova events may lead to a heterogeneous distribution of the neutron-rich iron-group isotopes in the dust in the Galaxy. Processing of that dust in the interstellar medium will tend to homogenize the isotopes as supernova shocks sputter atoms from the dust which then reaccrete onto other dust grains. If that homogenization process is not too efficient, however, the precursor dust in the Solar System might indeed have been quite isotopically heterogeneous so that the anomalies in the FUN CAIs could be understood.

Unraveling the details of the history of the neutron-rich iron-group isotopes is clearly a large problem that will require years, if not decades, of work. In this thesis I contribute to this grand problem by focusing on the issue of production of these isotopes in type Ia supernovae. In particular, I developed some tools to study the nucleosynthesis in low-entropy explosive
environments in which electron capture is changing the degree of neutron richness. To carry out this project, we developed Nucnet Tools and Nucnet Projects.

In this thesis I will describe the simple type Ia model and show the results in Chapter 2. This will give the initial abundances. Then I’ll use the chemical condensation code to estimate the possible chemical forms condensed in the supernova outflows. This will be discussed in Chapter 3. I’ll show how dusts grow in the expanding materials of supernovae in Chapter 4. Together with the results in Chapter 3 we will get the equilibrium chemical forms and the sizes of grains that might condense. Finally I will follow up with a simple GCE description to roughly estimate the reservoirs in the Solar System in Chapter 5. The summary and conclusion will be in Chapter 6.
CHAPTER 2
SIMPLE SNIA MODEL

Type Ia supernovae (SNIa) occur in binary systems in which one of the stars is a white dwarf while the other can be a giant star or another white dwarf. We just take the one white dwarf case and do not consider double degenerate case (merger of two white dwarfs) which is rare. And since our focus is on the nucleosynthesis, the detailed composition and mechanism might not affect the final result much. Thus we just make the white dwarf consisting of 50% Carbon-12 and 50% Oxygen-16 in mass and apply a simple set of hydrodynamic equations to describe it as shown in [Yu 2010].

A white dwarf is the remnant of a star that has completed its normal life cycle, say, after a red giant star phase for example (See Appendix F for more discussion of white dwarfs). It is composed mostly of electron-degenerate matter and the pressure inside mainly depends on the density but not temperature as in regular stars. If the companion of a white dwarf is a giant star, the white dwarf may gradually accrete mass from it. Once the white dwarf has accreted enough matter the degenerate pressure can no longer support the star. The mass limit is called Chandrasekhar limit, which is about 1.44 solar masses. Then it will contract and release the gravitational potential energy which would heat up the whole star, since the temperature gradient is small in a white dwarf. Once the temperature passes the carbon burning threshold, the whole star will encounter a thermonuclear explosion that incinerates the whole star. In our simple model, we just give the white dwarf a big initial mass of 1.5 solar masses and a high initial temperature of 1.5 billion Kelvin to let it explode.

In this chapter I will show a variety of results from our simple model.

2.1 White Dwarf Equations

The simple SNIa model is a 1-zone, 0-dimension model. We let the white dwarf (to explode) be a uniform, isotropic sphere with radius $R$. Thus the temperature and density do not depend on the radius of the white dwarf.
I am going to list the hydrodynamic equations below, which describe the white dwarf. The detailed derivations are shown in [Yu 2010].

\[
\frac{dx}{dt} = y
\]  
\[
\frac{dy}{dt} = \frac{P_0}{\rho_0 R_0^2} \left[ \frac{P}{P_0} x^2 - \frac{1}{x^2} \right]
\]

where \( x \equiv \frac{R}{R_0} \), \( y \equiv \frac{v}{R_0} \) and \( R_0 \) is the initial radius of the white dwarf.

For thermodynamic part, we evolve the entropy approach instead of temperature as in my master’s work:

\[
\frac{d(s/k_B)}{dt} = \frac{1}{k_B T} \frac{dq}{dt} - \sum_i \frac{\mu_i}{k_B T} \frac{dY_i}{dt}
\]

The entropy is useful because it is computationally a more stable quantity when the abundances are near equilibrium.

This is the first order ordinary differential equation for the change of entropy per nucleon with time, together with eq(2.1) and eq(2.2) forming a full series of equations that determine the behavior of the white dwarf.

There are two terms in the \( \frac{dq}{dt} \) term on the right hand side of eq(2.3) that determine how entropy changes. The first term is the heat loss mostly by neutrinos. The second term is the entropy lost by photons (radiation). We roughly account for this as discussed below.

### 2.2 Entropy Generation

The entropy generation is computed from the chemical potential of the species and their rate of change, as determined from the coupled nuclear reaction network. We also include the entropy loss by the escape of neutrino and photons. The neutrino entropy loss comes from the portion of energy in weak decays released into neutrinos that freely stream out of the star. We compute this from our weak interaction rates. To compute the photon entropy loss, we estimate the mean free path of photons in our supernova and then assume the object radiates as a black body losing the fraction of the energy corresponding to the ratio of the photon mean free path divided by the current radius.
2.3 Explosion and Nucleosynthesis

To solve the three first order ordinary differential equations (2.1, 2.2, 2.3), which determine the evolution of size, velocity and temperature, we used `gsl_odeiv_step_rk4`, the 4th order (classical) Runga-Kutta methods.

For each timestep, we evolve the three equations first. And the run the network to get the entropy generation and abundance changes. We use both $x, y, s$ and species abundances to control the timestep.
Figure 2.1 shows how the size of the star changes with time. This calculation and the following few are all with an initial density of $9 \times 10^9 \text{g/cm}$. In this figure the normalized radius $x$ starts to increase around $10^{-2}$ seconds and becomes $10^8$ times of original in about one year ($3 \times 10^8$ seconds).

![Graph showing normalized radius change with time](image)

Figure 2.1 The normalized radius change with time for a calculation of the simple type Ia model.

Figure 2.2 shows the change of velocity with time. The expanding speed of the star shoots up at about $10^{-5}$ seconds after the calculation starts and becomes significantly fast ($10^8 \text{cm/s}$) around $10^{-2}$ seconds. Due to the weak interaction (as shown below) the velocity...
varies a little bit and peaks around 1 second, and then levels at about $3 \times 10^8$ cm/s, $\approx 1\%$ of speed of light.

\[
\rho_0 = 9 \times 10^9 \text{g/cm}^3, \ T_0 = 1.5 \times 10^9 \text{K}, \ M = 1.5 \ M_{\text{sun}}
\]

![Graph](image)

**Figure 2.2** The velocity change with time for a calculation of the simple type Ia model. The final speed gets up to about 1% of speed of light.

**Figure 2.3** shows the temperature change with time. The uniform temperature of the star starts to shoot up at about $2 \times 10^{-5}$ seconds. This is because of the carbon burning. The system tends to be in the quasi-statistical equilibrium (QSE) in a short period of evolution. Once the system has a chance to relax to nuclear statistical equilibrium, the temperature will drop a little bit after the first peak in Figure 2.3. Then the weak interactions take over at such high temperatures. The electron captures will release energy to heat up the materials up to 11
billion Kelvin. Then the star responds to the pressure change and starts to expand and cool down. See Appendix [E] for more details about weak interactions.

\[ \rho_0 = 9 \times 10^9 \text{ g/cm}^3, \quad T_0 = 1.5 \times 10^9 \text{ K}, \quad M = 1.5 \text{ M}_{\odot} \]

Figure 2.3 The temperature change with time for a calculation of the simple type Ia model.

Figure 2.4 shows the temperature change with time for calculations of 3 different initial densities. Comparing with Figure 2.3, this figure plots the temperature in logarithmic scale, which reveals the hidden feature at low temperatures. We can see that at later time the system will be heated up to some extent. This is due to the decay of radioactive nuclide in the outflows. We also notice that for different initial densities the temperature curves look different. As we will see later in Figure 2.7, this is because the different radioactive mass fractions for each density model.
$\rho_0 = 2 \times 10^7 \text{ (g cm}^{-3}\text{)}$

$\rho_0 = 4 \times 10^9 \text{ (g cm}^{-3}\text{)}$

$\rho_0 = 9 \times 10^9 \text{ (g cm}^{-3}\text{)}$

Figure 2.4 The temperature change with time for a calculation of the simple type Ia model for various initial densities.

Figure 2.5 shows the temperature and density relationships for models with different initial densities. The density on the horizontal axis is plotted reversely, which indicates the expanding direction is to the right. This figure is useful to predict the possible condensation conditions at low temperature for different calculations. Generally the atoms in the outflow start to condense without being broken up by the energetic photons at about 1000 Kelvin. This means for certain trajectories, if the temperature stays high for a long time (due to the heating by decays) the density becomes too low for atoms to stick together when it is cool enough.
Figure 2.5 The temperature change with density for a calculation of the simple type Ia model for various initial densities.

Figure 2.6 shows the mass fraction change of selected species for different initial densities. At low densities the weak interaction rates are low, which means there is hardly electron captures happening to make the system neutron-rich. So the most abundant species are with even proton neutron numbers, such as $^{28}$Si and $^{56}$Ni. As the density goes up the electron captures start to take effect. The most abundant species becomes more and more neutron-rich. There is a threshold for the maximum possible density for this model, which is about $9 \times 10^9 g/cm^3$. Beyond this density the star would collapse instead of explosion. Right at the edge of the threshold,
there are a lot of $^{48}\text{Ca}$ and $^{50}\text{Ti}$ produced together. Notice that we plot the radioactive species in dash line in this figure.

Figure 2.6 The mass fraction change with initial densities for calculations of the simple type Ia model.

Figure 2.7 shows the mass fraction of radioactive nuclei versus initial density for this simple Ia model. We can see that for low densities ($10^7 - 5 \times 10^8 g/cm^3$) and high densities ($8 \times 10^9 - 9 \times 10^9 g/cm^3$) there are a lot of radioactive nuclide. For inter-medium densities there are few.

Figure 2.8 shows the mass fraction of select species in a mass coordinate. The density-radius profile of the white dwarf is chosen to be a polytrope with polytropic index of 3. We apply
The mass fraction of radioactive nuclei vs. initial densities for calculations of the simple type Ia model.

a central density of $9 \times 10^9 g/cm^3$ in this calculation. (See Appendix F for more information about white dwarf structures.) The horizontal axis is the enclosed mass at a certain radius in solar masses. Zero is the center and the maximum is the surface of the star. We can see that near the center $^{48}\text{Ca}$ and $^{50}\text{Ti}$ are produced abundantly together, while near the surface most of the yields are $^{56}\text{Ni}$, which will decay to $^{56}\text{Co}$ and then $^{56}\text{Fe}$ to provide the light curve of supernovae. In our simple model the whole star is uniform and burnt out thoroughly. In reality and other complicated models, there will be unburned carbon and oxygen at the surface. The neutron-rich materials in the center can be dredged up to the surface and mix with carbon and oxygen. See Chapter 3 for discussion about this.
Figure 2.8 The mass fraction of selected isotopes vs. mass coordinate for a polytropic profile of white dwarf.

Figure 2.9 shows the similar result as shown in Figure 2.8. Just in this calculation we let the star expands half slower. We use the parameter $\alpha$ to vary the hydrodynamic equations. We can see that for a slower expansion, the system has more time to make more neutron-rich isotopes. Comparing to other more realistic supernova models, the slower expansion seems reasonable. This means we may get more neutron-rich isotopes out of the dense type Ia supernova than what we get from the simple model.

In this chapter we described a variety of results from the simple type Ia supernova model. The results show that for dense supernova a significant amount of $^{48}$Ca and $^{50}$Ti can be produced together.
Figure 2.9  The mass fraction of selected isotopes vs. mass coordinates for a polytropic profile of white dwarf, with slower expansion (half of the speed).
CHAPTER 3
CHEMICAL EQUILIBRIUM CONDENSATION

To investigate the possible chemical forms of the ejecta from our simple Ia model, we apply a chemical condensation code. The particular code we use was designed by L. Grossman in 1972 and originally programmed by J. Lattimer in 1978. Now it is maintained by A. Fedkin from University of Chicago and B. S. Meyer from Clemson University. Nucnet Tools \footnote{Nucnet Tools is a set of C/C++ codes useful for studying element formation in stars. For more information, see Appendix I} is integrated into the chemical condensation code to make it easier to access the abundances in zones in the format of xml files. Also the code now is able to include decays during the condensation calculation.

The condensation code calculates the chemical forms of materials assuming the system has enough time to attain equilibrium at given temperature and pressure. To solve for equilibrium abundances, the code equates chemical potentials between species in a fashion similar to nuclear equilibrium [Yu 2010]. Because of the assumption of equilibrium, the code does not include individual chemical reaction rates.

We use our trajectories from the simple Ia model as the input. The condensation code interpolates temperatures and pressures from the input trajectories. As described in Figure 2.5, the radioactive isotopes would heat up the outflows. Due to re-heating, the trajectory may have multiple densities with the same temperature but different times. This causes problems since the condensation code evolves as the temperature cools down and uses the interpolated temperature to get the time. We have modified the code to handle this issue.

3.1 C/O Free Trajectories

In this chapter we use the yields from our Ia models as the input for the composition of the system. Table 3.1 lists some of our results. We tried different initial densities for the Ia model. The most abundant solids for each calculation are listed in atom fractions, which
are defined as the atoms in the chemical form divided by the total atoms in the outflow. The calculations evolves from high temperature to low temperature. The table lists the final chemical forms and the corresponding atom fractions. We see that for these certain conditions, the outflow could condense to alloys or metal nuggets. For low initial density trajectories, iron nugget account for most of the mass. Note that since we allow decays to happen, all $^{56}\text{Ni}$ has been transformed into iron. For higher initial density trajectories, alloys start to dominate. For the trajectory with initial density of $9 \times 10^9 \text{g/cm}^3$ most calcium condenses into a $\beta$ (body-centered-cubic) crystal. In this equilibrium calculation, the calcium atoms starts to condense when the temperature drops to about 600 K. However at this late time (about 100 days after explosion) the density will be low (about $10^{-17}\text{g/cm}^3$), and it is doubtful that calcium atoms can really condense. In this case, the calcium would be ejected as free atoms.

Our interest is in the correlation of Ca and Ti. In these calculations there is no such obvious correlation. It seems that calcium is hard to combine with other metals if there are only metals around as in our yields. Whereas titanium tends to alloy with other metals such as iron and nickel, calcium does not. So pure metal outflows are promising for the Ca-Ti correlation.

These results are from the yields of our simple Ia model. We assumed an ideal white dwarf that the whole star burns out simultaneously and thoroughly. For a real carbon-oxygen white dwarf, there is temperature gradient and there would some unburned carbon and oxygen at the surface layers. If there is some carbon and oxygen mixing in the outflow the final chemical equilibrium forms differ from those calculated here. In the next chapter we will add some carbon and oxygen manually to the input to explore this effect.
<table>
<thead>
<tr>
<th>Density g/cm³</th>
<th>Fe</th>
<th>Si</th>
<th>TiC</th>
<th>Ni₃Ti</th>
<th>Ni</th>
<th>Cr</th>
<th>Co</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 × 10⁸</td>
<td>7.1 × 10⁻¹</td>
<td>1.2 × 10⁻⁶</td>
<td>2.9 × 10⁻⁷</td>
<td>2.5 × 10⁻⁸</td>
<td>5.9 × 10⁻⁷</td>
<td>3.3 × 10⁻²</td>
<td>2.4 × 10⁻¹</td>
</tr>
<tr>
<td>5 × 10⁸</td>
<td>3.6 × 10⁻⁴</td>
<td>7.5 × 10⁻¹</td>
<td>1.4 × 10⁻⁵</td>
<td>8.1 × 10⁻⁵</td>
<td>8.3 × 10⁻⁷</td>
<td>2.4 × 10⁻³</td>
<td>1.6 × 10⁻¹</td>
</tr>
<tr>
<td>2 × 10⁹</td>
<td>1.5 × 10⁻⁸</td>
<td>6.2 × 10⁻¹⁴</td>
<td>2.2 × 10⁻⁷</td>
<td>6.5 × 10⁻⁸</td>
<td>3.1 × 10⁻¹²</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5 × 10⁹</td>
<td>3.8 × 10⁻⁸</td>
<td>4.1 × 10⁻¹⁶</td>
<td>3.8 × 10⁻⁸</td>
<td>6.1 × 10⁻¹⁶</td>
<td>2.7 × 10⁻⁹</td>
<td>3.3 × 10⁻⁷</td>
<td>6.3 × 10⁻³</td>
</tr>
<tr>
<td>7 × 10⁹</td>
<td>3.8 × 10⁻⁸</td>
<td>4.1 × 10⁻¹⁶</td>
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<td>6.3 × 10⁻³</td>
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<td>4.4 × 10⁻⁸</td>
<td>4.4 × 10⁻⁸</td>
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<td>4.4 × 10⁻⁸</td>
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</tr>
<tr>
<td>9 × 10⁹</td>
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<td>4.4 × 10⁻⁸</td>
<td>4.4 × 10⁻⁸</td>
<td>4.4 × 10⁻⁸</td>
<td>4.4 × 10⁻⁸</td>
<td>4.4 × 10⁻⁸</td>
<td>4.4 × 10⁻⁸</td>
</tr>
</tbody>
</table>

Table 3.1: Solid forms for different initial densities of Ia model.
3.2 C/O Trajectories

Nicolas Dauphas et al. (private communication) recently propose that perovskite (CaTiO$_3$) is the carrier of $^{48}$Ca and $^{50}$Ti. We repeated the above calculations with manually added carbon and oxygen in the outflows to observe if there is any change. In reality and in more complicated 3D supernovae models there are unburned carbon and oxygen mixing with the outflows; thus, the test calculation is meaningful.

We take the yield from the trajectory with a density of $9 \times 10^9$ g/cm$^3$ and add extra carbon/oxygen. The percentage of carbon/oxygen indicates the mass fraction of added carbon/oxygen given the original total mass fraction is 1. So the new total mass fraction is greater than unity and the chemical condensation code normalizes it. As we can see in Table 3.2 CaTiO$_3$ is formed and could account for more than 5% of total atoms. We tried several carbon-oxygen mixtures. It shows that the production of perovskite prefers more oxygen and less carbon. Also perovskite starts to condense at about 1500 Kelvin (1350 K for 10%C/10%O and 1865 K for 0%C/10%O). This means there is a chance for the chemical to really form in an environment with a density of about $1 \times 10^{-15}$ g/cm$^3$. Note that perovskite is among the earliest formed condensates.

Also Table 3.2 shows that other than perovskite titanium tends to form carbide while calcium tends to form oxide. If there is only oxygen added and no carbon, calcium will go into perovskite and oxide while titanium will favor the alloy with iron. If there is only carbon and no oxygen titanium will form carbide while calcium will become crystal.

To summarize the condensation test, we compare the two cases: with and without carbon-oxygen in the outflows. For C/O free trajectories, Ca condenses by itself and it happens at low temperature (late time). In this case, there is no obvious correlation with Ti. And as discussed above, at such a late time the density is too low and the condensation may not actually happen. Both are not promising for a Ca-Ti carrier. In the added C/O case, for some certain carbon-oxygen mixtures, we get a condensate (perovskite) that combines Ca and Ti. And it condenses at a high temperature (early time), which means a high density environment. In this case it is possible to really grow such dust grains to some certain size, which will be discussed in Chapter 4.
Table 3.2 Solid forms with manually added carbon and oxygen, for ρ = 9 × 10^9 g/cm^3 trajectory.

<table>
<thead>
<tr>
<th>C</th>
<th>O</th>
<th>Atom fractions</th>
</tr>
</thead>
<tbody>
<tr>
<td>10%</td>
<td>10%</td>
<td>C 8.4 × 10^{-2}</td>
</tr>
<tr>
<td>5%</td>
<td>10%</td>
<td>NiTi 5.8 × 10^{-2}</td>
</tr>
<tr>
<td>10%</td>
<td>5%</td>
<td>TiC 2.1 × 10^{-8}</td>
</tr>
<tr>
<td>10%</td>
<td>5%</td>
<td>CaO 2.4 × 10^{-8}</td>
</tr>
<tr>
<td>5%</td>
<td>5%</td>
<td>FeSi 1.9 × 10^{-8}</td>
</tr>
<tr>
<td>0%</td>
<td>10%</td>
<td>FeC 3.5 × 10^{-8}</td>
</tr>
<tr>
<td>10%</td>
<td>0%</td>
<td>FeTi 1.4 × 10^{-9}</td>
</tr>
<tr>
<td>10%</td>
<td>0%</td>
<td>Ca 2.7 × 10^{-8}</td>
</tr>
<tr>
<td>10%</td>
<td>0%</td>
<td>C 1.8 × 10^{-1}</td>
</tr>
<tr>
<td>10%</td>
<td>0%</td>
<td>NiTi 1.3 × 10^{-1}</td>
</tr>
<tr>
<td>10%</td>
<td>0%</td>
<td>TiC 1.3 × 10^{-1}</td>
</tr>
<tr>
<td>10%</td>
<td>0%</td>
<td>FeTi 1.4 × 10^{-1}</td>
</tr>
</tbody>
</table>

Atom fractions
CHAPTER 4
DUST FORMATION

In Chapter 3, we discussed the chemical forms into which the outflows would condense if the system always attains chemical equilibrium. Equilibrium calculations, however, do not indicate the size of condensates that might grow in type Ia supernova outflows. In this chapter, we study the dynamic dust formation, assuming single type of atom for simplicity.

4.1 Abundance Change

For a reaction:

$$1 + 2 \rightarrow 3 + \gamma$$

we can write the number density change of species $1$ as:

$$\frac{dn_1}{dt} = -\lambda_{12} n_1 n_2 + \lambda_{\gamma} n_3$$

(4.1)

where $\lambda_{12}$ is the reaction rate in the unit of $cm^3 s^{-1}$ and $\lambda_{\gamma}$ is the photo-dissociation rate of species $3$ with the unit of $s^{-1}$.

In a expanding or a collapsing system the number densities change with volume. We would like to study a quantity that does not depend on volume directly so that we use the fraction of each species in number instead of number density:

$$Y_i \equiv \frac{n_i}{n_{total}}$$

(4.2)

where $Y_i$ is called the abundance of species $i$, $n_i$ is the number density of species $i$ and $n_{total}$ is the number density of the unit particles, here the number density of total atoms. So $Y_i$ here indicates the number of species $i$ per atom. And

$$n_{total} = n_{atom} = n_{baryon} \times Y_{atom}$$
where \( n_{\text{baryon}} = \rho N_A \) is the baryon number density and \( Y_{\text{atom}} \) is the atom fraction, i.e. number of atoms per baryon. Take pure \(^{12}\text{C}\) for example, \( Y_{\text{atom}} = 1/12 \). So Eq. (4.1) can be rewrite as

\[
\frac{dY_i}{dt} = -\lambda_{12} n_{\text{atom}} Y_2 + \lambda_3 Y_3 = -\lambda_{12} \rho N_A Y_{\text{atom}} Y_1 Y_2 + \lambda \gamma Y_3
\]

(4.3)

where \( \rho \) is the mass density and \( N_A \) is the Avogadro number. Then what we need to study is how the abundance of each species changes with time.

### 4.2 Condensation Effective Rates

For a single kind of atom, we study the effective condensation rate here. The condensation here means one atom attaches to an existing multi-atom particle:

\[
P_i + P \rightarrow P_{i+1} + \gamma
\]

(4.4)

where \( P_i \) denotes a particle with \( i \) atoms in it. Here we are neglecting the photo-dissociation for large stable particles.

We assume that the condensation rate is proportional to the surface area (or cross section) of the larger particle, which goes like \( N^{2/3} \), i.e.

\[
\lambda \propto A \propto N^{2/3}
\]

or

\[
\lambda_i = \lambda_1 N_i^{2/3}
\]

(4.5)

where \( \lambda \) is the rate, \( A \) is the surface area and \( N \) is the number of atoms in the particle.

To make the calculation of particles with a large atom number possible, we introduce the “bin” after a continuous network. There will a number of particles in a bin and we assume steady state within a bin. The rate out of a bin is like

\[
\lambda_{\text{bin,last}} Y_{\text{bin,last}} = \lambda_{\text{eff,bin}} Y_{\text{bin}}
\]

\[
Y_{\text{bin}} = \sum_{i \in \text{bin}} Y_i
\]

\[
\lambda_{\text{eff,bin}} = \lambda_{\text{bin,last}} \left( \frac{Y_{\text{bin,last}}}{Y_{\text{bin}}} \right)_{ss} = \lambda_{\text{bin,last}} \left( \frac{1}{\sum_{i \in \text{bin}} Y_{\text{bin,last}}} \right)_{ss}
\]
For steady state,
\[
\frac{Y_i}{Y_j} = \frac{\lambda_i}{\lambda_j}
\]
so,
\[
\lambda_{\text{eff}}^{\text{bin}} = \lambda_{\text{bin, last}} \left( \frac{1}{\sum_{i \in \text{bin}} \lambda_{\text{bin, last}} / \lambda_i} \right) = \frac{1}{\sum_{i \in \text{bin}} \lambda_i} = \frac{1}{\sum_{i \in \text{bin}} N_i^{-2/3}}
\]
If we apply the integral approximation,
\[
\lambda_{\text{eff}}^{\text{bin}} \approx \lambda_1 \left( \int_{\text{bin, first}}^{\text{bin, last}} x^{-2/3} \, dx \right)^{-1} = \lambda_1 \frac{1}{N_{\text{bin, last}}^{1/3} - N_{\text{bin, first}}^{1/3}} \quad (4.6)
\]
We estimate \( \lambda_1 \) as the rate at which two single atoms collide together with thermal velocity:
\[
\lambda_1 = <\sigma_1 v> = \pi R^2 \sqrt{3 k_B T / m} \quad (4.7)
\]
where \( \sigma_1 \) is the cross section for a single atom and \( R \) is the radius of a single atom, \( v \) is the thermal velocity which is taken to be the average value in 3 dimensions, \( k_B \) is the Boltzmann constant, \( T \) is the temperature and \( m \) is the mass of a single atom.

For a detailed discussion of an alternative approach to our steady-state assumption, please refer to Appendix [G]. I have not implemented this approach computationally—it is for future work.

### 4.3 Atom Conservation

The abundance change rates of \( Y_{\text{bin}, i} \), \( Y_{\text{bin}, i+1} \) and \( Y_1 \) due to reaction \( \text{Bin}_i + XP_1 \rightarrow \text{Bin}_{i+1} + \gamma \) are
\[
\frac{dY_{\text{bin}, i}}{dt} = -\lambda_{\text{eff}}^{\text{atom}} Y_{\text{bin}, i} Y_1
\]
\[
\frac{dY_{\text{bin}, i+1}}{dt} = \lambda_{\text{eff}}^{\text{atom}} Y_{\text{bin}, i} Y_1
\]
\[
\frac{dY_1}{dt} = X (-\lambda_{\text{eff}}^{\text{atom}} Y_{\text{bin}, i} Y_1)
\]
where \( X \) is the factor to be determined that ensures the total atom number is conserved. Atom conservation requires
\[
N_{\text{bin}, i} \times \frac{dY_{\text{bin}, i}}{dt} + N_{\text{bin}, i+1} \times \frac{dY_{\text{bin}, i+1}}{dt} + \frac{dY_1}{dt} = 0.
\]
So we have

\[ X = N_{\text{bin}, i+1} - N_{\text{bin}, i} \]

Similarly the abundance change rates of \( Y_{\text{last}} \), \( Y_{\text{bin}, 1} \) and \( Y_1 \) due to reaction \( P_{\text{network, last}} + XP_1 \to \text{Bin}_1 + \gamma \) are

\[
\frac{dY_{\text{last}}}{dt} = -\lambda_{\text{last}} n_{\text{atom}} Y_{\text{last}} Y_1 \\
\frac{dY_{\text{bin}, 1}}{dt} = \lambda_{\text{last}} n_{\text{atom}} Y_{\text{last}} Y_1 \\
\frac{dY_1}{dt} = (-\lambda_{\text{last}} n_{\text{atom}} Y_{\text{last}} Y_1) \times (N_{\text{bin}, 1} - N_{\text{last}})
\]

4.4 Network Matrix

Let us look at the reaction between the last species in the continuous network and the first bin, the changes of the Newton-Raphson root-finding functions are (denoting \( n_{\text{atom}} \) as \( n_a \)):

\[
f_{\text{last}} + = \lambda_{\text{last}} n_a Y_{\text{last}} Y_1 \\
f_1 + = (\lambda_{\text{last}} n_a Y_{\text{last}} Y_1)(N_{\text{bin}, 1} - N_{\text{last}})
\]

To find the abundance changes in the continuous network, we need to solve the matrix

\[
AX = B
\]

The matrix element changes due to this reaction are

\[
A_{\text{last, last}} + = \lambda_{\text{last}} n_a Y_1 \\
A_{\text{last, 1}} + = \lambda_{\text{last}} n_a Y_{\text{last}} \\
A_{1, \text{last}} + = (\lambda_{\text{last}} n_a Y_1)(N_{\text{bin}, 1} - N_{\text{last}}) \\
A_{1, 1} + = (\lambda_{\text{last}} n_a Y_{\text{last}})(N_{\text{bin}, 1} - N_{\text{last}})
\]

The right-hand-side vector changes are

\[
B_{\text{last}} + = -f_{\text{last}} = -\lambda_{\text{last}} n_a Y_{\text{last}} Y_1 \\
B_1 + = -f_1 = -(\lambda_{\text{last}} n_a Y_{\text{last}} Y_1)(N_{\text{bin}, 1} - N_{\text{last}})
\]
Now we look at the reactions between bins. Bin\(_i\) + (\(N_{bin,i+1} - N_{bin,i}\))\(P_1\) → Bin\(_{i+1}\), where \(i\) goes from 1 to \(N - 1\) with \(N\) as the number of bins.

\[
\left(\frac{dY_1}{dt}\right)_i = (-\lambda_{bin,i}^{eff} n_a Y_{bin,i} Y_1)(N_{bin,i+1} - N_{bin,i})
\]

\((f_1)_i \leftrightarrow (\lambda_{bin,i}^{eff} n_a Y_{bin,i} Y_1)(N_{bin,i+1} - N_{bin,i})
\]

\((A_{1,1})_i \leftrightarrow (\lambda_{bin,i}^{eff} n_a Y_{bin,i})((N_{bin,i+1} - N_{bin,i})
\]

\((B_1)_i \leftrightarrow -(f_1)_i = -(\lambda_{bin,i}^{eff} n_a Y_{bin,i} Y_1)(N_{bin,i+1} - N_{bin,i})
\]

We first solve the matrix equation for current \(Y_{bin,i}\), and then compute the abundance changes in bins using the new abundances in the network (as showed below). Then feed the new bin abundances back to the matrix. We iterate until convergence.

### 4.5 Bin Abundances Change

Now we consider the abundance changes in bins for each reaction discussed above. We are going to solve these changes implicitly. For \(Y_{bin,1}\),

\[
\frac{Y_{bin,1}(t + \Delta t) - Y_{b1}(t)}{\Delta t} = \lambda_{last} n_a Y_{last}(t + \Delta t)Y_1(t + \Delta t) - \lambda_{bin,1}^{eff} n_a Y_{bin,1}(t + \Delta t)Y_1(t + \Delta t)
\]

\[
Y_{bin,1}(t + \Delta t) = \frac{\lambda_{last} n_a Y_{last}(t + \Delta t)Y_1(t + \Delta t)\Delta t + Y_{bin,1}(t)}{1 + \lambda_{bin,1}^{eff} n_a Y_1(t + \Delta t)\Delta t}
\]

Similarly for \(Y_{bin,i}\) as \(i\) goes from 2 to \(N - 1\):

\[
Y_{bin,i}(t + \Delta t) = \frac{\lambda_{bin,i-1}^{eff} n_a Y_{bin,i-1}(t + \Delta t)Y_1(t + \Delta t)\Delta t + Y_{bin,i}(t)}{1 + \lambda_{bin,i}^{eff} n_a Y_1(t + \Delta t)\Delta t}
\]

For \(Y_{bin,N}\) we don’t have any destructive terms for now,

\[
Y_{bin,N}(t + \Delta t) = \lambda_{bin,N-1}^{eff} n_a Y_{bin,N-1}(t + \Delta t)Y_1(t + \Delta t)\Delta t + Y_{bin,N}(t)
\]

With the set up describe above we are able to calculate the dust growth to large size. Figure 4.1 shows the dust size distribution with the application above. In this calculation we just use a generic type of atom and let them collide with each other to grow. The trajectory is from our simple Ia model with initial density of \(9 \times 10^9 g/cm^3\). In this figure we can see that
the number of atoms in a molecule can go up to $10^7 - 10^8$, which corresponds to a dust grain size of about 0.05 microns. Notice we are using the bins to calculate large molecules.

From Chapter 3, we saw that our high density type Ia supernova trajectory could condense perovskite if there is carbon and oxygen present. From the results in this chapter, we might expect that perovskite to be of the order 0.01 to 0.1 microns in size. A serious question is whether such perovskite grains could survive the shocks present in the exploding star, but, if so, these grains could carry coupled $^{48}$Ca and $^{50}$Ti into the solar system and give rise to the isotopic signatures in FUN CAIs.

Appendix G provides a more detailed discussion on large dust growth using graph theory.

For more details on dust growth in a core-collapse supernova, and especially the reaction network at low atom number, see Appendix H.
Figure 4.1 Dust size distribution for a Ia trajectory.
Galactic Chemical Evolution (GCE) is the study of the evolution of gas into stars and of the chemical composition of a galaxy. Various species are generated during stellar evolution. Some of them will be locked into low mass stars, which evolve slowly, or into compact objects which are left behind stellar explosive events. Some of them will be ejected into the interstellar medium (ISM) and become the ingredients of the next generation of stars. The newer generation of stars will then be enriched, relative to the previous generation, in heavier species like carbon and oxygen. These so called primary species will alter the evolution path of stars and help produce secondary species, which can only be synthesized when some certain primary species are present. Both primary and secondary species will travel through the Galaxy and get together with others to collapse to form new stars. So the chemical composition of stars depends on how the species travel and what chemical form they are in. Studying the chemical composition of current and early solar system will help us understand the chemical evolution history of the galaxy.

Figure 5.1 shows a basic diagram of GCE. The schematic graph gives the simple relationship between Galactic Halo Gas, Disk Gas and Stars. The infall of halo gas $f(t)$ feeds the disk gas which in turn will form stars with a timescale $\tau_s$. When stars die they will return part of their mass to the disk gas or interstellar medium with a rate of $R/\tau_s$, where $R$ is the return fraction. The simple graph demonstrates how the yields from previous stars become the ingredient of the next generation of stars.

Figure 5.2 emphasizes the role of rare type Ia supernovae in the GCE. The specific yields from such rare Ia may form dust with fingerprints of these rare Ia supernovae. Also the Ias will interact with regular gas and Ia dust. Some of the rare Ia dusts may go into stars which will bring in the heterogeneity of the neutron-rich iron-group isotopes.
Models of GCE can be simple or sophisticated. At minimum, a GCE model requires stellar properties and yields, a stellar initial mass function (IMF), a star formation rate (SFR), and gaseous flows. Included in realistic stellar yields should be the contribution of rare type Ia supernovae that likely make $^{48}\text{Ca}$. An even more sophisticated model would include the chemical form in which the isotopes traverse the Galaxy. These details are beyond the scope of the present thesis; however, we do have some preliminary ingredients, as computed in chapters 2 and 4. This allows us to make a rough estimation of the CAI formation with heterogeneous neutron-rich iron-group isotope inputs due to the rareness of dense type Ia supernovae.

![Diagram of Galactic chemical evolution]

Figure 5.1 Simple model of Galactic chemical evolution. Galactic halo gas falls in with rate $f(t)$ to form the Galactic disk. Stars form from the disk gas on the timescale $\tau_*$ while stars return gas to the disk with the rate $R/\tau_*$, where $R$ is the return fraction.

From Figure 2.8 and 2.9 we can estimate an average yield as the input of the ingredient composition. The mass fractions of Calcium and Titanium that we are interested in are listed
Figure 5.2  An extension of the simple Galactic chemical evolution model in Figure 5.1 to include rare type Ia supernovae and a reservoir of dust from such supernovae. $\tau_{Ia}$ is the timescale for the rare type Ia supernova, and $\tau_d$ is the interstellar dust destruction timescale. $f_d$ and $f_g$ are the fraction of mass ejected from rare Ia events that go, respectively, into dust and gas.

The average solar abundances are from [Lodders 2003]. Then we can create two reservoirs. One is with the Ia yield abundances. The abundances of the other can be calculated to make the combination to be solar abundances, given the mass fraction of $^{48}$Ca is
Table 5.1  Calcium and Titanium isotope mass fractions for solar system and Ia yields

<table>
<thead>
<tr>
<th>Species</th>
<th>Solar</th>
<th>Ia yield</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{48}\text{Ca}$</td>
<td>$1.38 \times 10^{-7}$</td>
<td>$6.14 \times 10^{-5}$</td>
</tr>
<tr>
<td>$^{40}\text{Ca}$</td>
<td>$5.99 \times 10^{-5}$</td>
<td>$4.32 \times 10^{-4}$</td>
</tr>
<tr>
<td>$^{50}\text{Ti}$</td>
<td>$1.64 \times 10^{-7}$</td>
<td>$2.60 \times 10^{-3}$</td>
</tr>
<tr>
<td>$^{48}\text{Ti}$</td>
<td>$2.15 \times 10^{-6}$</td>
<td>$9.87 \times 10^{-6}$</td>
</tr>
</tbody>
</table>

zero. Figure 5.3 shows a result of the anomalies that would result from different mixtures of the two reservoirs.

The results in Figure 5.3 assume the type Ia reservoir is completely characterized by the full yield. In fact, as seen in chapter 3, we might expect only a fraction of the ejected matter to enter this reservoir. This, plus the fact that this calculation does not include modification of the reservoir by dust destruction and growth processes in the interstellar medium, means these results are quite preliminary.
Figure 5.3  Correlation between $^{48}$Ca and $^{50}$Ti for a two reservoir calculation.
FUN CAIs show roughly correlated excesses and deficits in the neutron-rich iron-group isotopes such as $^{48}\text{Ca}$ and $^{50}\text{Ti}$. In this thesis we are trying to understand and propose a possible explanation of these effects.

From nucleosynthesis we know that these neutron-rich iron-group isotopes tend to be formed in low-entropy expansions of neutron-rich matter, which probably occur in dense Type Ia supernovae. We followed the nucleosynthesis with simple but realistic models of dense Type Ia supernovae and confirmed the production of these isotopes in inner zones of supernovae. The density near the center of the exploding white dwarf can be very high ($\sim 9 \times 10^9 \text{g/cm}^3$) so that the electron capture rates get really large leading to more neutronization and the formation of $^{48}\text{Ca}$ and $^{50}\text{Ti}$. Supernovae with such a dense core are rare ($\sim 2\%$ of total Type Ia’s), but they produce large quantities of these isotopes (a few percent in mass) once it occurs. Our models expand faster than some of the more realistic 3-dimension models. We tried slower expansion and found that more time for electron capture makes more such neutron-rich isotopes. So these rare dense Type Ia supernovae are good candidates for the source of these neutron-rich iron-group isotopes.

Then we applied the chemical condensation code to explore the outcome chemical forms of the expanding matter from the supernovae. The code assumes equilibrium in the system which is not the real case. But it shines a light on what may happen during the expansion. With unburned carbon and oxygen mixed in the outflows, we found that perovskite ($\text{CaTiO}_3$) would condense at an early time and a high temperature (about 1500 Kelvin). Perovskite is among the first few to condense. This means it is highly possible that this condensate is really formed during the expansion. Perovskite contains calcium and titanium together which makes it a perfect carrier of these neutron-rich isotopes.

To estimate the dust grain size this perovskite can grow we built a generic atom model. We applied the graph theory to bin the dust of large atom numbers with effective rates. Our
finding is that the number of atoms in a molecule can grow up to $10^7 - 10^8$ which corresponds to a dust grain size of about 0.05 microns.

From the results above, we might expect that perovskite to be of the order 0.01 to 0.1 microns in size. If such perovskite grains could survive the shocks present in the exploding star, these grains could carry coupled $^{48}\text{Ca}$ and $^{50}\text{Ti}$ into the solar system. Since these grains are rare and of large amount of these isotopes, they will bring the heterogeneous isotopic composition to the early solar system and give rise to the isotopic signatures in FUN CAIs.

Our conclusion is that the rarity of the dense Type Ia’s is reflected in the FUN CAIs. More detailed Galactic Chemical Evolution simulations in the future would make the statement even stronger.
Appendix A

Chondrites

Chondrites are stony meteorites that have round grains "chondrules" in them. See Figure A.1 for example. It is a slice from the Allende meteorite. These chondrules seem survived from the melting process and retain their original composition.

Figure A.1 A slice from the 4.5-billion-year-old Allende meteorite. This rock was formed along with the solar system. Figure from wikipedia. (http://en.wikipedia.org/wiki/File:Allende_meteorite.jpg)
CI chondrites, a small group of meteorites, have the most primitive compositions, meaning that physical and chemical processes that formed the meteorites did not significantly change their elemental compositions. This conclusion comes from plots like Figure A.2, which shows the abundances of elements in CI chondrites versus the abundance in solar photosphere. Elements on the solid line in Figure A.2 are present in the same abundance in the Sun and in CI chondrites. Except for those volatile elements that exist in the gas phase at room temperature and elements that were burned out of the Sun by the first stages of nuclear burning (like Li), essentially all elements are with the same relative abundance in the Sun and the CI chondrites. Since most of the meteorites were from the collisions of asteroids, which are generally small and have not experienced significant fractionation like the Earth, this correlation clearly indicates that the mixing during the early stages of the solar system was quite efficient.

Meteorite experimental works provide another way to explore the composition of the Solar System. Not only these works can be performed very accurate (in fact most of the solar abundances are obtained from meteorite measurement), they also give the isotopic information which can hardly be extracted from the spectra of the Sun’s photosphere. Studying chondrites and other extraterrestrial objects such as presolar grains and star dusts will give us more knowledge about the outer space besides the astronomical observation.
Figure A.2  Elemental abundances in CI chondrites compared to abundances in the solar photosphere. For comparison purposes, the abundance of Si is set at $10^6$ Si. The bulk compositions of the CI chondrites and the solar photosphere show an amazing correlation, with a few key exceptions. Combined, these data sets provide our best estimate for bulk solar elemental abundances. H and the noble gases are not shown. Figure and caption from Lauretta, A Cosmochemical View of the Solar System, Elements, Vol. 7, PP. 11-16.
Appendix B
Fractionation

Although the mixing in the early solar system was very efficient, the compositions of different objects nowadays are quite different. This is because most of the objects in our solar system have experienced various fractionation, both elementally and isotopically, to different extent.

B.1 Elemental Fractionation

The Earth’s atmosphere is an example of element fractionation. It is abundant in nitrogen and oxygen (in the form of N\textsubscript{2} and various oxygen molecules such as O\textsubscript{2} and ozone) and significantly depleted in hydrogen and helium. This is because the gravity of Earth is strong enough to retain the former species but any H\textsubscript{2} or He introduced into the Earth’s atmosphere leaks out into space on geological time scales. Another example is the Earth’s core/mantle separation. Iron and nickel, due to their high density, preferentially sank to the core during the Earth’s molten phase while silicates preferentially floated to the surface. The Earth thus has a Fe/Ni core and a silicon rich mantle. Chemistry and gravity combine to separate the elements strongly in planets.

B.2 Isotopic Fractionation

By contrast, isotopic fractionation is generally small in planetary samples. There are many processes that cause isotopic fractionation, and they are generally characterized as mass dependent or mass independent. An example of a mass-dependent process is water vapor condensation in a rain cloud. It is an experimental rule of thumb that, in equilibrium, the denser the phase of a material, the more it tends to be enriched in the heavier isotopes of a constituent element. Thus, in equilibrium, ice will tend to be enriched in $^{18}$O compared to liquid water and liquid water will be enriched in $^{18}$O compared to vapor. Thus, a rain drop will tend to be rich in $^{18}$O relative to the vapor it condenses from.

Another mass-dependent fractionation process is kinetic fractionation, which occurs when chemical reactions occur out of equilibrium, especially when the reaction products become physically separated from the reactants. For example, if a rock melts, the lighter isotopes of
silicon might escape (as silicate molecules) preferentially because they are lighter and move faster than silicates containing heavier silicon atoms.

An example of mass-independent fractionation is self-shielding of CO. If UV radiation impinges on a cloud of CO, the cloud will be thicker to C\textsuperscript{16}O than to C\textsuperscript{17}O or C\textsuperscript{18}O because the \textsuperscript{16}O is so much more abundant (that the other two isotopes. Deep in the core of the cloud, then, the UV intensity at the frequencies that can dissociate C\textsuperscript{16}O are much reduced compared to those than can dissociate C\textsuperscript{17}O or C\textsuperscript{18}O. We could thus expect \textsuperscript{17}O and \textsuperscript{18}O to preferably be in atomic form deep in the cloud core. If some other chemical process locks up the oxygen into, say, ice, that ice will be preferentially enriched in the heavy isotopes of oxygen. This process has been proposed as the source of the 5% enrichment in the heavy isotopes of oxygen in Earth’s ocean water compared to the inferred isotopic composition of the Sun.

We know from the presolar grains recovered from primitive meteorites that much of the ejecta from these stars were highly anomalous in their isotopic composition compared to the Solar System average composition.

B.3 Oxygen

Oxygen isotope abundance variations in meteorites are very useful in elucidating chemical and physical processes that occurred during the formation of the solar system [Clayton 1993].

Fig. B.1 shows the oxygen three isotope plot. The $\delta^{18}$O notation is defined as (like Eq. ??, same for \textsuperscript{17}O):

\[
\delta^{18}O = \left[ \frac{(18O/16O)_{sample}}{(18O/16O)_{standard}} - 1 \right] \times 1000
\] (B.1)

The SMOW stands for Standard Mean Ocean Water. The CAIs lie on the slope 1 line, while the Earth and Moon lie on the slope 0.5 line and they are \textsuperscript{17,18}O-rich compared to the CAIs and apparently the Sun, which lies at the left bottom conner. The evolution path of oxygen isotopes seem to be like this: it starts from the left bottom conner and spreads along the slope 1 line due to self-shielding (mass-independent). (see Sec. B.2) The different positions of CAIs along the line indicate their formation sites in the solar nebula. For the terrestrial objects they share the similar initial oxygen isotope ratio and spread along the slope 0.5 line.
due to mass-dependent fractionation. See Sec. B.4 for a rough estimation. It’s just like Robert Clayton’s words, “the Sun is not anomalous, you are!”

CAIs seem to be condensates from the solar gas and are $^{16}$O-rich. Also the FUN CAIs do not seem to be much different in their oxygen from the “regular CAIs”, although they lie on a slope 0.5 fractionation line with regular CAIs.

**B.4 Derivation of Slope 0.5 Line**

To simply illustrate the idea of fractionation, we consider an oxygen atom at one end of a spring (in molecules). The oscillation energy is then proportional to the frequency $\omega$:

$$E \propto \omega \sim \sqrt{\frac{1}{m}} \quad (B.2)$$

The last step has applied the harmonic oscillation approximation.

For oxygen there are three stable isotopes: $^{16}$O, $^{17}$O, $^{18}$O. So

$$\sqrt{\frac{1}{m}} = \sqrt{\frac{1}{m_{16} + \Delta m}} = \sqrt{\frac{1}{m_{16}} \left(1 + \frac{\Delta m}{m_{16}}\right)^{-1/2}} = \sqrt{\frac{1}{m_{16}} \left(1 - \frac{\Delta m}{2m_{16}}\right)}$$

where $\Delta m = 0$ for $^{16}$O, 1 for $^{17}$O and 2 for $^{18}$O, in the unit of atomic mass unit (roughly). The last step is for $\Delta m \ll m_{16}$. For energy we have:

$$E = E_{16} \left(1 - \frac{\Delta m}{2m_{16}}\right)$$

For Maxwell-Boltzmann distribution, we can write the number ratio of $^{17}$O to $^{16}$O as:

$$\frac{^{17}O/^{16}O_{\text{standard}}}{^{16}O/^{16}O_{\text{standard}}} = \frac{e^{-E_{17}/kT}}{e^{-E_{16}/kT}} = e^{\exp \left[\frac{E_{16}}{kT} \frac{\Delta m}{2m_{16}}\right]} = 1 + \frac{E_{16} \Delta m}{kT 2m_{16}}$$

In the last step the oscillation energy could be considered similar to $kT$ and $\Delta m \ll m_{16}$ is applied. The $\delta$ notation is usually defined as:

$$\delta^{17}O = \left[\frac{(^{17}O/^{16}O)_{\text{sample}}}{(^{17}O/^{16}O)_{\text{standard}}} - 1\right] \times 1000$$

So for two samples, we have

$$\delta^{17}O_2 - \delta^{17}O_1 = \frac{(^{17}O/^{16}O)_2}{(^{17}O/^{16}O)_{\text{standard}}} - \frac{(^{17}O/^{16}O)_1}{(^{17}O/^{16}O)_{\text{standard}}} \times 1000 = \frac{\Delta m}{2m_{16}} \left[\left(\frac{E_{16}}{kT}\right)_2 - \left(\frac{E_{16}}{kT}\right)_1\right] \times 1000$$
Figure B.1  Oxygen three-isotope plot showing representative compositions of major primary components of solar system matter, the solar wind (SW), and our preferred value for the Sun. All data fall predominantly on a single mixing line characterized by excesses (lower left) or depletions (upper right) of 16O relative to all samples of the Earth and Moon. Plotted are the most 16O-enriched solar system samples: an unusual chondrule (47); individual platy hibonite grains (55), which are ultra-refractory oxides from carbonaceous chondrites (CC); water inferred to have oxidized metal to magnetite (56) in ordinary chondrites (OC); very 16O-depleted water from the CC Acfer 094 (3), and whole CAIs from CC (19); and chondrules from CC and OC (19), bulk Earth (mantle), and Mars (SNC meteorites). The mass-dependent fractionation trajectory of primary minerals in FUN inclusions and the pure 16O (slope 1.0) line (57) are also shown. Figure and caption from McKeegan et al. 2011

So the slope is:

\[
\frac{\delta^{17}O_2 - \delta^{17}O_1}{\delta^{18}O_2 - \delta^{18}O_1} = \frac{\Delta m_{17}}{\Delta m_{18}} = \frac{1}{2}
\]
Appendix C

Chronology

Determining the ages of events and placing them in chronological order constitutes one of the major areas of research in cosmochemistry. There are several different approaches to determine the timing of events. Among them radiometric age dating is a powerful chronological tool.

The number of decays in a given period of time is proportional to the number of atoms present:

$$- \frac{dN}{dt} = \lambda N$$  \hspace{1cm} \text{(C.1)}

where $\lambda$ represents the probability that an atom will decay within a stated period of time and $\lambda N$ gives the rate of decay at a time. The numerical value of $\lambda$ is unique for each radionuclide and is expressed in units of reciprocal time. If we integrate Eq. (C.1) we get the remaining number of atoms at time $t$:

$$N = N_0 e^{-\lambda t}$$  \hspace{1cm} \text{(C.2)}

where $N_0$ gives the starting number of atoms at time $t = 0$.

The number of daughter atoms ($D^*$) produced by the decay of the parent isotope at any given time is

$$D^* = N_0 - N = N(e^{\lambda t} - 1)$$  \hspace{1cm} \text{(C.3)}

In most natural systems, the number of atoms of the daughter nuclide ($D$) consists of initial atoms already present in the system ($D_0$) plus those resulting from radioactive decay ($D^*$):

$$D = D_0 + D^* = D_0 + N(d^{\lambda t} - 1)$$  \hspace{1cm} \text{(C.4)}

Both $D$ and $N$ are measurable quantities and $D_0$ is a constant whose value can either be assumed or calculated from other data. Solving the equation above for $t$ gives the data:

$$t = \frac{1}{\lambda} \ln \left[ \frac{D - D_0}{N} + 1 \right]$$  \hspace{1cm} \text{(C.5)}

---

1 This appendix is based on Cosmochemistry, Harry Y. McSween, Jr. and Gary R. Huss, Cambridge 2010.
There are several requirements that need to be met to make sure that the radiometric date provides a valid age.

1. A specific event is required that homogenized the isotopic compositions of the parent and daughter element. It assures that additions to the amount of daughter isotope reflect only parent element and the time passed.

2. The system, e.g. a rock or mineral, must remain closed.

3. The decay constant ($\lambda$) must remain constant over the age of the solar system and the galaxy, and be accurately known.

4. The initial abundance of the daughter element $D_0$ is possible to assign with a realistic value.

With the formalism discussed above, one can study a wide variety of systems to produce a radiometric date.

C.1 Half-life

The rate of decay of a radionuclide is often described in terms of its half-life. The half-life ($T_{1/2}$) is the time required for one-half of a given number of radioactive atoms to decay. So

$$\frac{1}{2}N_0 = N_0 e^{-\lambda T_{1/2}} \quad (C.6)$$

$$T_{1/2} = \frac{\ln 2}{\lambda} = \frac{0.693}{\lambda} \quad (C.7)$$

Note that the half life is smaller than the mean life $\tau$:

$$\tau = \frac{1}{\lambda} = \frac{T_{1/2}}{0.693} \quad (C.8)$$

C.2 Long-lived Radionuclides

Long-lived radionuclides are those with half-lives long enough that still a significant fraction of the original atoms in the early solar system are present today. Long-lived radionuclides can give absolute ages of events back to the formation of the solar system.

Let’s take lead-lead dating as an example to demonstrate how it works. Lead-lead dating is a method for dating geological samples, normally based on ‘whole-rock’ samples of material such as granite. It is important for dating meteorites and the age of the Earth.
Uranium has two long-lived isotopes, $^{235}\text{U}$ and $^{238}\text{U}$, that decay to $^{207}\text{Pb}$ and $^{206}\text{Pb}$, with half-lives of $0.7038 \times 10^9$ years and $4.468 \times 10^9$ years respectively:

$$^{238}\text{U} \rightarrow ^{206}\text{Pb} + 8^4\text{He} + 6\beta^- \quad (C.9)$$

$$^{235}\text{U} \rightarrow ^{207}\text{Pb} + 7^4\text{He} + 4\beta^- \quad (C.10)$$

With the progress of time, $^{206}\text{Pb}$ and $^{207}\text{Pb}$ accumulate as the parent isotopes decay at a constant rate. While $^{204}\text{Pb}$ stays the same as it is the only non-radiogenic lead isotope. So the ratio of radiogenic Pb versus non-radiogenic Pb shifts with time:

$$\frac{^{207}\text{Pb}}{^{204}\text{Pb}} = \left(\frac{^{207}\text{Pb}}{^{204}\text{Pb}}\right)_0 + \frac{^{235}\text{U}}{^{204}\text{Pb}} \left(e^{\lambda_{235}t} - 1\right) \quad (C.11)$$

$$\frac{^{206}\text{Pb}}{^{204}\text{Pb}} = \left(\frac{^{206}\text{Pb}}{^{204}\text{Pb}}\right)_0 + \frac{^{238}\text{U}}{^{204}\text{Pb}} \left(e^{\lambda_{238}t} - 1\right) \quad (C.12)$$

The $^{207}\text{Pb}*/^{206}\text{Pb}*\text{ ratio}$ is insensitive to recent fractionation between parent and daughter elements caused either by natural process or by laboratory treatments such as chemical etching. Uranium-235 decays six times faster than $^{238}\text{U}$ and only about 1% of the original abundance of $^{235}\text{U}$ in the solar system is still present. This means that the $^{207}\text{Pb}*/^{206}\text{Pb}*\text{ ratio}$ evolved rapidly during the early stage of the solar system. Therefore the precision of the date obtained from the $^{207}\text{Pb}*/^{206}\text{Pb}*\text{ ratio}$ increases with the age of the sample.

The equation for the $^{207}\text{Pb}*/^{206}\text{Pb}*\text{ isochron}$ can be obtained by combining Equations C.11 and C.12:

$$\frac{^{207}\text{Pb}}{^{204}\text{Pb}} - \frac{^{207}\text{Pb}}{^{204}\text{Pb}}_0 = \frac{^{235}\text{U}}{^{238}\text{Pb}} \left[\frac{e^{\lambda_{235}t} - 1}{e^{\lambda_{238}t} - 1}\right] \quad (C.13)$$

where $^{235}\text{U}/^{238}\text{U} = 1/137.88$. If the $^{238}\text{U}$-$^{206}\text{Pb}$ and $^{235}\text{U}$-$^{207}\text{Pb}$ dates are concordant, this equation represents a family of straight lines (isochrons) with slopes of

$$m = \frac{1}{137.88} \left[\frac{e^{\lambda_{235}t} - 1}{e^{\lambda_{238}t} - 1}\right] = \left(\frac{^{207}\text{Pb}^*}{^{206}\text{Pb}}\right)_0 \quad (C.14)$$

and pass through the point

$$\left(\frac{^{207}\text{Pb}}{^{204}\text{Pb}}\right)_0, \left(\frac{^{206}\text{Pb}}{^{204}\text{Pb}}\right)_0$$
The determination of an age using the Pb-Pb isochron method relies on the assumption that all samples that define the isochron had the same initial lead isotopic composition, formed at the same time and remained close to uranium and lead until the very recent past.

![Pb-Pb Isochron](Pb-Pb Isochron.png)  
**Figure C.1** After the Pb-Pb isochron used by Patterson (1956). The diagram represented a major breakthrough in the use of lead isochrons when it was published in 1956. It presented the analysis of three stony meteorites and two iron meteorites. It shows that they fell on the same isochron. It also shows that a sample of modern ocean sediment fell on the same isochron. The isochron age reported by Patterson was 4.55 Giga years (Gy), and it becomes 4.48 Gy when applying the revised decay constants for the isotopes involved. Figure and caption from http://hyperphysics.phy-astr.gsu.edu/hbase/nuclear/pbpb.html

In Figure C.1 we can see that for different samples they have different initial U/Pb ratio. But the radiogenic non-radiogenic Pb ratios fall on a straight line for the same age. Using the slope then we can determine the age of the Earth. Since $^{235}$U decays to $^{207}$Pb faster, the growth curve is like the one shown in the figure.

### C.3 Short-lived Radionuclides

The short-lived radio-nuclide $^{26}$Al (half life 0.73 million years, decay to $^{26}$Mg) was found in CAIs. The ratio of the daughter isotope to a stable isotope of the same element
(\frac{^{26}\text{Mg}}{^{24}\text{Mg}} \text{ in Fig. C.2}) \text{ increases as the radioactive isotope decays. Because of its short half life, the existence of } ^{26}\text{Al in CAIs is the evidence that it was alive in the early solar system. And due to the short time scale, it provides a high resolution way to study the early history of the solar system.}

\begin{align*}
\frac{^{26}\text{Mg}}{^{24}\text{Mg}} &= \frac{^{26}\text{Mg}_0}{^{24}\text{Mg}} + \frac{^{26}\text{Mg}^*}{^{24}\text{Mg}} = \frac{^{26}\text{Mg}_0}{^{24}\text{Mg}} + \frac{^{26}\text{Al}}{^{27}\text{Al}} \frac{^{27}\text{Al}}{^{24}\text{Mg}}
\end{align*} \quad (C.15)

An interesting phenomenon is that \(^{26}\text{Al}\) and neutron-rich iron-group anomalies seem “mutually exclusive” (Andy Davis’s words). In FUN CAIs there is little \(^{26}\text{Al}\), but it shows excesses and deficits in n-rich iron-group isotopes, which is not found in regular CAIs. Then the question comes out: Did the FUN CAIs form before \(^{26}\text{Al}\) came into the Solar System, or was the \(^{26}\text{Al}\) heterogeneously distributed?
Magnesium isotopic ratios measured in different minerals with different ratios of aluminum to magnesium from a refractory inclusion in the meteorite Allende. Magnesium shows excesses in the isotope $^{26}\text{Mg}$ that are correlated with the aluminum/magnesium ratio, indicating that the $^{26}\text{Mg}$ excesses originated from the decay of the radioactive isotope $^{26}\text{Al}$. This finding is evidence for the initial presence of $^{26}\text{Al}$ in early solar system objects. [Lee et al. 1976]
Appendix D

Production of $^{48}$Ca

The short beta-decay half of $^{45}$Ca (162.2 days) and even shorter half of $^{47}$Ca (4.536 days) prevent $^{48}$Ca from being produced in the same environment. The site of $^{48}$Ca synthesis is suspected to be a subset of thermonuclear supernovae (type Ia supernovae) that achieve high enough densities to have significant electron capture during the explosion (e.g., [Meyer et al. 1996 | Woosley 1997]). Because the matter in these explosions has low entropy per nucleon (typically less than 0.1 $k_B$, where $k_B$ is Boltzmann’s constant, per nucleon), the nuclear abundances are characterized by an overabundance of heavy nuclei relative to nuclear statistical equilibrium. This permits production of abundant $^{48}$Ca when nuclear statistical equilibrium would require even larger production of $^{66}$Ni, an isotope with nearly the same degree of neutron richness [Hartmann et al. 1985].

Neither s-process (slow-neutron-capture-process) nor r-process (rapid-neutron-capture-process) nucleosynthesis could produce $^{48}$Ca, as shown in the network flow diagrams below.

Figure D.1 to Figure D.4 show a typical s-process calculation. The s-process is a nucleosynthesis process that occurs at relatively low neutron density and intermediate temperature conditions in stars. At such conditions the decay rates are faster than the neutron capture rates so that the radioactive nuclei do not have enough time to capture another neutron to make heavier isotopes before they decay away. In this calculation we applied a constant density of 1500 g/cm$^3$ and a constant temperature of 0.2 billion K. In the figures the proton numbers of nuclei increase vertically and neutron numbers horizontally. The yellow isotopes are stable, while white ones are radioactive. The three green ones are also stable and are the neutron-rich iron-group isotopes that we are interested in. We put $^{38}$Ar and $^{60}$Fe as anchors to keep the graph consistent. We can see from the figures that the reaction flow does not pass $^{48}$Ca due to the short decay time of $^{45}$Ca and $^{47}$Ca. Whereas $^{50}$Ti and $^{54}$Cr are in the pathway.

Figure ?? and Figure ?? show a typical r-process calculation. The r-process is an nucleosynthesis process that occurs in core-collapse supernovae and is responsible for the creation of approximately half of the neutron-rich atomic nuclei heavier than iron. The environment is of high neutron density and high temperature so that the neutron capture rates are much faster.
than the decay rates. In this calculation we applied an initial density of about $3 \times 10^5$ g/cm$^3$ and an initial temperature of about 7 billion K and let the materials expand and cool down. The colors of species are of the same meanings as in Figure D.1. The three green ones are still $^{48}$Ca, $^{50}$Ti and $^{54}$Cr. We can see that the nuclei are pushed to the right (neutron-rich) and decay back later. There is no significant radiogenic $^{48}$Ca produced.

So neither of these two major nucleosynthetic sites are responsible for the production of $^{48}$Ca.
Figure D.2  S-process production 2

time(\text{yr}) = 1.259 \times 10^4  \quad T_0 = 0.2  \quad \rho(\text{g/cm}) = 1500  \quad \text{flow}_{\text{avg}} = 1.722 \times 10^{-17}

Figure D.3  S-process production 3

time(\text{yr}) = 7.157 \times 10^4  \quad T_0 = 0.2  \quad \rho(\text{g/cm}) = 1500  \quad \text{flow}_{\text{avg}} = 3.1 \times 10^{-18}
Figure D.4  S-process production 4
Figure D.6  R-process production 2
Appendix E

Weak Nuclear Statistical Equilibrium and the Production of Neutron-Rich Iron-Group Isotopes

This work is by Tianhong Yu and Bradley S. Meyer [PoS(NIC XII)213].

E.1 Abstract

Calcium-48, $^{50}$Ti, and $^{54}$Cr are neutron-rich iron-group isotopes that show roughly correlated excesses and deficits in certain calcium-aluminum-rich inclusions (CAIs) in primitive meteorites. These isotopes are produced in high-temperature, low-entropy-per-nucleon environments such that the nuclear population are governed by a quasi-statistical equilibrium with too many heavy nuclei compared to nuclear statistical equilibrium. Such environments are present in dense thermonuclear (Type Ia) supernovae. Production of these isotopes also requires an electron fraction $Y_e$ approximately equal to 0.42, which is set by electron captures during the explosion. We use NucNet Tools, an open-source suite of tools for nucleosynthesis, to study nucleosynthesis in high-density, low-entropy environments appropriate for Type Ia supernovae and follow the neutronization of the matter by weak interactions. We study how the nuclear populations evolve towards and into dynamical weak statistical equilibrium. Realistic expansion timescales for dense Type Ia supernova matter do not allow the material to reach dynamical weak statistical equilibrium. Nevertheless, such expansions are able to generate low enough $Y_e$ to produce $^{48}$Ca. The conditions in these expansions are extreme and thus probably rare in Galactic history, but, when they do occur, they produce copious amounts of $^{48}$Ca and the other neutron-rich species. For this reason, it is likely that the abundance of these isotopes in interstellar dust is quite heterogeneous. Because the CAIs formed from interstellar dust precursors, they inherited this heterogeneity.

E.2 Introduction

Primitive Solar System hibonites and FUN (Fractionated and Unknown Nuclear effects) CAIs (calcium-aluminum-rich inclusions) show correlated excesses and deficits in neutron-rich iron-group elements (e.g., [Meyer and Zinner 2006]). These isotopes are robustly produced in low-entropy expansions of neutron-rich matter [Meyer et al. 1996], and such expansions likely occur in rare, dense, thermonuclear (Type Ia) supernovae [Woosley 1997].
In this brief paper we explore several low-entropy expansions and follow the neutronization that occurs due to weak interactions on free nucleons and nuclei. We compare network calculations to corresponding calculations of dynamical weak statistical equilibrium to study the extent to which the network calculations attain this equilibrium. For realistic supernova timescales, the expansions do not attain dynamical weak statistical equilibrium, but they do reach a degree of neutron richness sufficient to make neutron-rich iron-group isotopes like \(^{48}\text{Ca}\), \(^{50}\text{Ti}\), and \(^{54}\text{Cr}\).

### E.3 Dynamical Weak Nuclear Statistical Equilibrium

Given sufficient time, a system undergoing nucleosynthesis can evolve until the nuclear species are in full equilibrium under assembly from free nucleons. This is the condition of nuclear statistical equilibrium (NSE), for which the chemical potential for a nuclear species with atomic number \(Z\) and mass number \(A\) is related to that for free neutrons \(\mu_n\) and free protons \(\mu_p\) by

\[
\mu(Z, A) = Z\mu_p + (A - Z)\mu_n. \tag{E.1}
\]

A related equilibrium is quasi-statistical equilibrium (QSE) in which nuclei are in equilibrium under exchange of nucleons, but the total number of heavy nuclei \((Z > 2)\) is not that required by NSE because the three-body reactions assembling heavy nuclei are too slow \cite{Meyer1996}. In this case, the chemical potential for a heavy nucleus is given by

\[
\mu(Z, A) = \mu_h + Z\mu_p + (A - Z)\mu_n. \tag{E.2}
\]

where \(\mu_h\) is the chemical potential of the heavy nuclei as a whole.

The NSE and QSE described above consider the total neutron-to-proton ratio to be fixed. Weak interactions can change this quantity so that the system can evolve to weak equilibrium. If neutrinos are trapped in the material, the system can evolve to weak nuclear statistical equilibrium (here called WSE) such that there is an equilibrium under the interchange of neutrons and protons via weak reactions. In this case there is the additional condition relating the chemical potentials of protons, electrons, neutrons, and electron-type neutrinos:

\[
\mu_p + \mu_e = \mu_n + \mu_{\nu_e} \tag{E.3}
\]
In WSE, nuclear abundances per nucleon $Y(Z,A)$ evolve until their chemical potentials satisfy Eq. (E.1) and the electron-to-nucleon ratio $Y_e$ satisfies Eq. (E.3).

Densities are typically not sufficient in white dwarf star cores to trap neutrinos, however. In such matter, nuclear populations evolve not to WSE but rather to a dynamical weak nuclear statistical equilibrium (here called dWSE) [Arcones et al. 2010]. In this case, the nuclear abundances obey Eq. (E.1), but the constraint on the electron-to-nucleon ratio $Y_e$ is instead given by the condition that the time rate of change of $Y_e = 0$. Because of the extremely low abundance of positrons in degenerate material, positron capture and $\beta^+$ decay are both small in white-dwarf star matter so that this dWSE arises when the total electron capture rate in the matter (which decreases $Y_e$) equals the total $\beta^-$ decay rate (which increases $Y_e$).

**E.4 Network Calculation**

We study the nucleosynthesis of matter expanding from high temperature and density using NucNet Tools, an open-source suite of tools we have written to study nucleosynthesis [?]. Our network calculations use reaction rates from the Joint Institute for Nuclear Astrophysics database at http://www.jinaweb.org. We supplement these rates with weak-interaction rates from [Langanke and Martínez-Pinedo 2001]. For nuclei that do not yet have microscopic weak rate estimates available, we use the approximate rate formulation in [Arcones et al. 2010].

We ran a set of calculations that began with 50% by mass of $^{12}\text{C}$ and 50% by mass $^{16}\text{O}$. The matter began at a mass density $\rho$ of $9 \times 10^9$ g cm$^{-3}$ and a temperature of $T_9 = T/10^9 \text{K} = 10$. We considered the density to expand exponentially with time $t$ such that $\rho(t) = \rho(0) \exp(-t/\tau)$, where $\tau$ is the density e-folding timescale. We considered the entropy of the matter to be dominated by relativistic particles such that $\rho \propto T_9^3$. We also ran some more detailed models that account for energy generation that we will describe in a future paper. These models show that $\rho \propto T_9^3$ is a reasonable parameterization for these studies.

Fig. E.1 shows the time evolution of the electron-to-nucleon ratio $Y_e$ for $\tau = 0.1, 1, 10,$ and 1000 seconds. Also shown on this curve is the instantaneous dWSE value of $Y_e$. This is the electron-to-nucleon ratio the matter would evolve to if the expansion were arrested and the matter allowed to evolve at the fixed temperature and density at that point in the expansion.
expansion from $T_9 = 10, \rho = 9 \times 10^9 \text{ (g/cm}^3\text{)},$ with 50% $^{12}\text{C}$ and 50% $^{16}\text{O}$

![Graph](image)

Figure E.1 The evolution of the electron-to-nucleon ratio $Y_e$ as a function of $T_9 = T/10^9 \text{ K}$ in expansions of various density e-folding timescale $\tau$. Also shown as the red curve is the dynamical weak statistical equilibrium (dWSE) $Y_e$ for the corresponding density and temperature. The slow expansions come close to attaining dWSE at high temperature and density but diverge from dWSE at lower temperature when the weak rates decrease dramatically. The faster expansions never attain dWSE.

This quantity is computed by finding the value of $Y_e$ at that temperature and density such that the NSE has a rate of change of $Y_e$ equal to zero. The dWSE $Y_e$ is low ($Y_e \approx 0.38$) early in the calculation because the density and, hence, the electron chemical potential is high. This favors electron capture and drives the dWSE $Y_e$ down. As the matter expands and cools, the density
drops. This lowers the electron chemical potential, which lowers the typical electron-capture rate and increases the dWSE $Y_e$.

As Fig. E.1 shows, slow expansion (large $\tau$) allows the system $Y_e$ to keep pace with the dWSE $Y_e$ better than the faster expansions. For $\tau = 1000$ s, the matter attains dWSE at $T_9 = 10$ and evolves in dWSE until the network diverges from dWSE near $T_9 = 5$ and freezes out at about $T_9 = 4$. In contrast, the faster expansions experience a drop from the initial $Y_e = 0.5$ early due to electron capture but freezeout near their final $Y_e$ at about $T_9 = 8$.

![Figure E.2](image_url)  
Figure E.2  The total electron-capture and $\beta^-$ decay rates as a function of time during the fixed temperature and density calculations. The system attains dWSE when the two rates become equal. Note that the lower density calculation takes a longer time to reach dWSE because the overall rates are lower.

To study the evolution of $Y_e$ during these calculations, we made two calculations of matter with initial mass fractions of 50% $^{12}$C and 50% $^{16}$O evolving at fixed temperature and density drawn from points in the expansions shown in Fig. E.1. The first calculation is for $T_9 = 8$ and $\rho = 4.6 \times 10^9$ g cm$^{-3}$. The left panel of Fig. E.2 shows the total electron capture and total $\beta^-$ decay rate during this calculation. Initially electron capture dominates beta decay and causes the $Y_e$ to drop. As the material becomes neutron rich, however, $\beta^-$ decay becomes
Figure E.3 The total electron-capture and $\beta^-$ decay rates as a function of the material’s electron-to-nucleon ratio $Y_e$ during the fixed temperature and density calculations. Initially the electron captures dominate $\beta^-$ decay. As the material becomes more neutron rich, the $\beta^-$ decay rates increase and the electron-capture rates decrease. When they become equal, the rate of change of $Y_e$ becomes zero and the material reaches dWSE.

important. After $\sim 10$ s, the total electron capture rate equals the total $\beta^-$ decay rate and the matter attains dWSE. This explains why both the $\tau = 10$ s and $\tau = 1000$ s expansions are near dWSE at $T_9 = 8$ – the expansion timescale is longer than or comparable to the timescale to attain dWSE.

The second calculation is for $T_9 = 5.5$ and $\rho = 1.5 \times 10^9$ g cm$^{-3}$. The right panel of Fig. E.2 shows the total electron capture and $\beta^-$ decay rates for this calculation. This figure is similar to that for the previous calculation. The difference is that the overall rates are smaller because of the lower density (and electron chemical potential) which results in a longer timescale for evolution to dWSE (larger than $\sim 100$ s). The long timescale for evolution to dWSE means that, even for the $\tau = 1000$ s expansion, the network has difficulty keeping pace with the changing dWSE $Y_e$ at this temperature and density.

Fig. E.3 shows the total electron capture and $\beta^-$ decay rates for the two fixed temperature and density calculations as a function of $Y_e$ instead of time. This figure shows how, as
the material neutronizes, the total electron capture rate declines and the total $\beta^-$ decay rate increases. Once they meet, the rate of change of $Y_e$ goes to zero and the system reaches dWSE.

Four movies that accompany this paper show the evolution of the elemental abundances in the four expansions as compared to those in QSE, NSE, and dWSE. Two other movies show the evolution of the elemental abundances for the two fixed temperature and density calculations. In the movies, it is clear that the nuclear populations evolve quickly into QSE, then NSE, and finally, on a longer timescale (if the expansion is not too fast), into dWSE.

Fig. E.4 shows the mass fractions of the most abundant species in the $\tau = 1$ s expansion. This timescale is comparable to the explosion timescales expected in Type Ia supernovae. The dominant products are clearly $^{66}$Ni, $^{60}$Fe, $^{50}$Ti, $^{48}$Ca, and $^{54}$Cr. These five species constitute nearly 86% of the mass from this expanding matter. About 14% of the final mass is in $^{48}$Ca. Expansions from lower density do not reach as low a $Y_e$ and, hence, produce much less $^{48}$Ca. This result confirms that $^{48}$Ca production is robust when high densities and timescales of seconds are present in expanding matter.

E.5 Conclusion

Significant production of $^{48}$Ca in expansions of low-entropy matter requires $Y_e \approx 0.42$. As we showed, densities near $\rho = 9 \times 10^9$ g cm$^{-3}$ and expansion timescales of $\sim 1$ s can drive matter with $Y_e \approx 0.5$ down to this level and lead to robust $^{48}$Ca synthesis. This occurs despite the fact that such relatively fast expansions never attain dynamical weak statistical equilibrium.

While Type Ia supernovae are fairly frequent events in the Galaxy and significant producers of the Solar System’s supply of iron, a density as high as $9 \times 10^9$ g cm$^{-3}$ is rare in white dwarf stars (e.g., Woosley 1997), the progenitors of these explosions. This means that Type Ia supernova production of $^{48}$Ca is probably rare. Nevertheless, as our calculation shows, these rare events would make tremendous amounts of $^{48}$Ca. Because of this, our expectation is that this isotope is rather heterogeneously distributed in the dust in the interstellar medium. When such dust was inherited by the early Solar nebula, the isotopically heterogeneous dust formed into solids such as hibonites and FUN CAIs, which then naturally show isotopic anomalies in the neutron-rich iron-group isotopes.
expansion from $T_9=10$, $\rho=9\times10^9$ (g/cm$^3$), $\tau=1$ (s), with 50% $^{12}$C and 50% $^{16}$O

Figure E.4 Mass fractions as a function of $T_9$ in the $\tau = 1$ s expansion.

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Appendix F

White Dwarf

A white dwarf is the compact object left after a low to medium mass star evolves to its end. The white dwarf may consist of carbon, oxygen, neon and magnesium, but it is supported by the degenerate pressure of electrons. We will discuss the properties of degenerate matter in F.1.

F.1 Degenerate Matter

To describe the properties of matter, people usually use the concept of "the equation of state" (EoS). The equation of state is the function that relates the pressure to the density, particle mass and temperature of a matter. The net pressure can be divided into three components, pressure from radiation, pressure from ions and pressure from electrons. The latter may not obey the ideal gas law due its light weight which makes it become degenerate easier.

We introduce adiabatic index $\gamma$ to study the equation of state. For a fixed composition and a certain temperature, the pressure has a simple relation with the density:

$$P \propto \rho^\gamma \quad (F.1)$$

$$\gamma = \frac{\rho}{P} \frac{dP}{d\rho} = \frac{d\ln P}{d\ln \rho} \quad (F.2)$$

We show the variation of $\gamma$ with different densities in Figure [F.1]. In this calculation we use a single composition of carbon-12 and a fixed temperature of $10^4$ Kelvin.

One way to determine whether the electron matter is degenerate or not is comparing the thermal de Broglie wavelength of electrons with the space between the neighbor electrons. If the thermal wavelength gets bigger than the latter, it means the quantum effects begin to dominate. This will lead to degenerate state. A rough estimation of the thermal wavelength can be:

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m_e E_k}} = \frac{h}{\sqrt{2m_e^2 k_B T}} = \frac{h}{\sqrt{3m_e k_B T}} \quad (F.3)$$

where $h$ is Planck’s constant, $p$ is the momentum, $m_e$ is mass of electron, $E_k$ is the kinetic energy, $k_B$ is Boltzmann constant and $T$ is the temperature in Kelvin. For electrons at $10^4$ Kelvin $\lambda \sim 10^{-7}$cm, which corresponds a density of $2.6 \times 10^{-3}$g/cm$^3$. This can be calculated
from the following relation:

$$n_e = 1/\lambda^3 = \rho N_A Y_e$$  \hspace{1cm} (F.4)

where $n_e$ is the electron number density, $\rho$ is the mass density of the matter, $N_A$ is the Avogadro constant and $Y_e$ is defined as electron numbers per baryon in the system, which is 0.5 in this calculation.

So for low densities ($\rho < 10^{-3} \text{g/cm}^3$) both the carbon ions and the electrons can be treated as ideal gas. The pressure from matter then is

$$P_{\text{matter}} = \rho N_A Y_T k_B T$$  \hspace{1cm} (F.5)
where $Y_i$ can be $Y_e$ or $Y_{carbon}$ which is 1/12. In either case the pressure is proportional to the density. So where the pressure from matter dominates ($\rho$ from about $10^{-9}$ to $10^{-3}$ g/cm$^3$), from Equation F.1 we get $\gamma = 1$ as shown in Figure F.1.

When the density drops the pressure from matter decreases. Below a certain density the pressure from radiation would dominate.

$$P_{\text{radiation}} = \frac{1}{3} a T^4$$

where $a$ is the radiation constant ($a = 4\sigma/c = 7.5647 \times 10^{-15}$ ergs cm$^{-3}$ K$^{-4}$, where $\sigma$ is Stephan Boltzmann constant). At this condition we have $P_{\text{radiation}} = 2.5 \times 10^1$ dyn/cm$^2$. If we let the pressure from matter be the same value we get a density of about $6 \times 10^{-11}$ g/cm$^3$. So below this density the net pressure will be dominated by the radiation which does not depend on density. From Equation F.1 we know that $\gamma$ will approach zero when the density drops further (see Figure F.1).

Now let’s look at the degenerate case. To calculate the pressure we need to apply the pressure integral [Clayton 1968]:

$$P = \frac{1}{3} \int n(p)vpd^3p$$

where $n(p)$ is the number density as a function of momentum $p$, $v$ is the velocity. For complete degenerate electrons

$$P = \frac{1}{3} \int_0^{p_F} \frac{G}{h^3} vpd^3p$$

where $p_F$ is Fermi momentum which indicates the momentum of electrons near the surface of Fermi sea, $G$ is the multiplicity which is 2 for electrons. This can be divided into two cases: relativistic and non-relativistic.

For non-relativistic case we have $v = p/m$ so the pressure is like

$$P_{\text{NonRel}} \propto \int_0^{p_F} p^4 dp \propto p_F^5$$

For relativistic case $v = c$, so

$$P_{\text{Rel}} \propto \int_0^{p_F} p^3 dp \propto p_F^4$$
For degenerate matter we have

\[ p_F = \left( \frac{3h^3}{8\pi} n \right)^{1/3} \propto \rho^{1/3} \]  

(F.11)

So we have

\[ P_{\text{NonRel}} \propto \rho^{5/3} \]  

(F.12)

\[ P_{\text{Rel}} \propto \rho^{4/3} \]  

(F.13)

Thus we get \( \gamma = 5/3 \) for complete degenerate and non-relativistic matter, \( \gamma = 4/3 \) for complete degenerate and relativistic matter as shown in Figure F.1.

To determine when the electrons become relativistic, we compare the Fermi kinetic energy (\( \sim p_F c \)) with the rest mass energy of electrons (\( m_e c^2 \)). When the two equal to each other the density is about \( 2 \times 10^6 \text{g/cm}^3 \). As we can see in Figure F.1 \( \gamma \) starts to move from \( 5/3 \) to \( 4/3 \) at around such a density.

To summarize this section, we list the four cases here:

1. At low densities the pressure is dominated by radiation and does not depend on the density.
2. For higher densities the pressure is dominated by matter which can be treated as ideal gas.
3. For even higher densities the matter becomes degenerate and the pressure is proportional to the density to the \( 5/3 \) power.
4. For highest densities the matter become degenerate and relativistic. The pressure is proportional to the density to the \( 4/3 \) power.

\[ \text{F.2 White Dwarf Structure and Mass Limit} \]

White dwarfs are supported by degenerate electron pressure. As a white dwarf accretes matters from its companion, it gets more massive and denser (which will be discussed later). The electrons in the white dwarf then convert from non-relativistic to relativistic gradually. Once all the electrons become relativistic the white dwarf uses up its “potential” and the degenerate pressure cannot support any more masses. Thus the white dwarf becomes unstable and the variation in size will cause the temperature change which basically remained constant before. The increase of temperature will ignite carbon burning through out the whole white dwarf in our model and cause it explode.
To describe the structure of white dwarfs we built a TOV solver. In astrophysics, the Tolman-Oppenheimer-Volkoff (TOV) equation constrains the structure of a spherically symmetric body of isotropic material which is in static gravitational equilibrium, as modeled by general relativity. The TOV equation is

$$\frac{dP(r)}{dr} = -\frac{G}{r^2} \left[ \rho(r) + \frac{P(r)}{c^2} \right] \left[ M(r) + 4\pi r^3 P(r) c^2 \right] \left[ 1 - \frac{2GM(r)}{c^2 r} \right]^{-1} \quad \text{(F.14)}$$

Here $r$ is a radial coordinate, $\rho(r_0)$ and $P(r_0)$ are the density and pressure, respectively, of the material at $r = r_0$. The equation is derived by solving the Einstein equations for a general time-invariant spherically symmetric metric. Together with the mass continuity equation

$$\frac{dM(r)}{dr} = 4\pi \rho(r) r^2 \quad \text{(F.15)}$$

and proper boundary conditions we can solve the problem numerically.

Figure F.2 shows a typical relation between the mass of white dwarf and its central density calculated by our TOV solver. We can see that the mass gets its maximum at a central density about $10^{10}$ g/cm$^3$. This mass limit is called Chandrasekhar limit. Beyond that density the mass starts to decrease. However this hardly happens because beyond the threshold density the white dwarf is not stable any more. For even higher densities neutrons start to become degenerate to support the star. The mass-density curve would jump horizontally to a much higher density from the summit.

We tried to use the classical Newton’s Law to calculate the white dwarf structure to see the difference. At classical conditions the TOV equation [F.14] reduces to:

$$\frac{dP(r)}{dr} = -\frac{GM(r)}{r^2} \rho \quad \text{(F.16)}$$

Figure F.3 shows some comparison between TOV and Newtonian solver. The figure plots the density change in mass coordinates. For low central density calculations, the difference is not quite noticeable. For high density of $10^{10}$ g/cm$^3$ the Newtonian result has a larger white dwarf mass. The general relativity effects on white dwarf seem not very significant.
An analytical way to solve the classical equations $F.16$ and $F.15$ is to use polytropes. It is assumed that there is a polytropic relation between pressure and density:

$$P = K \rho^{n+1/n} \tag{F.17}$$

where $K$ and $n$ are real, positive constants and $n$ is called a polytropic index. If we apply this we will eventually get a Lane-Emden equation. Also comparing this to Equation $F.1$ we can get the relation between adiabatic index and polytropic index:

$$\gamma = \frac{n + 1}{n} \tag{F.18}$$

Figure $F.4$ shows a comparison between TOV solver and polytropes. It also shows the density distribution in mass coordinates. It shows that for a low central density of $10^7 \text{g/cm}^3$ a
polytrope with index of 2 does not differ much from the full TOV calculation. From Equation F.18 and the discussion of the previous section we know that polytropic index of 1.5 corresponds to a non-relativistic degenerate matter and 3 for a relativistic degenerate matter. So Figure F.4 shows a condition between non-relativistic and full relativistic degenerate cases. In Figure 2.8 and 2.9 we applied a polytropic white dwarf structure with index of 3.
Figure F.4  Compare TOV solver with polytropes.
Appendix G
Growing Large Dust Grains

In this appendix, I present a graph branching derivation of a computationally efficient means of growing dust grains of arbitrarily large size. It is possible to use network calculations that follow all species up to those with $\sim 10^4$ atoms, but following larger species requires a different approach. I do not use this approach in §4, but I record it here for possible future use.

To treat this problem, we follow the time evolution of a network with branchings \cite{Wang2009}. In such a case, we analyze the abundance $Y_i(t + \Delta t)$ of a species $i$ in a linear network at time $t + \Delta t$ in terms of branchings of a directed graph. The vertices of the graph are the species in the network. The directed arcs in the graph are the reactions between the species. Since the network solutions at $t + \Delta t$ are in terms of the abundances at $t$, an arc from vertex $i$ to vertex $j$ gives the contribution of vertex $j$ at time $t$ to the abundance of $i$ at time $t + \Delta$.

As a consequence of this, and because of the rules of branching weights, the weight of the arc from $i$ to $j$ is $\ln(\rho_{ji}\Delta t)$, where $\rho_{ji}$ is the rate of the reaction from $j$ to $i$. Note that direction of the arc is opposite that of the reaction in time.

A branching $B$ in a graph is a set of arcs in the graph such that there are no cycles in the graph and no vertex has indegree (that is, the number of arcs entering a vertex) larger than one. The weight $w(B)$ of a branching $B$ is the sum of the weights of all the arcs in the branching.

With these preliminaries in mind, the abundance of species $i$ in the network at $t + \Delta t$ is

$$Y_i(t + \Delta t) = \frac{\sum_{B:(i)} \exp\{w(B)\} Y_{B}^{(i)}(t)}{\sum_B \exp\{wB\}}$$  \hspace{1cm} (G.1)

The symbol $B : (i)$ indicates a branching rooted at $i$, that is, a branching such that vertex $i$ has no arcs entering it. The symbol $Y_{B}^{(i)}(t)$ is defined as

$$Y_{B}^{(i)}(t) = \sum_{j : \{(i) \rightarrow j\}_B} Y_j(t)$$  \hspace{1cm} (G.2)

where the symbol $j : \{(i) \rightarrow j\}_B$ means any vertex $j$ for which there is a path from root $i$ to $j$ in branching $B$. 
We now turn to the problem of forming large dust grains. We consider a network that may be split into two subnetworks—one has complicated interactions among the subnetwork members and the other has a simple capture chain. Fig. G.1 shows a simple six species example. Species 1 through 3 interact via capture and destruction reactions. Species 4 through 6 only interact via capture reactions. We may thus split up the network into two subnetworks, \( C_1 \) and \( C_2 \), and the parent digraph for branchings is then that in Fig. G.2.

We now consider the general case. We imagine the \( n \) species in \( C_1 \) to be labeled 1 through \( n \) and the species in \( C_2 \) to be labeled \( n + 1 \) to \( N \). We also consider that \( C_1 \) and \( C_2 \) are linked via a capture from \( n \) to \( n + 1 \). If we focus on a subnetwork consisting of \( C_2 \) plus species \( n \), the possible exponential sum of branchings is

\[
\sum_{B_2} \exp\{w(B_2)\} = \prod_{i=n}^{N} (1 + \lambda_i \Delta t) \quad (G.3)
\]

because each reaction in the subnetwork will either contribute an arc (weight \( \ln (\lambda_j \Delta t) \)) or not (weight zero) to a given branching. Consider now the full network. We build up branchings from a sub-branching within \( C_1 \) and within \( C_2 \) and links between them. If a branching contains
the arc from $C_2$ to $C_1$, that is, from $n + 1$ to $n$, the sub-branch for the subnetwork $C_1$ must be rooted at $n$ because there can only be one arc entering $n$. On the other hand, if the branching does not include the arc from $n + 1$ to $n$, the sub-branching within $C_1$ can be rooted at any of the vertices in $C_1$. The exponential sum of all branchings will then be

$$
\sum_B \exp\{w(B)\} = \sum_{B_1:\{(k\in C_1)\subset C_1}} \exp\{w(B_1)\} \prod_{i=n+1}^{N} (1 + \lambda_i \Delta t) + \sum_{B_1:\{(n)\subset C_1}} \exp\{w(B_1)\} \lambda_n \Delta t \prod_{i=n+1}^{N} (1 + \lambda_i \Delta t)
$$

where $B_1 : \{(k)\subset C_1\}$ indicates the branching $B_1$ is rooted at $k \in C_1$ and is entirely contained in $C_1$.

We begin by considering the abundance of species $n$. The abundance of species $n$ at $t + \Delta t$ is given by Eq. (G.1). Since the relevant branchings must be rooted at $n$, they cannot contain any arcs entering vertex $n$; thus, we find

$$
Y_n(t + \Delta t) = \frac{\sum_{B_1:\{(3)\subset C_1}} \exp\{w(B_1)\} \prod_{i=n+1}^{N} (1 + \lambda_i \Delta t) Y_{B_1}^{(n)}}{\left(\sum_{B_1:\{(k\in C_1)\subset C_1}} \exp\{w(B_1)\} + \sum_{B_1:\{(n)\subset C_1}} \exp\{w(B_1)\} \lambda_n \Delta t\right) \prod_{i=n+1}^{N} (1 + \lambda_i \Delta t)}
$$

This reduces to

$$
Y_n(t + \Delta t) = \frac{\sum_{B_1:\{(n)\subset C_1}} \exp\{w(B_1)\} Y_{B_1}^{(n)}}{\sum_{B_1:\{(k\in C_1)\subset C_1}} \exp\{w(B_1)\} + \sum_{B_1:\{(n)\subset C_1}} \exp\{w(B_1)\} \lambda_n \Delta t}
$$

We now consider the abundance of species $j > n$. Since the relevant branchings must be rooted at $j$, they cannot contain the arc entering vertex $j$. The other question we address about the relevant branching is whether it includes the from $n + 1$ to $n$. Branchings that do not include that arc will include the factor $\sum_{B_1:\{(k\in C_1)\subset C_1}} \exp\{w(B_1)\}$. Branchings that do include that arc will include the factor $\sum_{B_1:\{(n)\subset C_1}} \exp\{w(B_1)\} \lambda_n \Delta t$. The contribution to the numerator in Eq. (G.1) will be

$$
N_j = \sum_{l=n+1}^{j} Y_l(t) \left( \prod_{m=n+1}^{l-1} (1 + \lambda_m \Delta t) \right) \left( \prod_{p=l}^{j-1} \lambda_p \Delta t \right) \left( \prod_{q=j+1}^{N} (1 + \lambda_q \Delta t) \right)
$$
because the branching must have a path from $l$ to $j$ for $Y_l(t)$ to contribute to $Y_j(t+\Delta t)$. The result is that

\[
Y_j(t+\Delta t) = \frac{\left(\sum_{B_l:((k\in C_l)\in C_1}\exp\{w(B_l)\} + \sum_{B_l:|(n)\in C_1}\exp\{w(B_l)\}\lambda_n\Delta t\right) N_j}{\left(\sum_{B_l:((k\in C_l)\in C_1}\exp\{w(B_l)\} + \sum_{B_l:|(n)\in C_1}\exp\{w(B_l)\}\lambda_n\Delta t\right) \prod_{i=n+1}^N (1 + \lambda_i \Delta t)} + \sum_{B_l:|(n)\in C_1}\exp\{w(B_l)\}\lambda_n\Delta t \frac{Y_{B_l}^{(n)} \left(\prod_{p=n+1}^{i-1} \lambda_p \Delta t\right)}{\prod_{i=n+1}^N (1 + \lambda_i \Delta t)}
\]

(G.8)

This reduces to

\[
Y_j(t+\Delta t) = \sum_{l=n+1}^j \frac{Y_l(t)}{1 + \lambda_j \Delta t} \left(\prod_{p=l}^{j-1} \frac{\lambda_p \Delta t}{1 + \lambda_p \Delta t}\right) + Y_n(t + \Delta t) \left(\frac{\lambda_n \Delta t}{1 + \lambda_j \Delta t}\right) \left(\prod_{p=n+1}^{j-1} \frac{\lambda_p \Delta t}{1 + \lambda_p \Delta t}\right)
\]

(G.9)

When $\Delta t \to 0$, we see $Y_j(t+\Delta t) \to Y_j(t)$ while when $\Delta t \to \infty$, we find $Y_j(t+\Delta t) \to \frac{\lambda_j}{\lambda_j} Y_n(t+\Delta t)$. Eq. (G.9) gives the abundance of a species $j > n$ at $t + \Delta t$ in terms of species $Y_n(t + \Delta t)$ and species with index $k < j$ at $t$. We now consider allowing only certain species with $j > n$ to have non-zero abundance. We label these $j_1, j_2, \text{and so forth}$. With our assumption, we insist that species with index $k$ such that $n < k < j_1$ have zero abundance. We thus find

\[
Y_{j_1}(t + \Delta t) = \frac{Y_{j_1}(t)}{1 + \lambda_{j_1} \Delta t} + Y_n(t + \Delta t) \left(\frac{\lambda_n \Delta t}{1 + \lambda_{j_1} \Delta t}\right) \left(\prod_{p=n+1}^{j_1-1} \frac{\lambda_p \Delta t}{1 + \lambda_p \Delta t}\right)
\]

(G.10)

Similarly, species with index $k$ such that $j_1 < k < j_2$ have zero abundance; thus,

\[
Y_{j_2}(t + \Delta t) = \frac{Y_{j_2}(t)}{1 + \lambda_{j_2} \Delta t} \prod_{p=j_1}^{j_2-1} \frac{\lambda_p \Delta t}{1 + \lambda_p \Delta t} + Y_n(t + \Delta t) \left(\frac{\lambda_n \Delta t}{1 + \lambda_{j_2} \Delta t}\right) \left(\prod_{p=n+1}^{j_2-1} \frac{\lambda_p \Delta t}{1 + \lambda_p \Delta t}\right)
\]

(G.11)

This can be written

\[
Y_{j_2}(t + \Delta t) = \frac{1 + \lambda_{j_1} \Delta t}{1 + \lambda_{j_2} \Delta t} \prod_{p=j_1}^{j_2-1} \frac{\lambda_p \Delta t}{1 + \lambda_p \Delta t} Y_{j_1}(t + \Delta t) + \frac{Y_{j_2}(t)}{1 + \lambda_{j_2} \Delta t}
\]

(G.12)

which, in turn, becomes

\[
Y_{j_2}(t + \Delta t) = \frac{\lambda_{j_1} \Delta t}{1 + \lambda_{j_2} \Delta t} \prod_{p=j_1+1}^{j_2-1} \frac{\lambda_p \Delta t}{1 + \lambda_p \Delta t} Y_{j_1}(t + \Delta t) + \frac{Y_{j_2}(t)}{1 + \lambda_{j_2} \Delta t}
\]

(G.13)
A similar analysis holds for subsequent species such that

\[
Y_{jm}(t + \Delta t) = \frac{\lambda_{jm-1}}{1 + \lambda_j \Delta t} \prod_{p=jm-1+1}^{jm-1} \left( \frac{\lambda_p \Delta t}{1 + \lambda_p \Delta t} \right) Y_{jm-1}(t + \Delta t) + \frac{Y_{jt}(t)}{1 + \lambda_j \Delta t} \tag{G.14}
\]

Note that it is important to distinguish between the symbols \(j_{m-1}\), which is the \((m - 1)\text{th}\) non-zero species in our approximation, and \(j_m - 1\), which is the species with index one less than \(j_m\). We are in fact interested in an effective rate for capture from \(j_{m-1}\) to \(j_m\), so we compute

\[
\frac{Y_{jt}(t + \Delta t) - Y_{jt}(t)}{\Delta t} = \frac{\lambda_{jm-1}}{1 + \lambda_j \Delta t} \prod_{p=jm-1+1}^{jm-1} \left( \frac{\lambda_p \Delta t}{1 + \lambda_p \Delta t} \right) Y_{jm-1}(t + \Delta t) - \frac{\lambda_{jm}}{1 + \lambda_j \Delta t} Y_{jm}(t + \Delta t) \tag{G.15}
\]

From this we infer an effective capture rate from \(j_{m-1}\) to \(j_m\) as

\[
\lambda^\text{eff}_{j_{m-1}, jm} = \frac{\lambda_{jm-1}}{1 + \lambda_j \Delta t} \prod_{p=jm-1+1}^{jm-1} \left( \frac{\lambda_p \Delta t}{1 + \lambda_p \Delta t} \right) \tag{G.16}
\]

Eq. (G.15) is still incomplete in our treatment because the capture term out allows for a single capture. This is inconsistent with our assumption that species with index \(k\) such that \(j_m < k < jm+1\) have zero abundance. We thus modify Eq. (G.15) to read

\[
\frac{Y_{jt}(t + \Delta t) - Y_{jt}(t)}{\Delta t} = \lambda^\text{eff}_{j_{m-1}, jm} Y_{jm-1}(t + \Delta t) - \lambda^\text{eff}_{jm, jm+1} Y_{jm}(t + \Delta t) \tag{G.17}
\]

This reduces the problem to a simple capture chain with effective capture rates given by Eq. (G.16).

Since the network is nonlinear, smaller species are consumed to create larger species. If we imagine capture is purely of single atoms and that larger species are made of a single type of atomic species \(a\), the contribution to the change in the abundance of single atoms when species \(jm-1\) captures to \(jm\) will be

\[
\frac{Y_a(t + \Delta t) - Y_a(t)}{\Delta t} = -(N_{jm} - N_{jm-1}) \left( \lambda^\text{eff}_{jm-1, jm} Y_{jm-1}(t + \Delta t) - \lambda^\text{eff}_{jm, jm+1} Y_{jm}(t + \Delta t) \right) \tag{G.18}
\]

where \(N_{jm-1}\) is the number of atoms \(a\) that make up species \(jm-1\) and \(N_{jm}\) is the number of atoms \(a\) that make up species \(jm\).
To solve the network equations by the Newton-Raphson method, we define

\[ f_{jm} = \frac{Y_{jm}(t + \Delta t) - Y_{jm}(t)}{\Delta t} - \lambda_{jm}^{\text{eff}} Y_{jm-1}(t + \Delta t) + \lambda_{jm}^{\text{eff}} Y_{jm}(t + \Delta t) \]  

(G.19)

These (and the other coupled equations) are iterated on updated solutions at \( t + \Delta t \) until convergence (all \( f' \)'s = 0). We compute the necessary matrix elements as

\[ A_{jm,jm} = \frac{\partial f_{jm}}{\partial Y_{jm}(t + \Delta t)} = \frac{1}{\Delta t} + \lambda_{jm,jm+1}^{\text{eff}} \]  

(G.20)

and

\[ A_{jm,jm-1} = \frac{\partial f_{jm}}{\partial Y_{jm-1}(t + \Delta t)} = -\lambda_{jm,jm-1}^{\text{eff}} \]  

(G.21)

We also find the contribution to the right-hand-side vector \( b_{jm} = -f_{jm} \). As for the single atoms \( a \), the contribution to the function \( f_{a} \) is

\[ f_{a} = \frac{Y_{a}(t + \Delta t) - Y_{a}(t)}{\Delta t} + (N_{jm} - N_{jm-1}) \left( \lambda_{jm-1,jm}^{\text{eff}} Y_{jm-1}(t + \Delta t) - \lambda_{jm,jm+1}^{\text{eff}} Y_{jm}(t + \Delta t) \right) \]  

(G.22)

The contribution to the matrix element \( A_{a,jm} \) is

\[ A_{a,jm} = \frac{\partial f_{a}}{\partial Y_{jm}(t + \Delta t)} = -(N_{jm} - N_{jm-1}) \lambda_{jm,jm+1}^{\text{eff}} \]  

(G.23)

and to \( A_{a,jm-1} \) is

\[ A_{a,jm-1} = \frac{\partial f_{a}}{\partial Y_{jm-1}(t + \Delta t)} = (N_{jm} - N_{jm-1}) \lambda_{jm-1,jm}^{\text{eff}} \]  

(G.24)

The contribution to \( b_{a} \) is \(-f_{a}\). Once all matrix and vector elements are available, the matrix equation \( A\delta Y = b \) is solved, the vector \( Y(t + \Delta t) \) is updated as \( Y + \delta Y \) and the procedure is repeated until \( \delta X = 0 \).

To implement this procedure, we must compute the effective rate in Eq. (G.16). We first note we will take an individual reaction rate \( \lambda_{p} \) to be given by \( \lambda_{p} = N_{p}^{2/3} \lambda_{0} \). \( N_{p}^{2/3} \) is proportional to the surface area of species \( p \). \( \lambda_{0} \) itself depends on the abundance of free atoms and other factors like the sticking probability, which we assume to be the same for all species. With this in mind, we make the following approximation:

\[ \frac{\lambda_{p} \Delta t}{1 + \lambda_{p} \Delta t} = \frac{1}{1 + 1/\lambda_{p} \Delta t} \approx \exp \left( -\frac{1}{\lambda_{p} \Delta t} \right) \]  

(G.25)
With this approximation, we may compute the effective rate in Eq. \((G.16)\) as

\[
\lambda_{j_{m-1},j_{m}}^{\text{eff}} = \frac{\lambda_0 N_{j_{m-1}}^{2/3}}{1 + \lambda_0 N_{j_{m}}^{2/3} \Delta t} \exp \left( -\frac{1}{\lambda_0 \Delta t} \sum_{p=j_{m-1}}^{j_{m}-1} \frac{1}{N_p^{2/3}} \right) \tag{G.26}
\]

Since the number \(N_p\) in the sum in the exponential of this equation is typically a very large number, we approximate the sum as an integral:

\[
\sum_{p=j_{m-1}}^{j_{m}-1} \frac{1}{N_p^{2/3}} \approx \int_{N_{j_{m-1}}}^{N_{j_{m}}-1} \frac{dN}{N^{2/3}} = 3 \left( N_{j_{m}}^{1/3} - N_{j_{m-1}}^{1/3} \right) \tag{G.27}
\]

which finally yields

\[
\lambda_{j_{m-1},j_{m}}^{\text{eff}} = \frac{\lambda_0 N_{j_{m-1}}^{2/3}}{1 + \lambda_0 N_{j_{m}}^{2/3} \Delta t} \exp \left( -3 \frac{\left( N_{j_{m}}^{1/3} - N_{j_{m-1}}^{1/3} \right)}{\lambda_0 \Delta t} \right) \tag{G.28}
\]

The individual rate, in our species per atom notation, is \(\lambda_0 = N_A \langle \sigma v \rangle \rho Y_a\). When \(\lambda_0 \Delta t\) is large compared to \(N_{j_{m}}^{1/3}\), the exponential term does not cut off the effective rate significantly. When \(\lambda_0 \Delta t\) is small compared to \(N_{j_{m}}^{1/3}\) because either the density or \(Y_a\) is small, the exponential will cutoff the effective rate and limit the build up of heavy species.
Appendix H

Formation of C\textsubscript{n} Molecules in Oxygen-rich Interiors of Type II Supernovae

This work is by Tianhong Yu, Bradley S. Meyer and Donald D. Clayton [Yu et al. 2013].

H.1 Abstract

Two reaction-rate-based kinetic models for condensation of carbon dust via the growth of precursor linear carbon chains are currently under debate. The first involved forming C\textsubscript{2} molecules via radiative association of free C atoms; the second forms C\textsubscript{2} molecules by the endoergic reaction CO + C \rightarrow C\textsubscript{2} + O. Both are followed by C captures until the linear chain eventually makes an isomeric transition to ringed carbon on which rapid growth of graphite may occur. These two approaches give vastly different results. Because of the high importance of condensable carbon for current problems in astronomy, we study these competing claims with an intentionally limited reaction-rate network that shows clearly that initiation by C + C \rightarrow C\textsubscript{2} + \gamma is the dominant pathway to carbon rings. We propose an explanation for why the second pathway is not nearly as effective as its proponents calculated it to be.

Keywords: atomic processes — ISM: abundances — ISM: general — meteorites, meteors, meteoroids — supernovae: general — supernovae: individual (SN 1987A)

H.2 Introduction

Whether carbon dust can or can not condense in the interiors of expanding Type II supernovae is an important question for astronomy. Many have assumed, guided by chemical equilibrium, that carbon condensation can not occur unless carbon is more abundant than oxygen. That assumption limits C condensation to the He-burning shell of SNII. This rule-of-thumb was challenged when [Clayton et al. 1999] introduced a non-equilibrium kinetic theory by which carbon can condense thermally in gas having more abundant oxygen, opening the possibility of C condensation throughout the O-rich core. That initial theory has been amplified by several studies [Clayton et al. 2001, Deneault et al. 2003, Deneault et al. 2006, Clayton 2011, Clayton 2013]. Within their chemical model [Cherchneff and Dwek 2009, Cherchneff and Dwek 2010] raised questions about the most effective way of producing C\textsubscript{2} molecules, which is the first step to linear carbon chains. They discovered that the neutral-neutral reaction CO + C \rightarrow C\textsubscript{2} + O
has a reasonably large cross section $\langle \sigma v \rangle = k_{CO,C} = 8.6 \times 10^{-14} \text{ cm}^3 \text{ s}^{-1}$ at temperatures near 5000K despite being endothermic by 4.8eV. Although the CO target abundance for production of C$_2$ in this manner must be calculated, they stated that in their model at $T = 5000$ K it created C$_2$ much more rapidly than the slow radiative reaction C + C $\rightarrow$ C$_2$ + $\gamma$. Sensing high importance of this reaction for astronomy, they claimed in their list of conclusions; 2. A new pathway to the formation of carbon chains is active in the O-rich mass zone of the unmixed ejecta and is identified as the CO conversion to C$_2$ via collisions with C. [Cherchneff and Dwek 2009] were unable to evaluate the quantitative consequences because their reaction network terminated at C$_3$ and did not include the formation of linear carbon chains C$_n$ and their isomerization to carbon rings. [Cherchneff and Dwek 2010] subsequently did include linear chains to $n = 10$, which they took to isomerize instantly to ringed structure, following the published model [Clayton et al. 1999; Clayton et al. 2001].

Testing their calculated abundances for C$_n$ is but a secondary goal of the present study. Its overriding goal is to point out abundance differences of several orders of magnitude for the CO and C$_2$ molecules between the computations of these two groups and to resolve those differences if possible. This test has important consequences for condensation of carbon dust, changing prior expectations if the production of C$_2$ owing to the reaction C + C $\rightarrow$ C$_2$ + $\gamma$ severely underestimates the subsequent abundances of linear carbon chains. [Cherchneff and Dwek 2010] harbored that expectation owing to their belief that much more C$_2$ is made earlier near $T = 5000$ K and survives. Dust created by supernova expansions is currently under intense study owing to three types of astronomical observations: (1) of dust observed in single supernova remnants; (2) of dust observed in early low-metallicity galaxies; (3) of supernova-condensed carbon dust (SUNOCONs) extracted from meteorites. Each of these topics depends sensitively on how much carbon, both numbers and sizes, is able to condense in cooling SNII interiors. Therefore we study this competition carefully.

Crucial to this task is the lifetime $\tau_{CO}$ of CO molecules. Thermal dissociation of CO is dominated by thermal photons because radiative association of C and O dominates other reactions for the formation of CO at the densities within SNII. Each reaction and its inverse is subject to the quantum principle of detailed balance. The thermal photo-dissociation lifetime $\tau_{\gamma}$ is calculated from detailed balance with the radiative association reaction, as in Section 2.1
of Clay et al. 2001. Because of the large 11.1 eV binding energy of the CO molecule, \( \tau_{\gamma} \) is very temperature sensitive. For readers' numerical ease we will tabulate \( \tau_{\gamma} \) at selected key temperatures in Table 1 to follow. The flux and spectrum of newly injected Compton electrons [Clayton and The 1991] yields the lifetime \( \tau_e \) of CO molecules against inelastic scattering dissociation by Compton electrons caused by the \(^{56}\text{Co} \) radioactivity. In a gas of pure CO the mean energy per ion pair is defined as the energy of primary electrons divided by the number of pairs produced. Liu and Victor 1994 calculated the mean energy per ion pair in pure CO gas and obtained the result \( \Delta E = 32.3 \) eV deposited per dissociated CO pair, agreeing with the measurement of 32.2 eV by Klots 1968. So the efficiency of energetic electrons for dissociating CO seems well established. A lifetime \( \tau_{CO} \) near one week is typical in SN 1987A, but would be longer in SNII synthesizing less \(^{56}\text{Co} \) and at times greater than about 8 months.

H.3 The Physical Model and Network

Because our goal is to study the chemistry, we can take a very simple physical model of the expansion; namely, temperature \( T = 3800 K/(t/100d) = 3.30 \times 10^{10}/t(s) \) K, where \( t \) is the time elapsed since core collapse. We choose \( n_O = 10^{10} \) cm\(^{-3} \) and \( n_C = 10^9 \) cm\(^{-3} \) at the starting time \( t = t_{6000K} \) at \( T = 6000 \) K for our chemical network. From our model choice for \( T(t) \) we get \( t_{6000K} = 5.47 \times 10^6 \) s. At subsequent times \( n_O(t) = 10^{10} \) cm\(^{-3} \) \( (t/t_{6000K})^{-3} \) owing to homologous expansion. Let \( N \) be the number of any specific molecular species in a comoving, expanding, initially 1 cm\(^3 \) volume at 6000 K. The only change of \( N \) during expansion occurs through chemical reactions. \( N \) may be expressed as atom fraction \( Y \) of the initial total number \( N_O + N_C = 1.10 \times 10^{10} \) atoms. We intentionally choose an O-rich interior having \( N_O/N_C = 10 \), so that no carbon at all would be able to condense if that interior were governed by chemical equilibrium.

We use an intentionally limited set of chemical species because our goal is to study the controversy over the correct carbon chemistry pathway to the ringed isomers. We limit the present study to C, O, CO, C\(_2\), C\(_3\), ... C\(_8\) and C\(_8^r\), the ringed isomer of C\(_8\), to which we give a lifetime \( \tau_C^r = 10 \) s against thermal isomeric transition from linear C\(_8\) to ringed C\(_8^r\). In a sense the \( n = 8 \) ring is a dummy standing for all rings; but it is also reasonable in being the smallest ring that is widely expected (e.g. Takai et al. 1990). Those ringed molecules are the seeds
for carbon growth because their oxidation rates are much smaller than oxidation rates of linear
$C_n$ whereas their $C$ capture rates are fast. For purposes of this study we take ringed $C_8^r$ to
be indestructible, simply integrating its rate of production. Our strategy is to compute the
number $C_8^r$ remaining after expansion from two differing sources of $C_2$ initiating the linear $C_n$
chains. Those two source reactions are

- $C + C \rightarrow C_2 + \gamma$ [Clayton et al. 1999].
- $CO + C \rightarrow C_2 + O$ [Cherchneff and Dwek 2009; Cherchneff and Dwek 2010].

We take our reaction rates from the rate tables in [Cherchneff and Dwek 2009; Cherchneff
and Dwek 2010]. The rate for the second reaction is indeed much greater than that of the
first reaction above $T = 3000$ K; but it becomes increasingly the smaller of the two below
$T = 2500$ K. We include the thermal inverse reaction of every reaction, which we calculate as
in Eq.(3) of [Clayton et al. 2001]. See Table 1 below for sample thermal dissociation rates for
CO molecules. We also include in our network dissociation of CO by Compton electrons. CO is
the only molecule for which electron dissociation can be the dominant destruction mechanism.
For that rate we use $\tau_e(s) = 10^5 \exp((t - 10^6 s)/111d)$, not fit to any specific model but with
plausibility for SN1987A. It lengthens to $\tau_e = 10^6$ s near eight months. Because of their helpful
cataloging of reaction rate tables, and in order to compare results without rate differences, we
take the rates as given in the tables of [Cherchneff and Dwek 2009; Cherchneff and Dwek 2010].
As one example, we take the rate for $C + C \rightarrow C_2 + \gamma$ as the rate given by RA4 in Table 5 in
[Cherchneff and Dwek 2009], p. 649.

Our computational reaction network is \textit{libnucnet} ([Meyer and Adams 2007—see also
http://sourceforge.net/projects/libnucnet/] modified to follow the chemical rather than
nuclear reactions. This network code has been thoroughly tested on a wide variety of reaction
networks and problems. We scrupulously tested our network answers by hand calculations
capable of exposing coding errors.

H.4 The Function $n_{CO}(t)$

The interior core of C and O resulting from completed He burning in massive stars is a
mix of C and O atoms having bulk C/O $< 1$. Post explosive cooling of such matter will attempt
to associate C and O into CO molecules [Lepp et al. 1990]. The reaction $C + O \rightarrow CO + \gamma$ is one of
the crucial reactions of chemical astrophysics. Its rate $k_{CO}$ is intrinsically slow because quantum mechanics requires not only rearrangement of electronic shells but also simultaneous creation of a photon during the collision; nonetheless, the huge product $n_{C}n_{O}$ in the He-exhausted core ensures steady growth for the CO abundance until it is reversed by radioactive dissociation.

Evidently the abundance of CO within that zone during expansion attempts to balance these creation and destruction effects, doing so exactly at the time $t = t_{max}$ of maximum $n_{CO}$. [Clayton 2013] has discussed the shape of the function $n_{CO}(t)$. His Eq.(1), which is valid at constant density, approximates the growth of $n_{CO}$ by its leading terms:

$$\frac{dn_{CO}}{dt} = n_{C}n_{O}k_{CO} - \frac{n_{CO}}{\tau_{CO}} = 0 \quad (H.1)$$

at $t = t_{max}$. The maximum abundance reached by CO is in cgs units

$$n_{CO}(t_{max}) = n_{C}n_{O}k_{CO}\tau_{CO} \quad (H.2)$$

This amount is equal to that formed during its last mean lifetime $\tau_{CO}$ against dissociation. Eq. (H.2) is also highly accurate in circumstances where the time derivative in Eq. (H.1) is but a small difference between much larger creation and destruction terms. Such balance is often set up as an abundance approaches its true maximum. If $\tau_{CO}$ is taken to be $\tau_{\gamma}$ because the dissociation of CO is dominated for $T > 3500$ K by thermal photons, one obtains the expression for the abundance $n_{CO}^{eq}$ in thermal equilibrium: $n_{CO}^{eq} = n_{C}n_{O}k_{CO}\tau_{\gamma}$, and is also entered in Table 1.

Expressed instead in terms of number fractions $Y_{CO} = n_{CO}/n$ and $Y_{C} = n_{C}/n$ where $n$ is the number density of all atoms, Eq. (H.1) transforms to

$$\frac{dY_{CO}}{dt} = Y_{C}Y_{O}n_{CO} - \frac{Y_{CO}}{\tau_{CO}} \quad (H.3)$$

which is the form integrated by our network of coupled reactions. The number density $n$ is needed for the rate $n(cm^{-3})k_{CO}(cm^{3}s^{-1})$. In our numerical example we take $n_{O} = 10^{10}$ cm$^{-3}$ and $n_{C} = 10^{9}$ cm$^{-3}$ at $t_{6000K}$ as starting conditions for the chemical network. Subsequent values are $n = 1.1 \times 10^{10}$ cm$^{-3}$ $[t_{6000K}/t]^{3}$, where the expansion factor reduces the initial
Table H.1  Values of $\tau_\gamma$(CO) and related quantities at selected time $t$ and temperature $T$

<table>
<thead>
<tr>
<th>$t$ (s)</th>
<th>$t/t_{6000K}$</th>
<th>$T$ (K)</th>
<th>$\tau_\gamma$ (s)</th>
<th>$k_{CO}$ (cm$^{-3}$ s$^{-1}$)</th>
<th>$n_{CO}^{eq}$ (cm$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$5.47 \times 10^6$</td>
<td>1</td>
<td>6000</td>
<td>$4.22 \times 10^{-2}$</td>
<td>$3.13 \times 10^{-17}$</td>
<td>$1.32 \times 10^1$</td>
</tr>
<tr>
<td>$5.97 \times 10^6$</td>
<td>0.769</td>
<td>5500</td>
<td>$3.54 \times 10^{-1}$</td>
<td>$2.99 \times 10^{-17}$</td>
<td>$6.27 \times 10^1$</td>
</tr>
<tr>
<td>$6.57 \times 10^6$</td>
<td>0.578</td>
<td>5000</td>
<td>$4.46 \times 10^0$</td>
<td>$2.83 \times 10^{-17}$</td>
<td>$4.24 \times 10^2$</td>
</tr>
<tr>
<td>$7.30 \times 10^6$</td>
<td>0.422</td>
<td>4500</td>
<td>$9.70 \times 10^1$</td>
<td>$2.67 \times 10^{-17}$</td>
<td>$4.61 \times 10^3$</td>
</tr>
<tr>
<td>$8.21 \times 10^6$</td>
<td>0.296</td>
<td>4000</td>
<td>$4.43 \times 10^3$</td>
<td>$2.48 \times 10^{-17}$</td>
<td>$9.67 \times 10^4$</td>
</tr>
<tr>
<td>$9.38 \times 10^6$</td>
<td>0.198</td>
<td>3500</td>
<td>$5.86 \times 10^5$</td>
<td>$2.28 \times 10^{-17}$</td>
<td>$5.26 \times 10^6$</td>
</tr>
<tr>
<td>$1.09 \times 10^7$</td>
<td>0.125</td>
<td>3000</td>
<td>$3.77 \times 10^8$</td>
<td>$2.05 \times 10^{-17}$</td>
<td>$1.21 \times 10^9$</td>
</tr>
</tbody>
</table>

number density appropriately. Expansion factors are also in Table 1. Then Eq. (H.2) reads:

$$Y_{CO}(t_{max}) = Y_C Y_{Onk} n_{CO} \tau_{CO}$$  \hspace{1cm} (H.4)

which is valid during expansions.

The lifetime of CO against dissociation is a composite of two physical reactions. Letting $\tau_\gamma$ be the photodissociation lifetime owing to thermal photons and $\tau_e$ be the dissociation lifetime owing to fast Compton electrons, we have

$$\frac{1}{\tau_{CO}} = \frac{1}{\tau_\gamma} + \frac{1}{\tau_e}$$  \hspace{1cm} (H.5)

Which partial lifetime dominates the dissociation depends on the temperature. The radioactive lifetime $\tau_e$ is taken to be $\tau_e(s) = 10^5 \exp((t - 10^6s)/111d)$, but the thermal photodissociation lifetime $\tau_\gamma$ depends strongly on temperature owing to the large binding energy of the CO molecule. Table H.1 displays a short list of $\tau_\gamma$ at key temperatures as well as several related quantities.

One sees from Table H.1 that $\tau_\gamma$ dominates Eq. (H.5) for $T > 3500$ K, whereas Compton electron dissociation $\tau_e$ dominates below 3500 K. We start computation of our chemical network at $T = 6000$ K, so $n_{CO}(t)$ will initially be small and will grow as temperature declines owing to the lengthening of $\tau_\gamma$ with falling temperature. After $t = t_{max}$ the abundance of CO declines owing to the destruction rate $1/\tau_e$ exceeding the creation rate in Eq. (H.1) while the gas cools.
to temperatures at which carbon chains can grow and isomerize to rings [Clayton et al. 1999]. Such rings are taken to be the nucleation upon which graphite grows.

Figure [H.1] compares our network calculation of the abundance of CO molecules with the expectation of Eq. (H.2) with $\tau_{CO} = \tau_{\gamma}$ dominating the destruction of CO. Solid points display the equilibrium product $n_{CO}^{eq}$ calculated from the factors shown in Table [H.1] and from the number densities $n_C$ and $n_O$ after their initial values at $T = 6000$ K have been reduced by the expansion factor $(t/t_{6000K})^{-3}$. Tight agreement for $T > 4000$ K is immediately evident, demonstrating that for $T > 4000$ K the abundance of CO is almost exactly in thermal equilibrium. Eq. (H.2) validly describes the black dots in Fig. [H.1] because creation and destruction terms are very nearly balanced while $T > 4000$ K. Below 3500 K the abundance of CO becomes much smaller than the expectation $n_{CO}^{eq}$ of thermal equilibrium because the dissociation of CO comes to be dominated by Compton electrons. The dashed vertical line at $T = 3500$ K marks the approximate boundary between these two mechanisms for CO dissociation. Notice carefully in Fig. [H.1] that $n_{CO}$ grows slowly as $T$ falls, not reaching its final maximum until expansion has cooled to $T = 3500$ K. Although it is obvious that equilibrium CO increases as $T$ falls, assuming that to occur begs the question of achieving equilibrium. Our kinetic results demonstrate that CO does quickly achieve its equilibrium abundance above $T = 4000$ K, and Eq. (H.3) shows that equilibrium to increase as $\tau_{\gamma}$ lengthens. At its final maximum $n_{CO} = 1.5 \times 10^6$ cm$^{-3}$, corresponding to $Y_{CO} = 0.7 \times 10^{-3}$. The slow growth of $n_{CO}$ shown in Fig. [H.1] differs markedly from the results of [Cherchneff and Dwek 2009]. Their results (e.g. Fig. 11) show $n_{CO}$ climbing quickly near 6000 K to a large maximum number fraction near 0.1. That maximum would almost exhaust free carbon. Our results in Fig. [H.1] so differ from theirs that the difference must be resolved. [Clayton 2013] has analyzed the expectation of growth of $n_{CO}$ to a single maximum before declining, and our results are in line with that expectation.

These features are further detailed in Fig. [H.2] which shows the reaction currents (reactions per second per atom) into and out of CO. There exists a near steady state in that the production of CO is almost balanced by the two flows destroying CO. The destruction flow $Y_{CO}/\tau_{\gamma}$ almost balances the association flow above 4000K except for a tiny excess leading to the slow growth of $n_{CO}$ evident in Fig. [H.1]. In that temperature range the production by $C + O \rightarrow CO + \gamma$ is in equilibrium with the thermal radiation field, as Fig. [H.1] implied. The
Figure H.1  Comparison of the density of CO molecules calculated by the numerical network (curve) with the expectation $n_{CO}^{\gamma eq} = n_C n_O k_{CO} \tau_\gamma$ for an abundance $n_{CO}$ in thermal equilibrium (dots) with photons. Above $T=4000K$ the CO abundance is seen to be in an accurate thermal equilibrium, but at lower temperature $n_{CO}$ is increasingly smaller than thermal equilibrium would require. Instead of thermal photons, the destruction of CO becomes increasingly dominated by Compton electrons for $T < 3500$ K. One see in Fig. H.1 that $n_{CO,max}$ occurs near 3500K, which occurs near $10^7$ s (see Table H.1).
Flows into and out of CO illustrate the near steady state between creation and destruction and the transition region near 3500K between the two modes of destruction of CO. The destruction flow $n_{CO} n_{C} k_{CO\rightarrow C}$ is only $3.27 \times 10^{-16}$ atom$^{-1}$s$^{-1}$, too small to be visible in Fig. II.2.
decline of the flow creating CO occurs owing to expansion. The destruction flow \( n_{CO}/\tau_e \) almost balances the creation flow below 3500 K. The transition between destruction modes occurs near 3500 K. It is no coincidence that the maximum of \( n_{CO} \) occurs when Compton electrons begin to dominate CO dissociation, because \( n_{CO} \) would continue growing as long as thermal photons dominate CO dissociation. Fig. H.2 also shows the destructive flow by inelastic electrons to slightly exceed the production flow for \( T < 3500 \) K. That modest difference causes CO to decline following its maximum.

H.5 Abundances of C\(_2\)

Figure H.3 displays the number density \( n_{C_2} \) along with that of \( n_{CO} \). Our examination of flows into \( C_2 \) shows that the reaction \( CO + C \rightarrow C_2 + O \) competes with the reaction \( C + C \rightarrow C_2 + \gamma \) only in the range \( 3400 \) K \( < T < 3900 \) K, but falls steeply for greater or lesser temperature. At higher \( T \) the abundance of CO is too small to create \( C_2 \) in this way, and at smaller \( T \) the cross section for \( CO + C \rightarrow C_2 + O \) declines too precipitously. [Cherchneff and Dwek 2009] missed that because their calculated abundance of CO was much too large. At its maximum \( n_{C_2} = 0.1 \) cm\(^{-3}\) is only about \( 10^{-7} \) of \( n_{CO} \). The reason \( C_2 \) is so rare is that its dissociation rate by thermal photons is much faster than that for CO because the binding energy of \( C_2 \) is so much less than that for CO. The smaller value of \( \tau_\gamma \) causes the steady state with thermal radiation for \( C_2 \), as in Eq. (H.3), to be much smaller than that for CO, so \( n_{C_2} \) grows much more slowly than \( n_{CO} \). The Compton electron lifetime \( \tau_e \) never plays a role for \( C_2 \), but the lifetime against oxidation becomes faster that \( \tau_\gamma \) when \( T \) falls below 3500 K. That transition establishes the maximum in Fig. H.3. This \( n_{C_2} \) maximum differs greatly from results in [Cherchneff and Dwek 2009], where their Fig. 11 shows the maximum atom fraction of \( n_{C_2} \) to be near \( 10^{-5} \), equal to about \( 10^5 \) cm\(^{-3}\), almost 1% of their \( n_{CO} \) at that time. And their maximum for \( C_2 \) occurs near 7000 K, far too hot for \( C_2 \) to be abundant in the face of rapid photodissociation. The huge differences between these two computations require an explanation. We find it likely that [Cherchneff and Dwek 2009] inadvertently omitted photodissociation by thermal photons from their destruction rates.

Figure H.4 shows the abundances \( Y_i \) of each species in our small network as a function of time \( t - t_{6000K} \) after \( T = 6000 \) K. From Table H.1 start time is \( t_{6000K} = 5.47 \times 10^6 \) s. To
Figure H.3  Number densities of CO and of C\textsubscript{2} as functions of temperature. The maximum density of C\textsubscript{2} is 0.1 cm\textsuperscript{-3}. Both abundances grow much more slowly than in the calculation by [Cherchneff and Dwek 2009].
Figure H.4  The abundance (number per atom) of linear chains $C_n$ and of ringed isomer $C_8^R$.

We have scaled each $Y_n$ by the factor stated in the box.
display each $Y_i$ on a figure with reasonable ordinate resolution, we have scaled each $Y_n$ by the factor stated in the box. Many features are noteworthy: (1) $Y_C$ and $Y_O$ are constant because their small depletion is negligible on the scale shown; (2) maxima of $Y_{CO}$ and $Y_2$ occur at almost exactly the same time $t - t_{6000K} = 4 \times 10^6$ s, as was also seen in Fig. H.3; (3) $C_3$ has very small abundance, about $10^{-7}$ of $Y_2$, although much later $Y_3$ slowly grows modestly relative to much more abundant $C_2$; (4) the rise shapes of $Y_4$ through $Y_8$ are very similar because they are linked by a near steady state; (5) the ringed carbon abundance $Y_{r8}$ has similar abundance shape vs. time, but notice that it is actually much more abundant than linear $C_{7-8}$ and because it accumulates from isomeric transitions of $C_8$ and unlike $C_n$ does not suffer from fast oxidation [Clayton et al. 1999]. Each of these features is understandable in terms of the flows into and out of each species.

One sees from Fig. H.4 that the CO+C → $C_2$+O reaction plays no role in $C_8^r$ production from the fact that $C_8^r$ rises only for $t - t_{6000K} > 1.5 \times 10^7$ s, corresponding to $T < 2000$ K, despite $C_2$ and $C_3$ rising at much earlier times. Whatevsoever $C_2$ is made earlier plays no role in $C_8^r$ production because the ejection of C atoms from $C_n$ at higher $T$ prevents the flow to $C_8$. Only at $T < 2000$ K do those photodissociation reactions become so slow that $C_8$ can grow, which it does from the $C_2$ recently formed by the $C + C → C_2 + \gamma$ reaction near 2000 K. Fig. H.4 also shows that $Y_{r8}^r$ grows quickly to $10^{-16}$. Since available C is $Y_C = 0.1$, the ratio gives $10^{15}$ C/ring. This is enough to grow very large graphite.

Figure H.5 shows the shape of $C_n$ vs. $n$ for $C_3$ to $C_8$ at two different temperatures near 2000 K. As temperature declines, the curve flattens because photoejection from $C_n$ by thermal

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$T = 2031$K</th>
<th>$T = 1802$K</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_5(C, \gamma)C_6$</td>
<td>$1.67 \times 10^{-29}$</td>
<td>$4.79 \times 10^{-28}$</td>
</tr>
<tr>
<td>$C_6(\gamma, C)C_5$</td>
<td>$1.67 \times 10^{-29}$</td>
<td>$4.79 \times 10^{-28}$</td>
</tr>
<tr>
<td>$C_6(C, \gamma)C_7$</td>
<td>$2.41 \times 10^{-39}$</td>
<td>$2.12 \times 10^{-32}$</td>
</tr>
<tr>
<td>$C_7(\gamma, C)C_6$</td>
<td>$1.26 \times 10^{-40}$</td>
<td>$7.27 \times 10^{-40}$</td>
</tr>
<tr>
<td>$C_6(O, CO)C_5$</td>
<td>$3.61 \times 10^{-31}$</td>
<td>$2.90 \times 10^{-32}$</td>
</tr>
</tbody>
</table>
Figure H.5  Shape of log $10(Y_n)$ vs. $n$ for C$_3$ to C$_8$ at two different temperatures near 2000K. These shapes can be understood by the relative magnitudes of flows into and out of C$_n$. 
photons (or vibrations) weakens. These abundance ratios are almost in a steady state, but that steady state changes slightly as $T$ falls. These patterns show almost equal values for $Y_3$ because that curve is relatively flat with time near $t - t_{6000\text{K}} = 10^7 \text{s}$ (Fig. H.4). Table H.2 lists our computed reaction flows both in and out of C$_6$ at $T = 2031$ K and $T = 1802$ K. The reactions are specified there in the compact notation target(in,out)residual. We tabulate the flow magnitudes for C$_6$ to aid readers checking our numerical results. Fig. H.5 and Table H.2 are made to be studied together. Note that the abundances of C$_8$ are very small: $Y_8 = 10^{-36}$ at $T = 1802$ K. The isomeric transition from linear to ringed C$_8$, for which we estimate a lifetime $\tau = 10 \text{s}$, provides the nucleation for graphite growth.

We call attention to several conclusions to be drawn from Table H.2. Firstly, the strongest flows by a wide margin involving C$_6$ are C$_5 + C \rightarrow$ C$_6$, which is very fast ($k = 3 \times 10^{-10} \text{cm}^3\text{s}^{-1}$) because vibrational excitation of C$_6$ obviates the need for creating a photon [Clayton et al. 1999], and its inverse reaction which ejects a C atom. Furthermore, those two flows are equal to each other to three significant figures, illustrating the near steady state of the abundance pattern. Secondly, thermal dissociation of C$_6$ is very much faster than its oxidation, showing the small effect of oxidation on the abundance pattern. The destroying flows from C$_6$ to C$_5$ stand in the approximate ratio C$_6$(γ, C)/C$_6$(O, CO) = 5 \times 10^5$ at $T = 2031$ K and $2 \times 10^4$ at $T = 1802$ K. Dissociation by thermally excited vibrations dominates oxidation. What we here label (γ, C) is actually radiationless. Note that oxidation of C$_n$ molecules is not faster than C-ejection reactions. This unusual situation occurs because the C-capture reactions proceed by exciting vibrations of the C$_6$ molecule. That residual vibrational energy makes capture reactions fast rather than slow, but also makes the inverse C-ejection reactions caused by thermally excited vibrations to be much faster. Detailed balance gets the ratio right. The smaller value for that ratio at $T = 1802$ K occurs because oxidation maintains its effectiveness as $T$ drops but thermal disruption does not, being much more temperature sensitive. For this reason the abundance pattern is flatter and C$_6$ is approximately 3000 times more abundant at $T = 1802$ K than at $T = 2031$ K. It is for that reason that destruction flows in Table H.2 for C$_6$ are larger at the smaller temperature. The steady state shifts to new ratios as $T$ falls. Thirdly, calculation of the rates will be illustrated for sake of clarity by the flow C$_6$ + O \rightarrow CO + C$_5$. From Fig. H.5 one sees that at $T = 2031$ K the abundance $Y_6 = 10^{-33.3}$. The value of
\[ Y_O = 10^{10} \text{cm}^{-3}/1.1 \times 10^{10} \text{cm}^{-3} = 0.909, \] so the flow per atom per second (e.g., Eq. [H.3]) is
\[ \frac{dY}{dt} = Y_O (2031K)k(C_6 + O). \] Expansion from \( T = 6000 \text{ K} \) to \( T = 2031 \text{ K} \) has diluted the total number density \( n \) to 
\[ 1.1 \times 10^{10} \text{cm}^{-3}(2031 \text{K}/6000 \text{K})^3 = 4.27 \times 10^8 \text{cm}^{-3}. \] The fast oxidation reaction rate factor is
\[ k(C_6 + O) = 3 \times 10^{-10} \text{cm}^3\text{s}^{-1}. \] Gathering factors yields approximately 
\[ 4 \times 10^{-35} \text{ per atom per second in good approximation to the Table [H.2] flow entry 3.61 \times 10^{-35} \text{ per atom per second}.} \]

Our calculations have shown clearly that producing \( C_2 \) molecules near 5000 \text{ K} via the CO + C reaction [Cherchneff and Dwek 2009] is not a viable prospect for condensation of carbon dust via linear carbon chains. The abundance of CO is far too small for it to seed high-T \( C_2 \) production. The abundance of \( C_8 \) rings grows much later (Fig. [H.4]) near 2000\text{K}, as [Clayton et al. 1999, Clayton et al. 2001] had found. These rings grew from \( C_2 \) created by simple carbon association, \( C + C \rightarrow C_2 + \gamma \). Furthermore, the abundance of \( C_2 \) is very small near 5000 \text{ K} (Fig. [H.3]), primarily because its thermal dissociation rate is much too fast for it to have significant abundance at that high \( T \). What little \( C_2 \) is made at 5000 \text{ K} is immediately dissociated by thermal photons. Therefore its small steady-state abundance is inadequate for building abundances of \( C_3 \) and beyond.

**H.6 Contrast with [Cherchneff and Dwek 2009, Cherchneff and Dwek 2010]**

The large numerical differences between the results of [Clayton et al. 1999, Clayton et al. 2001] and those of [Cherchneff and Dwek 2009, Cherchneff and Dwek 2010] seem to be characterized by these differences:

1. Instead of growing large CO abundance near \( Y_{CO} = 0.1 \) at \( T = 5500 \text{ K} \) as in Fig. 11 of [Cherchneff and Dwek 2009], we find that \( Y_{CO} \) builds to a maximum of only \( 10^{-3} \), which it achieves only slowly (Fig. [H.3]), reaching that maximum only at \( T = 3500 \text{ K} \) rather than 5500 \text{ K}.

2. We find a maximum number density \( n_{C_2} = 0.1 \text{ cm}^{-3} \), only about \( 10^{-7} \) of \( n_{CO} \). We find \( C_2 \) to be rare at high temperature because its dissociation rate by thermal photons is very much faster than for CO owing to the smaller binding energy (6.3eV) of \( C_2 \). This \( n_{C_2} \) maximum differs greatly from results in [Cherchneff and Dwek 2009], where their Fig. 11 shows the maximum atom fraction of \( n_{C_2} \) to be near \( 10^{-5} \), equal to about \( 10^5 \text{ cm}^{-3} \), almost 1\% of \( n_{CO} \) at that time. Our \( C_2/CO \) abundance ratio is, in other words, only \( 10^{-5} \) of the same ratio calculated by [Cherchneff and Dwek 2009].
We reason that these big differences can be understood if [Cherchneff and Dwek 2009] had inadvertently omitted the thermal dissociation rates of small carbon molecules. Believing that to be the cause for the discrepancy, we tested that hypothesis by performing our own trial calculation involving only C, O, CO, C$_2$, and C$_3$, as they had done, and omitted the $\tau_\gamma$ destruction terms and the oxidation of C$_3$. Figure H.6 displays the result. The rapid rise of $Y_{CO}$ to about $10^{-2}$ at high temperature is very similar to Fig. 11 of [Cherchneff and Dwek 2009]. Similar also is $Y_2$, which grows quickly (Fig. H.6) to $2 \times 10^{-4}$ of $Y_{CO}$, whereas our Fig. H.3 shows the true value of $Y_{CO}$ to be only $10^{-8}$ at $T = 5500$ K and, considerably later, $Y_2/Y_{CO} = 10^{-7}$ at their maxima.

With photodissociation turned off, the destruction of C$_2$ occurs primarily by oxidation, C$_2$ + O $\rightarrow$ CO + C, whereas production of C$_2$ is by CO + C $\rightarrow$ C$_2$ + O, the reaction we study in this work. Those reactions strive to balance, which if achieved would establish a steady state ratio $Y_{CO}/Y_2 = 3.5 \times 10^4$. Fig. H.6 and their Fig. 11 do show approximately that value, but $Y_2$ declines faster than $Y_{CO}$ because of declining production of C$_2$ as T declines.

We could not expect detailed agreement with [Cherchneff and Dwek 2009], even if our hypothesis for the cause of the discrepancy is correct. Our calculation used O/C = 10 whereas they used O/C = 3 for the zone of their SNII model. The temperature profiles also differ, we using $T = 3800K/(t/100d)$ and they $T = 18500K/(t/100d)^{1.8}$. We believe that their $T$ is too hot owing to omission of CO cooling ([Liu and Dalgarno 1996], Fig. 5), which we tried to accommodate roughly by the choice $T = 3800$ K at $t = 100d$, which is about 50% of the temperatures published within models that do omit CO cooling. And owing to the factor $t^{-1.8}$, their $T$ falls through a specified temperature drop (say, 5000 K to 3000 K) more quickly than does our parameterization. Nonetheless, any $T$ profile declines though 5000 K and reaches 3000 K somewhat later, so basically similar abundance results are expected.

Such detailed differences are small in comparison with inclusion of thermal photodissociation. The similarity of our Fig. H.6 to Fig. 11 of [Cherchneff and Dwek 2009], and the huge differences of these figures from those of our network amounts in our minds to a resolution of the discrepancy.

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Figure H.6 Abundances for network containing only C, O, CO, C\textsubscript{2}, and C\textsubscript{3} when photodissociation of molecules is omitted. Rapid rise of $Y_{CO}$ to $10^{-2}$ near 5500 K and the ratio $Y_{CO}/Y_2$ near $10^4$ are similar to Fig. 11 of Cherchneff and Dwek 2009.
Appendix I

Figure Instructions

To make the figures in this thesis, one needs to checkout our nucnet-projects code and install certain libraries to compile our code. The instructions of installing these libraries can be found at Dr. Meyer’s tutorial: [http://sourceforge.net/u/mbradle/wiki](http://sourceforge.net/u/mbradle/wiki)

After install the necessary libraries, just create a projects directory:

```bash
mkdir projects
```

Change into the projects directory:

```bash
cd projects
```

Now checkout the project:

```bash
svn checkout https://subversion.assembla.com/svn/simple-Ia/trunk simple-Ia
```

Now change into the project directory and compile the code:

```bash
cd simple-Ia
make all_Ia
```

Upon successful compilation, there will be executables like `run_entropy`. Then download the data files:

```bash
make data
```

Then one can run the simple Ia calculation. For example to run a calculation with initial

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2 The code sits on assembla.com temporarily and will be moved to sourceforge.net eventually.
density of $9 \times 10^9 g/cm^3$, initial temperature of $1.5 \times 10^9 K$, star mass of 1.5 solar mass and only consider nuclei with proton number equal or smaller than 50:

```
./run_entropy ../nucnet-tools/data_pub/my_net.xml zone.xml out_9.0e9.xml 9.e9 "[z <= 50]"
```

The initial temperature and star mass are set in `zone.xml`. Also there are several other parameters that can be set in the xml file, like end time, initial time step, neutrino chemical potential, whether to use approximate weak rates, whether to include neutrino/photon entropy loss, whether to use screening, whether to use detailed weak rates, etc. After got an output xml file (`out_9.0e9.xml` in the example above), one can use the nucnet-tools examples to analyze it. To do this, the analysis examples need to be compiled:

```
cd ../nucnet-tools/examples/analysis
make all_analysis
```

```
cd -
```

Now let’s look at the instructions for making each figure.

**I.1 Figure 2.1**

To make the data for figure 2.1:

```
../nucnet-tools/examples/analysis/print_properties out_9.0e9.xml time x > x.txt
```

A line in x.txt gives the time (column 2) and the x value (column 3).

To create figure 2.1 plot column 3 of x.txt versus column 2 of x.txt.

**I.2 Figure 2.2**

To make the data for figure 2.2:

```
../nucnet-tools/examples/analysis/print_properties out_9.0e9.xml time y r_0 > v.txt
```
A line in v.txt gives the time (column 2), y (column 3) and the initial radius (column 4).

To create figure 2.2 plot column 3 times column 4 of v.txt versus column 2 of v.txt.

To make it a little bit easier, one may set the environmental variables. For bash:

```bash
export PATH=$PATH:../nucnet-tools/examples/analysis/
```

Then to do the same analysis:

```bash
print_properties out_9.0e9.xml time y r_0 > v.txt
```

Alternatively one can edit the .bash_rc or .bash_profile file in the home directory.

The reader may follow the instructions for each figure, or one can print out the properties to one file and choose the right columns to make corresponding figures. For example,

```bash
print_properties out_9.0e9.xml time t9 rho x y r_0 > prop_9.e9.txt
```

and the use prop.txt to make the plots.

### I.3 Figure 2.3

To make the data for figure 2.3

```bash
../nucnet-tools/examples/analysis/print_properties out_9.0e9.xml time t9 > T.txt
```

A line in T.txt gives the time (column 2) and T9 (column 3).

To create figure 2.3 plot $10^9$ times column 3 of T.txt versus column 2 of T.txt.

Other figures are generated in a similar way. Please contact the author for more information.
BIBLIOGRAPHY


