

To the Graduate Council:

I am submitting herewith a dissertation written by Suzanne T. Parete-Koon entitled “The QSE-Reduced Nuclear Reaction Network for Silicon Burning.” I have examined the final electronic copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Physics.

Michael Guidry

Major Professor

We have read this dissertation
and recommend its acceptance:

W. Raphael Hix

Witold Nazarewicz

Mark Littmann

Kate Jones

Accepted for the Council:

Carolyn R. Hodges

Vice Provost and
Dean of Graduate Studies

(Original signatures are on file with official student records.)

The QSE-Reduced Nuclear Reaction Network for Silicon Burning

A Thesis

Presented for the

Doctor of Philosophy

Degree

The University of Tennessee, Knoxville

Suzanne T. Parete-Koon

August 2008

Acknowledgments

Joining a research group is like joining a family. I have been very fortunate in the academic family that I have found at the University of Tennessee and Oak Ridge National Laboratory. I would like to thank my advisors Raph Hix and Mike Guidry for their guidance, time, patience, and support throughout the process of this work. I would also like to express my appreciation to my committee members (Witek Nazarewic, Mark Littmann, and Kate Jones) for taking the time to be on my committee, review my work, and provide helpful insight. I would like to thank Bronson Messer for help with FLASH and insightful discussions. Great thanks to Mark Littman, Marissa Mills, Betty Mansfield, Catherine Longmire, and Jack Neely for guiding my development as a science writer and introducing me to the world of science journalism. I would also like to thank my many academic siblings and cousins (Marc, Reuben, James S., James W., Dwayne, Jason, Jay, Ryan, Austin, Ted, Shuhua, Caroline, Meagan, both Eric L's, Elisha, Viktor, Andy, Will, Cara, Frankie, Luc D., Eun Ju, Nasrin, Val, and Erin) for their friendship and for keeping my life interesting (if not always quiet!). Special thanks also to Paul Lewis for pulling me out of my studies occasionally to look at real stars and supernova remnants and for the many all you-can-eat-ribs excursions.

My special thanks go to my husband, Tim Koon, who has supported me and often put his own ambitions on hold so that I could finish this degree. I also express my gratitude to my parents, Jo Wallace and Jesse Parete, my aunt Charlotte Wallace,

my in-laws, Jan and Steve Koon, and my grandparents, Jo and Jesse Parete Sr., and Carrie and Emmet Wallace, for their encouragement and support.

Development of the QSE-reduced network is a project that has been many years in the making, has had many authors, and may have many more. Therefore, I dedicate this work to all those who keep running when they know that the race is long.

Abstract

Iron and neighboring nuclei are formed by silicon burning in massive stars before core collapse and during supernova outbursts. Complete and incomplete silicon burning is responsible for the production of a wide range of nuclei with atomic mass numbers from 28 to 70. Because of the large number of nuclei involved, accurate modeling of these nucleosynthetic stages is computationally expensive. For this reason, hydrodynamic models of supernovae often employ a limited set of nuclei to track the nuclear energy generation until nuclear statistical equilibrium is reached. These limited approximations do not include many of the reaction channels important for the production of iron (Hix & Thielemann, 1996), making them a partial solution at best for energy generation during silicon burning (Timmes et al., 2000). Examination of the physics of silicon burning reveals that the nuclear evolution is dominated by large groups of nuclei in mutual chemical equilibrium before the global Nuclear Statistical Equilibrium (NSE) is reached and after temperatures drop below those needed to maintain NSE during explosive burning (Bodansky, Clayton, & Fowler, 1968). In this work a nuclear reaction network is built which takes advantage of Quasi Statistical Equilibrium (QSE) and NSE at the appropriate temperatures in order to reduce the number of independent variables calculated. This allows accurate prediction of the nuclear abundance evolution, deleptonization, and energy generation. Where conditions apply, the QSE-reduced network runs at least an order of magnitude faster and requires roughly a third as many variables as a standard nuclear reaction network

without a significant loss of accuracy. These reductions in computational cost make this network well suited for inclusion within hydrodynamic simulations, particularly in multi-dimensional applications.

Contents

1	Introduction	1
1.1	How Silicon Burns to Form Iron	3
1.1.1	Quasi Statistical Equilibrium	5
1.1.2	Silicon Burning Outcomes	8
1.2	Supernova Mechanisms	9
1.2.1	The Core Collapse Supernovae Mechanism	10
1.2.2	Thermonuclear Supernovae	13
2	Nuclear Reaction Network Fundamentals	18
2.1	Nuclear Reaction Rates	18
2.2	Nuclear Reaction Networks	22
3	The QSE-Reduced Network	25
4	Testing the QSE-reduced Network	34
4.1	Reducing the 299 Nuclide Network	38
4.1.1	Constant Conditions	38
4.1.2	Explosive Silicon Burning	43
4.2	Conclusion	73
4.3	Postlude	75
	Bibliography	76

List of Tables

4.1	Network Speed for Constant Conditions	42
4.2	Network Speed for Incomplete Silicon Burning	55
4.3	Network Speed for Complete Silicon Burning	64
4.4	Network Speed for Silicon Burning α -rich Freezeout	68

List of Figures

4.1	This shows the 1-group network configuration, where the evolution of all the species shown in black is follow by the two species, protons and neutrons, shown in red.	36
4.2	This shows the 2-group QSE-reduced network configuration. Independent species are shown in red. The large QSE group, stretching from magnesium to germanium, is shown in green, and the light QSE group is shown in black.	36
4.3	This shows the 3-group QSE-reduced network configuration. Independent species are shown in red. The silicon QSE group is shown in green, the iron-peak QSE group is shown in blue, and the light QSE group is shown in black.	37
4.4	This shows the 3*-group QSE-reduced network configuration. Independent species are shown in red. The silicon QSE group is shown in green, the iron-peak QSE group is shown in blue, and the light QSE group is shown in black.	37
4.5	A comparison between the full network (solid lines), the 3-group QSE-reduced network (circles), and the 2-group QSE-reduced network (crosses) for constant conditions is shown. A selection of important nuclei is shown.	39

4.6	Shown here are deviations of the abundances calculated with the 3-group QSE-reduced network from those calculated by the full network. The calculation with the original rate library is shown on the top panel and a calculation using the balanced rate library is shown on the lower panel. The circles are the dominant nuclei with mass fractions larger than 10^{-6} . The squares are mass fractions between 10^{-6} and 10^{-12} . The X's are mass fractions between 10^{-12} and 10^{-20}	41
4.7	An example of incomplete silicon burning is shown. The solid lines represent the full network calculation, the crosses the 2-group QSE-reduced network and the circles the 3-group QSE-reduced network. A vertical black line marks the time that corresponds to a temperature of 3.5 GK.	45
4.8	A comparison of the energy generation rate of the full network and the QSE-reduced network. The solid lines represent the full network calculation, the crosses the 2-group QSE-reduced network and the circles the 3-group QSE-reduced network. A vertical black line marks the time that corresponds to a temperature of 3.5 GK. The lower plot shows more detail for early times.	46
4.9	Ratios between abundances calculated with the QSE-reduced network and those calculated with the full network are shown for the case of incomplete silicon burning. Black symbols indicate the 3-group network and red symbols indicates the 2-group network. Circles are dominant nuclei with mass fractions greater than 10^{-6} . Squares are mass fractions between 10^{-6} and 10^{-12} and X's are mass fractions between 10^{-12} and 10^{-20}	48

4.10	Shown here are the ratios between abundances calculated by the QSE-reduced network and those calculated by the full network for incomplete silicon burning at 4 and 3.7 GK. Black symbols indicate 3-group and red symbols indicate 2-group. The 2-group network reproduces the abundances of the full network as the temperature drops to 4GK, but at lower temperatures the 3-group network gives the better match.	49
4.11	Shown here are ratios of abundances calculated with the QSE-reduced network and the full network for the case of incomplete silicon burning at 3.5 GK. Black symbols indicate the 3-group network and red symbols indicate the 2-group network. The 3-group network still matches the full network to 20% or better. Only the most abundant species of the 2-group network still match.	50
4.12	Shown are four variations for how the Adaptive QSE-reduced network can be tuned to switch between QSE group configurations during incomplete silicon burning.	52
4.13	Shown here is a comparison of the energy generation rate of the full network and the QSE-reduced network for incomplete silicon burning. A vertical black line marks the time that corresponds to a temperature of 3.5 GK. The lower plots show more detail for early and late times.	53
4.14	Shown here are the ratios between abundances calculated with the adaptive QSE-reduced network and those calculated by the full network for incomplete silicon burning. Black symbols indicate the 3-group network, red symbols indicate the Adaptive-1 run, and green symbols indicate the Adaptive-2 run. The shapes of the symbols have the same meaning as Figure 4.9.	54

4.15	Shown here are the ratios between abundances calculated with the adaptive QSE-reduced network and the full network for incomplete silicon burning. Black symbols indicate the 3-group network, red symbols indicate the Adaptive-3 run, and green symbols indicate the Adaptive-4 run.	56
4.16	An example of complete silicon burning is shown. The solid lines represent the full network calculation, the circles the QSE 3-group network, the crosses the QSE 2-group network, and the dotted lines the QSE 1-group network.	58
4.17	Shown here are the ratios of QSE-reduced to full network abundances for the case of complete silicon burning at early times. Here black symbols represent the 3-group network, red symbols represent the 2-group network, and green symbols represent the 1-group network. . .	59
4.18	Shown here are the ratios of QSE to full network abundances for the case of complete silicon burning at different times and temperatures. Black symbols represent the 3-group network, red symbols represent the 2-group network, and green symbols represent the 1-group network.	60
4.19	Ratio of the QSE-reduced to full network abundances for the case of complete silicon burning at 3.5 GK, where QSE is still valid. Black symbols represent the 3-group network, red symbols represent the 2-group network, and green symbols represent the 1-group network. . .	61
4.20	Shown here is a comparison of the energy generation rate of the full network, the 2-group network, and the adaptive QSE-reduced network. A vertical black line marks the time that corresponds to a temperature of 3.5 GK on both plots.	63

4.21	Shown here are the ratios of the abundances produced by the QSE-reduced networks to those produced by the full network for the case of complete silicon burning. Black symbols represent the 3-group network and red symbols represent the adaptive network. The two networks garner the same abundance results	65
4.22	An example of silicon burning with an α -rich freezeout is shown. The solid lines represent the full network calculation, the circles the 3-group QSE-reduced network, the crosses the 2-group QSE-reduced network, and the dotted lines the 1-group QSE-reduced network.	66
4.23	An example of silicon burning with an α -rich freeze out. A comparison of the energy generation rate during α -rich freeze out is shown. A vertical black line marks 3.5 GK.	67
4.24	Comparison of the QSE and the full network abundances for the case of silicon burning with an α -rich freezeout for early times and temperatures is shown. Black symbols represent the 3-group network, red symbols represent the 2-group network, and green symbols represent the 1-group network.	69
4.25	Comparison of the QSE-reduced and the full network abundances for the case of silicon burning with an α -rich freezeout at different times and temperatures is shown. Black symbols represent the 3-group network, red symbols represent the 2-group network, and green symbols represent the 1-group network.	70
4.26	Ratios of the Adaptive and 3-group QSE-reduced network abundances to those of the full network abundances for the case of silicon burning with an α -rich freeze out at 3.5 GK are shown. Black symbols represent th 3-group network and red symbols represent the adaptive network.	71

4.27	This shows the 2^* -group network configuration, where only two independent variables are used to follow the chemical evolution.	72
------	--	----

Chapter 1

Introduction

We study nucleosynthesis, the construction of the chemical elements, because it is one of the basic processes that made our existence possible. After the Big Bang, the early universe was composed of roughly 75% hydrogen and 23% helium by mass. (Rolfs & Rodney, 1988). For heavier elements like carbon, oxygen, and iron to form, the hydrogen had to be collected and heated to the point that its like-charged nuclei could fuse into heavier elements. Stars, which first coalesced about a billion years after the Big Bang, were just such collection points. A star is a natural nuclear fusion reactor that staves off the pull of its self-gravity with the energy produced in its core by nuclear fusion of hydrogen, helium, and other elements to form heavier elements. A star with an initial mass that is greater than 8-10 times the mass of our sun can fuse elements up to iron in its core. Before they became part of our solar system, many of the chemical elements that compose our bodies and our world were forged by massive stars.

Iron and other heavy elements form in the innermost regions of a star but, in most cases¹, they are trapped there by gravity so they can not mix with the rest of the universe while the star exists. Both observations and computational simulations

¹If mixing by convection dredges deep enough in AGB stars, the AGB stars' winds can carry heavy elements, such as carbon, off the stars and out into the universe.

indicate that supernovae, the cataclysmic explosions that occur at the end of massive stars' lives, or on carbon-oxygen white dwarfs in binary systems are the primary factories and distribution centers for the heavy elements between oxygen and iron (Schramm & Arnett, 1975).

The abundances of nuclei released by supernovae can be observed in the spectra of supernova remnants and in the light produced by the explosion. For example, the amount of ^{56}Ni produced in Supernovae 1987a was estimated by observing the gamma rays produced by its daughter nucleus ^{56}Co (Shigeyama et al., 1988). Since nickel is believed to be produced in the innermost regions of the supernova, its abundance contains information about the inner workings of the explosion (Arnett et al., 1989). It is vital that the computational models of supernovae include the accurate schemes for reproducing the abundances of the nuclei produced so that model calculations can be compared and constrained by observation.

Computational simulations of supernovae nucleosynthesis need to model the hydrodynamics, which includes the local temperature and density conditions, transport of particles, the abundance of each nuclear isotope, the energy generated or absorbed by the nucleosynthesis and the energy released by gravitational process. For core collapse supernovae, it is also important to include radiation transport of neutrinos and anti-neutrinos since they carry away most of the energy released by the implosion of the core. The amount of physics that can be input is limited by computational constraints of memory and processor speed. There are hundreds of species involved in the reactions that form the iron-peak elements, so modeling their nucleosynthesis is computationally expensive (Woosley & Weaver, 1995). To follow the nuclear energy generation at a reasonable computational speed, hydrodynamic models of supernovae often employ a limited set of nuclei such as an α -network² composed of 13

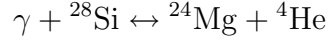
² α -nuclei are nuclei composed of multiples of ^4He . The nucleus of ^4He has two protons and two neutrons and is referred to as the α -particle. In alpha networks, nuclei are formed by captures of α -particles on α -nuclei. For example, $^4\text{He} + ^4\text{He} + ^4\text{He} \leftrightarrow ^{12}\text{C} + ^4\text{He} \leftrightarrow ^{16}\text{O} + ^4\text{He} \leftrightarrow ^{20}\text{Ne}$ etc.

to 14 nuclei from ${}^4\text{He}$ to ${}^{56}\text{Ni}$ or ${}^{60}\text{Zn}$ (Thielemann et al., 1996). The detailed nuclear evolution is then calculated later using temperature and density histories from the hydrodynamic simulations. This approach is called post-processing. Its success depends on how well the limited nucleosynthesis approach used in the hydrodynamic calculation estimated the nuclear energy generation and how important mixing is to the nucleosynthesis. Because their reactions are limited to equal numbers of protons and neutrons, α -networks can not follow the effects of electron captures on the overall neutronization³ of the matter (Timmes et al., 2000; Hix & Thielemann, 1996). The degree of neutronization affects the rate at which silicon is destroyed by altering the reaction paths (Hix & Thielemann, 1996). Studies of terrestrial iron-peak elements show that they have a low content of neutron-rich isotopes compared to that produced by recent supernovae simulations (Herant et al., 1994; Janka & Müller, 1995; Kifonidis et al., 2003). To allow models to better match observations, an efficient but more complete scheme for modeling iron formation *in situ* in hydrodynamic supernovae simulations is needed. In the following sections I will present such a scheme and demonstrate its utility and limitations.

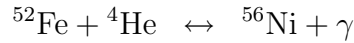
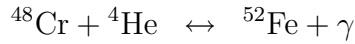
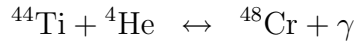
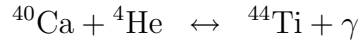
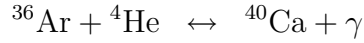
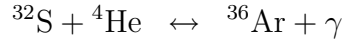
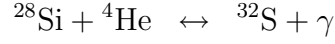
1.1 How Silicon Burns to Form Iron

It takes temperature in excess of 3 billion Kelvin, to allow silicon to fuse with lighter particles such as protons, neutrons, and α -particles to form heavier elements. At these high temperatures energetic photons are abundant and they bombard the silicon, knocking off protons, neutrons, and α -particles. An example of this process, called photodissociation, is given below where the γ symbol represents photons with energies of several MeV.

³Neutronization is the process of making the composition of nuclei more neutron rich, both in the number of free neutrons and those contained within the isotopes of the elements. In supernovae, the neutronization is accomplished by neutrino reactions that change protons into neutrons.



The particles released by photodissociation can undergo a sequence of reactions like:



i This sequence can continue above Nickel. Proton and neutron captures and their dissociations contribute to this sequence as well and often dominate, but for simplicity I have only shown α -reactions. As long as temperatures exceed 3 billion Kelvin (3 GK) each of these reactions run almost in chemical equilibrium, meaning that the forward rate of the reaction is about the same as the reverse rate. This is how the supply of light particles and energetic photons is maintained as silicon slowly melts through this sequence into iron. At high enough temperatures the rate of photodissociations and other collisions melt the composition entirely into protons, neutrons, and ${}^4\text{He}$.

Weak force reactions change neutrons into protons or vice versa in the nucleus. The ratio of protons to nucleons in the overall composition is called the electron fraction, Y_e .

$$Y_e = \sum_i Z_i/A_i X_i, \quad (1.1)$$

where Z_i is the proton number of species i , A_i is the atomic number, and X_i is the mass fraction. The most abundant nucleus produced during equilibrium will be the one with the highest binding energy which also has a ratio of protons to nucleons that matches the global Y_e . The electron fraction also affects how well the chemical equilibrium can be maintained at a given temperature and density since different compositions open faster and slower reaction channels (Hix & Thielemann, 1996). Explosive silicon burning occurs on timescales that are so short that the effect of the weak reactions on the global Y_e is limited.

1.1.1 Quasi Statistical Equilibrium

If all the reactions are in equilibrium, the composition is said to be in nuclear statistical equilibrium (NSE). Under hydrostatic conditions like those encountered in stellar interiors, NSE can be achieved at 3.5 GK, but for explosive burning, temperatures greater than 6 GK are required for NSE to keep up with the rapidly varying temperature and density. If some reactions remain out of equilibrium, then isolated groups of nuclei form, each with a unique equilibrium within itself. These are called quasi-statistical equilibrium (QSE) groups. A QSE group's membership is weakly dependent on temperature and density and strongly dependent on neutronization (Hix & Thielemann, 1996). The membership of these groups also varies with time as the composition approaches NSE. Whether the composition maintains NSE or QSE depends on the rate of change of the temperature and density. During explosive burning, QSE groups can be maintained for temperatures between 3 and 6 GK. Below 3 GK, the QSE groups fall apart because photodissociation of the nuclei is no longer occurring rapidly enough to balance the light particle captures. This is called freezeout.

The physics of chemical equilibrium follows from the chemical potential. For a group of nuclei in QSE, the chemical potential of any group member can be expressed

in terms of the sum of the chemical potentials of the proton, neutron, and one focal nucleus chosen from the group members:

$$\mu_{AZ} = \mu_{focal} + (Z_{AZ} - Z_{focal})\mu_p + (N_{AZ} - N_{focal})\mu_n \quad (1.2)$$

Here $(Z_{AZ} - Z_{focal})$ and $(N_{AZ} - N_{focal})$ are the number of protons and neutrons need to build the species AZ from the focal nucleus. For a group of particles obeying Boltzmann statistics, the chemical potential of each species can be written

$$\mu_{AZ} = m_{AZ}c^2 + k_B \ln \left[\frac{Y_{AZ}\rho N_a}{G_{AZ}} \left(\frac{2\pi\hbar^2}{m_u k_B T} \right)^{3/2} \right], \quad (1.3)$$

Where m_{AZ} is the mass of the species AZ , c is the speed of light, k_B is Boltzmann's constant, Y_{AZ} , is the abundance of the species AZ , G_{AZ} is the partition function, ρ is the density and T is the temperature.

Equation 1.3 can be substituted into equation 1.2 and solved to get an expression for the abundances of the i th element.

$$Y_{\text{QSE},focal}({}^AZ) = \frac{C({}^AZ)}{C(Y_{focal})Y_p^{Z-Z_{focal}}Y_n^{N-N_{focal}}}, \quad (1.4)$$

where I have defined

$$C({}^AZ) = \frac{G({}^AZ)}{2^A} \left(\frac{\rho N_A}{\theta} \right)^{A-1} A^{\frac{3}{2}} \exp \left(\frac{B({}^AZ)}{k_B T} \right) \quad (1.5)$$

and

$$\theta = \left(\frac{m_u k_B T}{2\pi\hbar^2} \right)^{3/2}.$$

A is the atomic number. N is the neutron number. $B({}^AZ)$ is binding energy of the nucleus AZ . N_A is Avogadro's number. Y_p and Y_n are the abundances of free protons and neutrons and the integers $(N_{AZ} - N_{focal})$ and $(Z_{AZ} - Z_{focal})$ are the

number of such nucleons needed to construct the nucleus AZ from the focal nucleus. Thus to follow the evolution of every member of a QSE group through conditions of the changing temperature and density, one only needs to track the abundances of protons, neutrons, and one focal nucleus.

For simplicity this expression was derived in the absence of electron screening of the nucleus. The presence of the electrons around a positively charged nucleus, reduces the Coulomb repulsion between the nucleus and other positively charged particles. Electron screening increases the probability of reaction between two positively charged nuclei and, therefore, the overall reaction rate for those species. Screening corrections for QSE were covered in Hix (1995) with the impact being a change in the binding energy to reflect the changed chemical potential of the protons and nuclei.

As will be shown in Section 4, the calculation speed of a nuclear reaction network varies nonlinearly with the size of the network. Thus, small reductions in the number of variables lead to large increases in speed. The first attempt to take advantage of this was by Bodansky, Clayton, & Fowler (1968), hereafter BCF. They used the principles of QSE to follow the evolution of a large group of nuclei stretching from magnesium through the iron-peak nuclei by following ${}^{28}\text{Si}$ and the lightest nuclei—protons, neutrons, and ${}^4\text{He}$ —whose reactions held the group in equilibrium. Their reduced network reproduced the most dominant abundances but did not reproduce the full abundance pattern or early behavior of the dominant species. Woosley et al. (1973) noticed that at lower temperatures the BCF large QSE group split in to two distinct groups, one centered around the iron-peak nuclei and one centered in the intermediate mass nuclei around silicon. This configuration of QSE garnered a better overall match to non-reduced network abundances. Woolsey also demonstrated that the time for the two QSE groups to merge back into the larger group explored by BCF could be determined. This led to further exploration of the factors that determined the number of groups and the group membership. Thielemann & Arnett

(1985) and Hix & Thielemann (1996) demonstrated that the path of the nuclear flow from the silicon group to the iron-peak group and the membership of these groups depends strongly on the amount of neutronization. Hix & Thielemann (1996) further demonstrated that for material which has undergone significant neutronization, the separation between the silicon and iron-peak groups persists through a significant part of the nuclear evolution. In spite of these complications, Hix & Thielemann (1999a) showed that QSE could provide a reasonable estimate of the abundances of many species during silicon burning, even under explosive conditions, where the photodisintegration reactions freeze out before their corresponding particle captures. This dissertation centers on building a QSE-reduced network that can be tuned to pick the proper QSE group size and membership for the hydrodynamic conditions.

1.1.2 Silicon Burning Outcomes

There are three primary types of silicon burning, which are determined by the evolution of the temperature and density conditions. These are complete silicon burning, with normal freezeout, complete silicon burning with α -rich freezeout, and incomplete silicon burning.

Complete silicon burning occurs at temperatures in excess of 5 billion Kelvin where almost all of the silicon is fused to iron-peak nuclei. For typical expansion rates, if the density exceeds $2 \times 10^8 \text{ g cm}^{-3}$, the triple alpha process, which combines three ^4He into ^{12}C , can run at a sufficient rate to fuse the α -particles that are not captured by heavier nuclei into carbon (Thielemann et al., 1990; Thielemann et al, 1986). As the temperature drops, the photodissociation-producing ^4He lags behind ^4He fusion and the alpha captures cease because of a lack of available helium. This is called normal freezeout. The composition at the end of normal freezeout is similar to that of the NSE, with only a few particle captures happening as the matter cools.

At densities below $2 \times 10^8 \text{ g cm}^{-3}$, the triple alpha process can not bind up the

large helium abundances as the temperature drops (Thielemann et al, 1986). This results in an excess of ^4He . The excess of helium allows further alpha captures to occur on heavy nuclei after NSE has frozen. Thus when conditions produce an α -rich freezeout, the NSE composition is distorted by the presence of nuclei made by excess alpha captures, such as ^{60}Zn as well as lighter nuclei like ^{44}Ti , made from the continued flow through the triple alpha process.

For typical supernova timescales, incomplete silicon burning happens for peak temperatures between 3 and 5 billion Kelvin. In this case, a significant fraction of the mass stays in silicon and its near nuclear neighbors. The composition can not form NSE because temperatures are not high enough to push enough reaction flow past extremely stable nuclei like ^{40}Ca in the available time. Instead QSE groups form and are maintained until a temperature decrease causes proton, neutron, and alpha reactions to freeze out.

In the next two sections, I will discuss core collapse and thermonuclear supernovae, the primary sites of explosive silicon burning.

1.2 Supernova Mechanisms

As mentioned in section 1.1, the terrestrial abundances of elements from silicon to iron and nickel result from supernovae. Because of their sudden appearance and extraordinary brightness, supernovae have been well documented throughout human history. Our current understanding is that there are two distinct mechanisms that produce these violent displays, the collapse of a stellar core or the thermonuclear disruption of a white dwarf.

1.2.1 The Core Collapse Supernovae Mechanism

Core collapse supernovae, which include events categorized observationally as Type II, Type Ib, and Type Ic, are gravity-powered events. The designation Type II denotes supernovae that have prominent hydrogen lines in their optical spectra, while Type I denotes those supernova that do not. However, 40 years of study have revealed that Type II, Type Ib, and Type Ic supernovae have a common mechanism with the observed differences resulting from differences in the stars' exteriors unrelated to the supernova mechanism.

Core collapse supernova spew metal-rich matter trapped in the gravitational well of a star into the interstellar medium; however the composition of the ejecta is greatly altered by the explosion. In addition to the elements up to iron and nickel, core collapse supernovae are believed to be the source of half the elements heavier than iron, which form by rapid capture of neutrons on heavier elements. This mode of nucleosynthesis is called the r-process. It occurs on heavy seed nuclei in a neutron-rich environment, such as inner ejecta of core collapse supernovae. The iron formation processes studied in this work sets the stage for the r-process, and determines the number and mass of heavy seed nuclei and the free neutron abundances.

As a massive star evolves, its primary core fuel, hydrogen, is fused to helium. As the fuel dwindles the star's core can not maintain the pressure needed to balance its self-gravity and the core begins to compress, causing a rise in its temperature. When the temperature becomes high enough and the matter dense enough, the helium ash left from the hydrogen fusion ignites and burns, producing the pressure needed to re-establish the core's hydrostatic equilibrium. The star repeats this process as it ages, burning successively heavier elements as its core fuel. Shells of successively heavier elements from the ash of each burning stage form around the core like sections of an onion. As the star contracts these shells ignite, repeating the nucleosynthesis that occurred in the core. The last stage of a massive star's life occurs when fusion of

silicon to iron becomes the core's primary energy source. Iron and its close nuclear neighbors are called the iron-peak elements because they form a peak in the solar abundance curve. They have the highest binding energy per nucleon of all nuclei, therefore fusion of the iron-peak nuclei absorbs energy rather than releasing it. As iron forms, the star no longer has an energy source to fight the relentless pull of its self-gravity. For a short time, the core is supported by a pressure derived from the quantum mechanical properties of its electrons, called electron degeneracy pressure. Electron degeneracy pressure is a consequence of the Pauli Exclusion Principle, which states that no two fermions⁴ can occupy identical quantum states. The gravity of the core compresses the electrons so that several electrons have almost the same position. To avoid violating the Pauli Exclusion Principle, the electrons must occupy significantly different momentum states. All the lowest available momentum states fill and the matter cannot compress any further without violating the Pauli Exclusion Principle (Kippenhann & Weigert, 1990). The highest momentum state occupied is called the Fermi momentum. The maximum mass that electron degeneracy pressure can support, which is roughly 1.4 solar masses for matter with equal numbers of protons and neutrons, is called the Chandrasekhar limit. The nuclear burning shells around the core continue fusing silicon, adding more iron mass to the core. Eventually the core exceeds the Chandrasekhar mass limit, which is $\tilde{1}$ solar mass for the neutron-rich core. The core collapses until its matter is roughly the same density as that of the nucleons in the nucleus. The electrons combine with protons in the core's atoms to form neutrons and neutrinos are released in the process.

The core is now a proto-neutron star supported against further collapse by neutron degeneracy pressure and the repulsive core of nuclear potential. Neutron degeneracy pressure is analogous to the electron degeneracy pressure, where the pressure is derived from the quantum mechanical properties of the nucleons. The in-falling

⁴Electrons and all $\frac{1}{2}$ -integer spin particles are fermions. Spin is the quantum number that specifies the intrinsic angular momentum of the electron.

matter rebounds off the incompressible core and sends a shock wave out through the rest of the star. In simulations, this shock stalls due to energy loss from escaping neutrinos and energy lost tearing apart highly bound nuclei into their constituent neutrons and protons (Arnett, 1996; Thompson et al., 2003). It is believed that flux of neutrinos from the cooling proto neutron star is so intense that enough neutrinos interact with the matter to redeposit about 1% of the escaping energy. This reenergizes the shock and ultimately drives the explosion (Bethe & Wilson, 1985).

Spherically symmetric simulations of supernovae, which use the best available physics, have not been able to produce an explosion with this mechanism (Mezzacappa et al., 2001). The most complete simulations of neutrino transport show that the amount of energy transferred from the escaping neutrons is too small to revitalize the explosion (Mezzacappa et al., 1998; Rampp & Janka, 2000). This does not necessarily indicate that this delayed shock mechanism is a failure, but rather that departures from spherical symmetry are important. Advances in computer technology have begun to make multi-dimensional models of supernovae with more realistic microphysics possible. These models allow for the effects of convection and mixing of the onion-like layers of different fuels within the supernova. Initially, many of the 2-D models exploded (Herant et al., 1994; Burrows et al., 1995) but as better physics for the neutrino transport was implemented, these models also failed (Buras et al., 2003). However, the most recent simulations show explosions at later times. Improved multi-dimensional techniques, a still more complete treatment of neutrino transport and better nuclear physics inputs are being applied to the problem to reach a conclusion about the mechanism.

With the problems producing explosions in these models, most explosive nucleosynthesis calculations have been performed with an artificially induced shockwave of the appropriate energies (see, e.g., Woosley & Weaver, 1986, 1995; Chieffi et al., 2003) or with the inner workings of the supernova replaced with a thermal energy bomb

(Thielemann et al., 1996; Nagataki et al., 1998). Simulations that match the observed properties of Supernova 1987a show that the innermost ejecta experience complete silicon burning with an α -rich freezeout and incomplete silicon burning (Thielemann & Nomoto, 1996), where QSE groups play a dominant role in the nucleosynthesis. Thermonuclear energy generation becomes vital to predicting the thermodynamics in the innermost ejecta because the nuclear energy released by the recombination of α -particles into iron group nuclei is comparable to the change of thermal energy in the gas caused by the expansion of the ejecta. This means that there is likely to be considerable feedback between the rate of these recombination reactions and the thermodynamic conditions that are causing them so the separation of the hydrodynamics from the nucleosynthesis implied by the post-processing approximation in simulations is problematic. For this reason, a fast but accurate nucleosynthesis scheme that can be coupled into multi-dimensional models of core collapse supernovae is highly desirable.

1.2.2 Thermonuclear Supernovae

Type Ia supernovae are believed to be thermonuclear explosions of carbon–oxygen white dwarfs (Hoyle & Fowler, 1960). Unlike core collapse supernovae, the energy for the explosion comes mostly from the nuclear reactions. The details of the mechanism that causes the explosion are still uncertain. Type Ia supernovae are among the most luminous stellar explosions, so it is possible to observe them at high redshifts (great distances). The designation Type Ia comes from their spectra, which lack hydrogen Balmer lines, lack helium lines and show a silicon absorption line near peak luminosity. Their light curves, showing the supernova’s brightness as a function of time, have distinctive characteristics and shape. Since light travels at a constant speed, the distance to a supernova is also a measure of how long ago it exploded. The redshift of the light also contains information about the relative expansion rate of the

universe since the explosion. Because of their luminosity and nearly homogeneous absolute brightness, Type Ia supernovae can shed light on the expansion rate of the universe and have been used as a tool for measuring cosmic distances.

A class of objects of known absolute magnitude can be used as a standard candle by which cosmic distance is measured. Type Ia supernovae do not have perfectly homogeneous absolute magnitudes at their maximum brightness, but extensive observational studies of many Type Ia supernovae light curves have indicated that there is a correlation between the shape of the light curves and the maximum brightness (Phillips, 1993; Hamuy et al., 1995; Reiss et al., 1996). In this way Type Ia supernovae are standardizable candles. However, better understanding of their mechanism is needed if we are to move beyond those empirical corrections and improve the standardization of the candles.

The three main models that have been suggested for the mechanisms that trigger the explosions are 1) a white dwarf that accretes mass from the Roche lobe overflow of an evolved companion star until the accreted matter pushes the mass of the white dwarf core over the Chandrasekhar limiting mass (Arnett, 1969; Nomoto et al., 1977; Khokhlov, 1991), 2) the merger of two carbon-oxygen white dwarfs (Tutukov & Yungelson, 1982; Iben & Tutukov, 1984; Webbink, 1984) and 3) detonation of helium on the surface of a low mass white dwarf (Nomoto, 1980; Woosley et al., 1980). Simulations of models one and two produce results similar to observations and mechanism. Model one is generally favored because of the relative rarity of double white dwarf systems and the difficulty in achieving the observed small scattering in luminosity (Höflich et al., 1996). Since the main energy source for the light curve is the decay of ^{56}Ni through ^{56}Co to ^{56}Fe (Nadyozhin, 1994), it is important that the models accurately reproduce the nucleosynthesis forming the iron-peak elements during the explosion if further understanding of the mechanism is to be achieved.

It is agreed that whatever the means of accretion, the added mass increases the

pressure in the core of the white dwarf, which raises the temperature near the center enough for $^{12}\text{C} + ^{12}\text{C}$ fusion to ignite (Arnett, 1996). This is followed by a period of convection during which temperatures increase due to the energy released by the fusion and additional pressure from the accreting material. After boiling for about 100 years, it is believed that fluctuations in density caused by the convection near the core cause temperatures high enough to allow fusion of oxygen and eventually silicon to ignite in a localized region (Timmes & Woosley, 1992). This burning region is called a flame. The initial laminar width of the flame front is believed to be on the order of thousandths of a millimeter (Timmes & Woosley, 1992). The exact ignition density and the location and number of points where the flame begins is still a source of significant debate, as simulations of the 100 year simmering phase are beyond current computational capabilities. (Thielemann et al., 2004).

After ignition it is believed that the flame begins to propagate subsonically as a deflagration through the core. The matter in the core is degenerate, which means that it does not expand until the thermal energy exceeds the Fermi energy, which is related to the Fermi momentum and is the highest energy level occupied by the core's degenerate electrons. Since there is no expansion, there is no cooling. The temperature in the burning region becomes so hot that the nuclear reactions run out of control. The localized heating drives convection which distorts the flame front and increases its surface area, enhancing the rate of burning. The flame accelerates through the white dwarf, fusing the majority of the nuclei into iron-peak elements. Whether the flame remains a deflagration or transitions to a supersonic detonation is an open question that is rather important to the nucleosynthesis. The flame speed effects how long the matter burns, which determines to what extent weak reactions can alter the electron fraction during the burning (Brachwitz et al., 2000). Timmes & Woosley (1992) found that models running with an abridged nuclear network underestimate the flame speed compared to those that run with a more complete set

of nuclei.

The temperature generated by the flame is ultimately high enough to break the degeneracy and a rapid expansion occurs that destroys the white dwarf and ejects matter into the interstellar medium. Observations indicate that the explosion’s kinetic energy is on the order of 1.3×10^{51} ergs (Thielemann et al., 2004). That 10^{26} times more energetic than the largest nuclear weapon ever detonated on Earth. Observations indicate that the complete thermonuclear disruption of the white dwarf produces predominantly iron-peak elements, like ^{56}Ni , typically in the amount of 0.6 to 0.8 solar masses, and smaller amounts of Si, S, Ar, and Ca. Models tuned to reproduce this composition indicate that both incomplete and complete silicon burning occurs in the flame. Many models produce an excess of neutron-rich iron-peak isotopes like ^{54}Fe and ^{58}Ni relative to solar abundances (Thielemann et al, 1986). Since the metals in our solar system are largely composed of the products of supernova nucleosynthesis, the solar abundances put strong constraints on how much neutron-rich matter is produced by supernovae. Parameterized 1-D models can be tuned to eliminate this problem, but it persists in self-consistent models (Thielemann et al., 2004).

Because the flame that ignites a thermonuclear supernova starts as a tiny spark and grows to the size of a planet, modeling a Type 1a is computationally challenging from the spatial standpoint alone. It is currently impossible to simultaneously model the scales of the whole white dwarf flame. Thus, sub-grid models of the initial flame are done separately using a resolution (grid) which is much finer than the resolution used to model the supernova explosion. These studies of the initial deflagration are then used to tune the initial energy and computational output of the supernova model. Even for sub-grid flame simulations the slow subsonic propagation speed of a deflagration front make following the flame with an explicit hydrodynamics code computationally demanding due to the spatial resolution needed to resolve the flame

and the enormous number of time steps that the calculation must be broken down into to accomplish this resolution for the entire flame front. There is little room in such calculations for the computational burden of nuclear reactions networks, however the nuclear reactions are the energy source driving the flame so they can not be entirely neglected.

Calder et al (2007) conducted a study of thermonuclear burning during carbon/oxygen fuel deflagrations, with the goal of producing a realistic flame model for simulations of Type Ia supernovae. Their study built on the advection-diffusion model of Khokhlov (1995), by following the burning through three different stages. The composition is assumed to be an equal mixture of ^{12}C and ^{16}O . During the first stage, carbon-carbon reactions form alpha particles, ^{16}O , ^{20}Ne , and ^{24}Mg . For the second stage, these species burn to the intermediate mass elements near silicon, producing conditions ideal for QSE. In the final stage, the QSE composition is followed into NSE, producing the iron-peak elements. Single zone studies with a 200 isotope network were used to supplement studies with the FLASH hydrodynamics code (Fryxell et al, 2000; Calder et al, 2002), where the main nuclear energy generation up to NSE was managed on an alpha nuclear reaction network. This approach was necessary because the full network was deemed too computationally expensive to run in situ in the flame model. Given the importance of the nuclear energy release and the need to follow the weak reactions in order to examine the production of neutron-rich iron-peak species, a faster but still accurate scheme for following the nuclear evolution is needed here too.

The QSE-reduced network described in the following sections is built with the aim of replacing alpha networks, where conditions of QSE apply.

Chapter 2

Nuclear Reaction Network Fundamentals

Prior to discussion of the QSE-reduced nuclear reaction network, it is useful to review the fundamentals of nuclear reaction networks.

2.1 Nuclear Reaction Rates

The most basic piece of information that can be determined about a nuclear reaction is its nuclear cross section. The cross section is defined as:

$$\sigma = \frac{\text{number of reactions target}^{-1}\text{sec}^{-1}}{\text{flux of incoming projectiles}} = \frac{r/n_j}{n_k v}. \quad (2.1)$$

The cross section is a measure of the probability per particle pair that a nuclear reaction will occur between the particles. It is used to calculate reaction rates and it can be determined in laboratory experiments where beams of particles bombard a target made of reactants to produce the desired reaction. To see how the reaction rate follows from the cross section, consider a gas made up of particles of two reactant nuclei j and k . Assume for simplicity that the relative velocity, v , between all

particles of j and k is constant. Arbitrarily j denotes the target nuclei and k the projectiles. Thus, all particles of j are considered to be at rest and all particles k are considered to have velocity v . The projectiles see an effective reaction area which is the product of the cross section for one target nucleus, j , multiplied by the number density n_j of the species j . The number of reactions occurring in the reaction area is proportional to the incident flux of projectiles, which is the product of the number density of k , n_k , and the velocity, v . The rate, r , of the reaction is simply the product of the reaction area and the incident flux.

$$r = \sigma v n_j n_k \quad (2.2)$$

In a gas, the relative velocity between particles varies over a wide range and the rate must be averaged over the velocity distribution. In this case, equation 2.2 is

$$r_{j,k} = \int \sigma(|\vec{v}_j - \vec{v}_k|) |\vec{v}_j - \vec{v}_k| d^3 n_j d^3 n_k. \quad (2.3)$$

The evaluation of this integral depends on the types of particles and distributions which are involved. For massive particles in astrophysical environments at sufficiently low densities, we may often assume that this velocity distribution is a Maxwell-Boltzmann distribution (Clayton, 1983) where,

$$d^3 n = n \left(\frac{m}{2\pi k_B T} \right)^{3/2} \exp\left(-\frac{mv^2}{2k_B T}\right) d^3 v, \quad (2.4)$$

allowing n_j and n_k to be moved outside of the integral. Equation. 2.3 can then be written as $r_{j,k} = \langle \sigma v \rangle_{j,k} n_j n_k$, where $\langle \sigma v \rangle$ is the velocity integrated cross section.

For thermonuclear reactions, these integrated cross sections have the form (Clayton, 1983; Fowler et al., 1967)

$$\langle j, k \rangle \equiv \langle \sigma v \rangle_{j,k} = \left(\frac{8}{\mu\pi} \right)^{1/2} (k_B T)^{-3/2} \int_0^\infty E \sigma(E) \exp(-E/k_B T) dE, \quad (2.5)$$

where μ denotes the reduced mass of the target-projectile system, E the center of mass energy, T the temperature and k_B is Boltzmann's constant.

When particle k in equation 2.3 is a photon, the distribution $d^3 n_k$ is given by Plank's distribution.

$$d^3 n_\gamma = \frac{8\pi}{c^3 h^3} \frac{E_\gamma^2}{\exp(E_\gamma/k_B T) - 1} dE_\gamma. \quad (2.6)$$

Plank's distribution gives the radiation density at a given temperature and wavelength of light. In the case of photodissociation reactions, it allows us to determine what fraction of the photons will have enough energy to dissociate light particles, such as protons, neutrons, and ^4He from larger nuclei.

The relative velocity for a photon is always c and thus the integral is separable, simplifying to

$$r_j = \frac{\int d^3 n_j}{\pi^2 (c\hbar)^3} \int_0^\infty \frac{c \sigma(E_\gamma) E_\gamma^2}{\exp(E_\gamma/k_B T) - 1} dE_\gamma \equiv \lambda_{j,\gamma}(T) n_j. \quad (2.7)$$

Due to the difficulty of measuring photodissociation cross sections, rather than evaluating the photodisintegration cross sections directly, nuclear reaction networks described in the next section, generally use the principle of detailed balance ¹ to express the photodissociation cross sections in terms of the capture cross sections for their inverse reactions, $l + m \rightarrow j + \gamma$ (Fowler et al., 1967). Thus $\lambda_{j,\gamma}(T)$ can be expressed

¹This works on the assumption that when a system is in equilibrium, its forward processes occur with the same frequency as its reverse processes.

$$\lambda_{j,\gamma}(T) = \left(\frac{G_l G_m}{G_j}\right) \left(\frac{A_l A_m}{A_j}\right)^{3/2} \left(\frac{m_u k_B T}{2\pi\hbar^2}\right)^{3/2} \langle l, m \rangle \exp(-Q_{lm}/k_B T). \quad (2.8)$$

Where $G = \sum_i (2J_i + 1) \exp(-E_i/k_B T)$ is the partition function, which accounts for the populations of the excited states of the nucleus, the A 's are the mass numbers of the nuclei involved, T is the temperature, $\langle l, m \rangle$ is the inverse reaction rate, and Q is the reaction Q -value, which is the energy released by the reaction,

$$Q_{lm} = (m_l + m_m - m_j)c^2 = -Q_j. \quad (2.9)$$

A wide variety of theoretical and experimental methods are employed to obtain the necessary data used to calculate each reaction rate over the range of temperatures and densities involved in astrophysical environments. The methods for measuring experimental nuclear rates and the kinds of experimental rate data currently available has been reviewed in detail by Rolfs & Rodney (1988); Thielemann (1998). Since experimental information is incomplete or non-existent for many of the thousands of rates needed for a basic nuclear reaction network, theoretical modeling of rates also plays a vital role.

Because the data for a reaction's forward and reverse rate may come from many different sources, and the relative amount of error between each source varies, the collective errors can have a profound effect on the accuracy of the reaction rate. Rate errors have a particularly strong effect for conditions that produce equilibrium. The temperatures that produce equilibrium are high so the rates are large and physically their forward and reverse reaction fluxes are oppositely equal. Small errors in the rates get magnified in the subtraction of the fluxes, causing flux cycles to form that leave the calculated abundances of the involved species out of true equilibrium.

In cases where the equilibrium is held between photodissociations and their reverse reactions, it is important that all the main reaction channels are present and

the reaction rates are accurate so that the methods of detailed balance can predict the correct equilibrium abundances for all the species at a given temperature.

2.2 Nuclear Reaction Networks

The set of coupled differential equations that link all the interdependent interactions for individual species of nuclei to the overall pattern of abundances of the nuclei involved is called a nuclear reaction network. Its purpose is to evolve the abundance of each nuclear species in time. The nuclear abundance of a species Y_i , tells what fraction of the total number of nuclei in the system belong to species i . It is defined as

$$Y_i = n_i/(\rho N_A), \quad (2.10)$$

where n_i is number density of species i , the mass density is ρ , and N_A is Avogadro's number.

The final abundance Y_i of any one species is dependent on the sum of the reactions that create or destroy it. For a set of abundances and the reaction rates that link them, the change in each abundance over time can be calculated by:

$$\dot{Y}_i = \sum_j \mathcal{N}_j^i \lambda_j Y_j + \sum_{j,k} \mathcal{N}_{j,k}^i \rho N_A \langle j, k \rangle Y_j Y_k + \sum_{j,k,l} \mathcal{N}_{j,k,l}^i \rho^2 N_A^2 \langle j, k, l \rangle Y_j Y_k Y_l,$$

where the three sums are over reactions which produce or destroy a nucleus of species i with 1, 2, and 3 reactant nuclei, respectively. $\lambda_j Y_j$ is the rate for single particle reactions such as decays, photodisintegrations, and electron and positron captures. $\langle j, k \rangle Y_j Y_k$ and $\langle j, k, l \rangle Y_j Y_k Y_l$ represent the rates for two and three particle reactions like proton, neutron, and alpha captures and the triple alpha process. The $\mathcal{N}$'s provide for proper accounting of numbers of nuclei so that double counting of the

number of reactions when identical particles react with each other is avoided.

To find the overall change in any Y_i during the simulation, the changes in Y_i are integrated over small increments in time. Charged particle captures and photodisintegrations accelerate as the temperature rises. Thus for high temperatures, particularly small time steps must be used to accommodate the rapid speed at which the charged particle captures and photodisintegrations change the abundances.

For the full set of nuclear abundances, the derivative is written as a finite change in $\vec{Y}$,

$$\dot{\vec{Y}}(t + \Delta t) = \frac{\vec{Y}(t + \Delta t) - \vec{Y}(t)}{\Delta t}. \quad (2.11)$$

Where $\dot{\vec{Y}}$ is given by equation 2.11. The solution to this fully implicit² equation can be found by finding the zeros of the following equation,

$$\vec{\mathcal{Z}}(t + \Delta t) \equiv \frac{\vec{Y}(t + \Delta t) - \vec{Y}(t)}{\Delta t} - \dot{\vec{Y}}(t + \Delta t) = 0 \quad (2.12)$$

using the Newton-Raphson method (see e.g., Press et al., 1992). A Taylor expansion in $\vec{\mathcal{Z}}$ yields:

$$\vec{\mathcal{Z}}(t + \Delta t) + \left(\frac{\partial \vec{\mathcal{Z}}(t + \Delta t)}{\partial \vec{Y}(t + \Delta t)} \right)^{-1} \Delta \vec{Y} + \text{higher order terms} \quad (2.13)$$

In the Backward Euler Method, the terms above first order in $\vec{\mathcal{Z}}$ are dropped, leaving

$$\vec{\mathcal{Z}}(t + \Delta t) = \left(\frac{\partial \vec{\mathcal{Z}}(t + \Delta t)}{\partial \vec{Y}(t + \Delta t)} \right)^{-1} \Delta \vec{Y}, \quad (2.14)$$

and solving for $\Delta \vec{Y}$,

²In equation 2.11 we consider the derivative of Y_i , $\dot{Y}_i$, at the time based on the trial time step, $(t + \Delta t)$, rather than at time t . This is the implicit form.

$$\Delta \vec{Y} = \left(\frac{\partial \vec{Z}(t + \Delta t)}{\partial \vec{Y}(t + \Delta t)} \right)^{-1} \vec{Z}, \quad (2.15)$$

where $\partial \vec{Z}/\partial \vec{Y}$ is the Jacobian matrix of $\vec{Z}$. The network iterates this equations until $\vec{Y}(t + \Delta t)$ converges. With multiple integrations per time step and many small timesteps at high temperature, this process becomes time consuming for a large Jacobian.

Since the heart of this nuclear reaction network is a matrix solution, the computational cost of solving it grows nonlinearly with the number of nuclei included in the calculation. Our standard nuclear reaction network was written by Hix and Thielemann (1999). For silicon burning, it uses a 299 by 299 element matrix to evolve 299 nuclei which are linked by over 3000 equations (Hix & Thielemann, 1996). Due to the numerical methods used to solve the matrix, our network speed is roughly proportional to the number of nuclear abundances raised to the third power (Press et al., 1992). Thus with 299 species it runs about 12 times slower than it would if it only had 119 species. Even small reductions in the number of variables, and thus the size of the Jacobian, bring large increases in computational speed.

Chapter 3

The QSE-Reduced Network

The goal of the QSE-reduced network is to solve the same set of abundances as a full nuclear reaction network in a more efficient way. The existence of QSE groups allows the calculation of a large set of abundances from a much smaller subset because all of the elements in a QSE group can be represented by just one focal nucleus, thereby reducing the Jacobian matrix.

As a first implementation, we assumed three QSE groups with fixed membership, one focused around ^{28}Si , one focused around ^{56}Ni , and one composed of protons and neutrons and isotopes of helium. By specializing equation 1.5 for nuclei in quasi equilibrium with ^{28}Si , the individual abundances can be calculated by:

$$Y_{\text{QSE,Si}}(^AZ) = \frac{C(^AZ)}{C(^{28}\text{Si})} Y(^{28}\text{Si}) Y_p^{Z-14} Y_n^{N-14} , \quad (3.1)$$

where I have again defined

$$C(^AZ) = \frac{G(^AZ)}{2^A} \left(\frac{\rho N_A}{\theta} \right)^{A-1} A^{\frac{3}{2}} \exp \left(\frac{B(^AZ)}{k_B T} \right) , \quad (3.2)$$

and

$$\theta = \left(\frac{m_u k_B T}{2\pi \hbar^2} \right)^{3/2} .$$

As with equation 1.5, A is the atomic number and N , is the neutron number. $G(^AZ)$ and $B(^AZ)$ are the partition function and the binding energy of the nucleus AZ , N_A is Avogadro's number, k_B is Boltzmann's constant, and ρ and T are the density and temperature of the plasma. Y_p and Y_n are the abundances of free protons and neutrons and the integers $(N - 14)$ and $(Z - 14)$ are the number of such nucleons needed to construct the nucleus AZ from ^{28}Si . A similar expression can be written for iron-peak nuclei in equilibrium with ^{56}Ni such that,

$$Y_{\text{QSE,Ni}}(^AZ) = \frac{C(^AZ)}{C(^{56}\text{Ni})} Y(^{56}\text{Ni}) Y_p^{Z-28} Y_n^{N-28}, \quad (3.3)$$

The lightest nuclei, neutrons, protons, and isotopes of helium form the third QSE group. They are held in equilibrium with each other by the balance of their reactions among the members of the silicon and iron-peak groups. It is the growth of this group to include all nuclei that indicates the approach to NSE. The equations for NSE are similar to QSE except all nuclei are in equilibrium with protons and neutrons:

$$Y_{\text{NSE}}(^AZ) = C(^AZ) Y_n^N Y_p^Z \quad (3.4)$$

The abundance of each species in NSE is determined only by its nuclear binding energy and partition function, plus the electron fraction, temperature, and density of the matter.

Combining the focal abundances for each QSE group and the nuclei that must still be evolved independently gives a reduced set of abundances, $\vec{Y}^{\mathcal{R}}$. For conditions where QSE applies, the full set of abundances, $\vec{Y}^{\mathcal{F}}$ is directly and simply related to $\vec{Y}^{\mathcal{R}}$ by the QSE abundances equations, like equation 3.1, 3.3, and 3.4. Direct evolution of $\vec{Y}^{\mathcal{R}}$ is possible (Hix, 1995), however the resulting equations are highly non-linear and require many Newton-Raphson iterations to converge. It is much more efficient to calculate time derivatives of each QSE group as a whole. For this

purpose, 4 group abundances are defined,

$$\begin{aligned}
Y_{NG} &= \sum_{i \in Lt \text{ group}} N_i Y_i + \sum_{i \in Si \text{ group}} (N_i - 14) Y_i + \sum_{i \in Fe \text{ group}} (N_i - 28) Y_i, \\
Y_{ZG} &= \sum_{i \in Lt \text{ group}} Z_i Y_i + \sum_{i \in Si \text{ group}} (Z_i - 14) Y_i + \sum_{i \in Fe \text{ group}} (Z_i - 28) Y_i, \\
Y_{SiG} &= \sum_{i \in Si \text{ group}} Y_i, \\
Y_{FeG} &= \sum_{i \in Fe \text{ group}} Y_i.
\end{aligned} \tag{3.5}$$

Physically, Y_{SiG} and Y_{FeG} represent the total abundances of the silicon and iron-peak QSE groups, while Y_{NG} and Y_{ZG} represent the sum of the abundances of free nucleons and those nucleons required to build the members of the QSE groups from the focal species. The integers $(N_i - 28)$ and $(Z_i - 28)$ are respectively the numbers of neutrons and protons required to build Y_i from focal nucleus ^{56}Ni . These four group abundances, combined with the independent abundances, form a new “group” abundance set, $\vec{Y}^{\mathcal{G}}$ which has the same number of members as $\vec{Y}^{\mathcal{R}}$.

To visually simplify the following derivation, a series of moments of the group abundance distributions is defined,

$$\mathcal{M}^j = \sum_{i \in j \text{ group}} Y_i, \quad \mathcal{M}_k^j = \sum_{i \in j \text{ group}} (k_i - k_f) Y_i, \quad \mathcal{M}_{k,\ell}^j = \sum_{i \in j \text{ group}} (k_i - k_f)(\ell_i - \ell_f) Y_i, \tag{3.6}$$

where j reflects which of the 3 QSE groups (Light, Si or Fe) is being summed over, while k and ℓ can be either the neutron number, N , or the proton number, Z . The subscript f refers to the focal element of the respective group, hence $N_f = Z_f = 14$ for the silicon group and $N_f = Z_f = 28$ for the iron group. These definitions are extended to the light group by defining $N_f = Z_f = 0$ for the Light group. As an example $\mathcal{M}_{RZN}^{Si} = \mathcal{M}_{NZ}^{Si} = \sum_{i \in Si \text{ group}} (N - 14)(Z - 14) Y_i$. In terms of the definitions

of equation 3.6, equation 3.5 becomes

$$\begin{aligned}
Y_{NG} &= \mathcal{M}_N^{Lt} + \mathcal{M}_N^{Si} + \mathcal{M}_N^{Fe} \equiv \mathcal{M}_N^* , \\
Y_{ZG} &= \mathcal{M}_Z^{Lt} + \mathcal{M}_Z^{Si} + \mathcal{M}_Z^{Fe} \equiv \mathcal{M}_Z^* , \\
Y_{SiG} &= \mathcal{M}^{Si} , \\
Y_{FeG} &= \mathcal{M}^{Fe} ,
\end{aligned} \tag{3.7}$$

where the superscript $*$ is used to indicate the sum over the 3 values which j can have, Lt, Si and Fe.

The time derivatives of these group abundances are calculated by replacing the abundances, Y_i in Eq. 3.5 with their time derivatives, $\dot{Y}_i$. For example,

$$\dot{Y}_{NG} = \sum_{i \in Lt \text{ group}} N_i \dot{Y}_i + \sum_{i \in Si \text{ group}} (N_i - 14) \dot{Y}_i + \sum_{i \in Fe \text{ group}} (N_i - 28) \dot{Y}_i \tag{3.8}$$

The $\dot{Y}_i$ can in turn be calculated from reaction rates via Eq. 2.11. Strong and electromagnetic reactions among the members of the QSE groups do not contribute to the group derivatives. For example, a neutron capture reaction connecting ^{56}Fe and ^{57}Fe does not contribute to $\dot{Y}_{NG}$, since the contribution to the sum over the iron group $[(31 - 28) - (30 - 28) = +1]\rho N_A \langle j, k \rangle Y_n Y(^{56}\text{Fe})$ is exactly canceled by the corresponding term in the sum over the Light group, $[-1]\rho N_A \langle j, k \rangle Y_n Y(^{56}\text{Fe})$. Thus, employing the group abundance set $\mathcal{G}$ in practice also reduces the number of reactions whose flux must be calculated since non-weak reactions between group members can be ignored, offering further computational efficiency.

Unfortunately, the rates for this remaining set of reactions are still functions of the full abundance set, $\vec{Y}^{\mathcal{F}}$. Since the time derivatives are not easily expressed in terms of the group abundance, $\vec{Y}^{\mathcal{G}}$, one must calculate $\dot{\vec{Y}}^{\mathcal{G}}$ from $\vec{Y}^{\mathcal{F}}$ or alternately, using the QSE relations defined in equations 3.1, 3.3 & 3.4, from the reduced set

$\vec{Y}^{\mathcal{R}}$. Thus, to evolve $\vec{Y}^{\mathcal{G}}$ over time, one must repeatedly solve for $\vec{Y}^{\mathcal{R}}$. By applying the QSE relations (Eqs. 3.1, 3.3 & 3.4) to Eq. 3.5, $\vec{Y}^{\mathcal{G}}$ is written as a function of $\vec{Y}^{\mathcal{R}}$, with as many independent equations as unknowns implying a unique relation between $\vec{Y}^{\mathcal{G}}$ and $\vec{Y}^{\mathcal{R}}$. Fortunately, with the exception of Y_n and Y_p , the relations between $\vec{Y}^{\mathcal{G}}$ and $\vec{Y}^{\mathcal{R}}$ are linear.

To evolve the group abundances, $\vec{Y}^{\mathcal{G}}$, by their time derivatives, $\dot{\vec{Y}}^{\mathcal{G}}$, an equation analogous to Eq. 2.11 is constructed and the same Newton-Raphson procedure is followed. In particular, Eq. 2.15 becomes

$$\Delta \vec{Y}^{\mathcal{G}} = \left(\frac{\partial \vec{Z}^{\mathcal{G}}(t + \Delta t)}{\partial \vec{Y}^{\mathcal{G}}(t + \Delta t)} \right)^{-1} \vec{Z}^{\mathcal{G}}. \quad (3.9)$$

Central to the calculation of $\Delta \vec{Y}^{\mathcal{G}}$ is the Jacobian of $\vec{Z}^{\mathcal{G}}$, $\partial \vec{Z}^{\mathcal{G}} / \partial \vec{Y}^{\mathcal{G}}$. From Eq. 2.12, one can write the elements of this Jacobian as

$$\frac{\partial Z_i^{\mathcal{G}}}{\partial Y_j^{\mathcal{G}}} = \frac{\delta_{ij}}{\Delta t} - \frac{\partial \dot{Y}_i^{\mathcal{G}}}{\partial Y_j^{\mathcal{G}}} \quad (3.10)$$

Thus solution of the system of equations requires knowledge of $\partial \dot{Y}^{\mathcal{G}} / \partial \vec{Y}^{\mathcal{G}}$, which can not be calculated directly since $\dot{Y}^{\mathcal{G}}$ can not be expressed in terms of $\vec{Y}^{\mathcal{G}}$. Instead the chain rule is used,

$$\frac{\partial \dot{Y}^{\mathcal{G}}}{\partial \vec{Y}^{\mathcal{G}}} = \frac{\partial \dot{Y}^{\mathcal{G}}}{\partial \vec{Y}^{\mathcal{R}}} \frac{\partial \vec{Y}^{\mathcal{R}}}{\partial \vec{Y}^{\mathcal{G}}} \quad (3.11)$$

to calculate the Jacobian. Analytically, the first term in the product on the right hand side of Eq. 3.11 is easily calculated from the sums of reaction terms, ignoring strong and electromagnetic reactions within the groups. For example,

$$\frac{\partial \dot{Y}_{NG}}{\partial Y_r} = \sum_{i \in Lt \text{ group}} N_i \frac{\partial \dot{Y}_i}{\partial Y_r} + \sum_{i \in Si \text{ group}} (N_i - 14) \frac{\partial \dot{Y}_i}{\partial Y_r} + \sum_{i \in Fe \text{ group}} (N_i - 28) \frac{\partial \dot{Y}_i}{\partial Y_r}, \quad (3.12)$$

while the required derivatives $\partial \dot{Y}_i / \partial Y_r$ are calculated in the same fashion as a con-

ventional network, i.e. by differentiating Eq. 2.11.

Calculation of individual elements of the second term on the right hand side of Eq. 3.11, $\partial Y_r / \partial Y_g$ (where $r \in \mathcal{R}$ and $g \in \mathcal{G}$) is more complicated. For the independent nuclei, $\mathcal{I}$, which are members of both $\mathcal{R}$ and $\mathcal{G}$, $\partial Y_r / \partial Y_g = \delta_{rg}$. Calculation of the remaining 16 terms which involve the focal QSE isotopes and the group abundances, $\partial Y_{n,p,^{28}\text{Si},^{56}\text{Ni}} / \partial Y_{NG,ZG,SiG,FeG}$, requires implicit differentiation of the definition of $\vec{Y}^{\mathcal{G}}$ with respect to $\vec{Y}^{\mathcal{G}}$, using equation 3.5 (or 3.7). For example, differentiating the four equations of Eq. 3.7 with respect to Y_{NG} produces a system of equations that begins with $\frac{\partial Y_{NG}}{\partial Y_{NG}} = 1$.

Using the definition of Y_{NG} given in equation 3.7 and equations equation 3.3 to express Y_i in terms of the QSE focal nuclei,

$$\begin{aligned}
\frac{\partial Y_{NG}}{\partial Y_{NG}} = & \sum_{i \in \text{Lt group}} C_i N_i [N_i Y_n^{N_i-1} Y_p^{Z_i} \frac{\partial Y_n}{\partial Y_{NG}} + Z_i Y_n^{N_i} Y_p^{Z_i-1} \frac{\partial Y_p}{\partial Y_{NG}}] \\
& + \sum_{i \in \text{Si group}} C_i (N_i - 14) [(N_i - 14) Y_n^{N_i-15} Y_p^{Z_i-14} Y_{^{28}\text{Si}} \frac{\partial Y_n}{\partial Y_{NG}} \\
& + (Z_i - 14) Y_n^{N_i-14} Y_p^{Z_i-15} Y_{^{28}\text{Si}} \frac{\partial Y_p}{\partial Y_{NG}} + Y_n^{N_i-14} Y_p^{Z_i-14} \frac{\partial Y_{^{28}\text{Si}}}{\partial Y_{NG}}] \\
& + \sum_{i \in \text{Fe group}} C_i (N_i - 28) [(N_i - 28) Y_n^{N_i-29} Y_p^{Z_i-28} Y_{^{56}\text{Ni}} \frac{\partial Y_n}{\partial Y_{NG}} \\
& + (Z_i - 28) Y_n^{N_i-28} Y_p^{Z_i-29} Y_{^{56}\text{Ni}} \frac{\partial Y_p}{\partial Y_{NG}} + Y_n^{N_i-28} Y_p^{Z_i-28} \frac{\partial Y_{^{56}\text{Ni}}}{\partial Y_{NG}}] . \quad (3.13)
\end{aligned}$$

Grouping terms with like partial derivatives and using equations 3.1 through 3.4 to reform the Y_i 's,

$$\begin{aligned}
\frac{\partial Y_{NG}}{\partial Y_{NG}} &= [\sum_{i \in Lt \text{ group}} N_i^2 Y_i + \sum_{i \in Si \text{ group}} (N_i - 14)^2 Y_i + \sum_{i \in Fe \text{ group}} (N_i - 28)^2 Y_i] Y_n^{-1} \frac{\partial Y_n}{\partial Y_{NG}} \\
&+ [\sum_{i \in Lt \text{ group}} N_i Z_i Y_i + \sum_{i \in Si \text{ group}} (N_i - 14)(Z_i - 14) Y_i \\
&\quad + \sum_{i \in Fe \text{ group}} (N_i - 28)(Z_i - 28) Y_i] Y_p^{-1} \frac{\partial Y_p}{\partial Y_{NG}} \\
&+ [\sum_{i \in Si \text{ group}} (N_i - 14) Y_i Y_{28Si}^{-1} \frac{\partial Y_{28Si}}{\partial Y_{NG}} \\
&\quad + [\sum_{i \in Fe \text{ group}} (N_i - 28) Y_i Y_{56Ni}^{-1} \frac{\partial Y_{56Ni}}{\partial Y_{NG}}]. \tag{3.14}
\end{aligned}$$

Applying the definition of $\mathcal{M}$ with superscript $*$ indicating the sum over Lt, Si and Fe terms,

$$\begin{aligned}
\frac{\partial Y_{NG}}{\partial Y_{NG}} &= [\mathcal{M}_{NN}^*] Y_n^{-1} \frac{\partial Y_n}{\partial Y_{NG}} + [\mathcal{M}_{NZ}^*] Y_p^{-1} \frac{\partial Y_p}{\partial Y_{NG}} \\
&\quad + [\mathcal{M}_N^{Si}] Y_{Si}^{-1} \frac{\partial Y_{28Si}}{\partial Y_{NG}} + [\mathcal{M}_N^{Fe}] Y_{Ni}^{-1} \frac{\partial Y_{56Ni}}{\partial Y_{NG}}. \tag{3.15}
\end{aligned}$$

Differentiating the remaining three equations of Eq. 3.7 with respect to Y_{NG} in similar fashion forms a matrix equation, $\mathcal{A}\vec{x} = \vec{b}$,

$$\begin{bmatrix} \mathcal{M}_{NN}^* & \mathcal{M}_{NZ}^* & \mathcal{M}_N^{Si} & \mathcal{M}_N^{Fe} \\ \mathcal{M}_{NZ}^* & \mathcal{M}_{ZZ}^* & \mathcal{M}_Z^{Si} & \mathcal{M}_Z^{Fe} \\ \mathcal{M}_N^{Si} & \mathcal{M}_N^{Si} & \mathcal{M}^{Si} & 0 \\ \mathcal{M}_Z^{Fe} & \mathcal{M}_Z^{Fe} & 0 & \mathcal{M}^{Fe} \end{bmatrix} \begin{bmatrix} Y_n^{-1} \frac{\partial Y_n}{\partial Y_{NG}} \\ Y_p^{-1} \frac{\partial Y_p}{\partial Y_{NG}} \\ Y^{(28Si)-1} \frac{\partial Y^{(28Si)}}{\partial Y_{NG}} \\ Y^{(56Ni)-1} \frac{\partial Y^{(56Ni)}}{\partial Y_{NG}} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}. \tag{3.16}$$

Solving Eq. 3.16 for the 4 unknowns gives

$$\begin{aligned}
\frac{\partial Y_n}{\partial Y_{NG}} &= \frac{Y_n}{\det \mathcal{A}} \left(\mathcal{M}^{Si} \mathcal{M}^{Fe} \mathcal{M}_{ZZ}^* - \mathcal{M}^{Si} \mathcal{M}_Z^{Fe^2} - \mathcal{M}^{Fe} \mathcal{M}_Z^{Si^2} \right) \\
\frac{\partial Y_p}{\partial Y_{NG}} &= \frac{Y_p}{\det \mathcal{A}} \left(\mathcal{M}^{Fe} \mathcal{M}_Z^{Si} \mathcal{M}_N^{Si} + \mathcal{M}^{Si} \mathcal{M}_Z^{Fe} \mathcal{M}_N^{Fe} - \mathcal{M}^{Si} \mathcal{M}^{Fe} \mathcal{M}_{NZ}^* \right) \\
\frac{\partial Y(^{28}\text{Si})}{\partial Y_{NG}} &= \frac{Y(^{28}\text{Si})}{\det \mathcal{A}} \left(\mathcal{M}^{Fe} (\mathcal{M}_{NZ}^* \mathcal{M}_Z^{Si} - \mathcal{M}_{ZZ}^* \mathcal{M}_N^{Si}) + \mathcal{M}_N^{Si} \mathcal{M}_Z^{Fe^2} - \mathcal{M}_Z^{Si} \mathcal{M}_Z^{Fe} \mathcal{M}_Z^{Fe} \right) \\
\frac{\partial Y(^{56}\text{Ni})}{\partial Y_{NG}} &= \frac{Y(^{56}\text{Ni})}{\det \mathcal{A}} \left(\mathcal{M}^{Si} (\mathcal{M}_{NZ}^* \mathcal{M}_Z^{Fe} - \mathcal{M}_{ZZ}^* \mathcal{M}_N^{Fe}) + \mathcal{M}_N^{Fe} \mathcal{M}_Z^{Si^2} - \mathcal{M}_Z^{Fe} \mathcal{M}_Z^{Si} \mathcal{M}_Z^{Si} \right)
\end{aligned} \tag{3.17}$$

where $\det \mathcal{A}$ is the determinant of the matrix on the left hand side of Eq. 3.16. Calculation of the twelve remaining unknowns proceeds in a similar manner, with ∂Y_{NG} in the denominator of $\vec{x}$ in Eq. 3.16 being replaced in turn by ∂Y_{ZG} , ∂Y_{SiG} and ∂Y_{FeG} while the $\vec{b}$ on the right hand side of Eq. 3.16 permutes through the remaining unit vectors.

Thus the reduced set Jacobian can be built and, via the equation. 3.9, the reduced set abundances updated. Then the QSE equations are solved for the focal abundances, which allows updating of all abundances in the full set. This process is repeated for each time step in the evolution.

The basic algorithm described above predates my involvement in this project. A prototype implementation was developed by Christian Freiburghaus, a graduate student at the University of Basel, Switzerland. However, this prototype delivered neither the speed nor accuracy desired. I spent a considerable amount of time improving this prototype and the result can be seen in Hix & Parete-Koon et al. (2007). In the interest of gaining better speed and accuracy, I decided to develop a completely new QSE-reduced network, based partially the old prototype, that would allow variation in the number of groups and their membership. This new code is also consistent with the existing conventional network, Xnet, allowing the possibility of smooth transitions between the QSE-reduced network and the conventional network as thermodynamic conditions change. My contribution to this project has

been an efficient and flexible implementation of this approach, allowing it to achieve the desired accuracy and computational efficiency, as I will demonstrate in the next section.

Chapter 4

Testing the QSE-reduced Network

The QSE-reduced network was tested under a variety of different initial conditions in order to demonstrate its speed and accuracy. First conditions of constant temperature and density were used to explore how the groups formed and persisted at different temperatures. These runs are similar those that the network would perform inside of instellar evolution simulations where the hydrodynamic conditions vary on a timescale of hours.

To approximate the evolution of the density and temperature during a supernova explosion, the widely used prescription introduced by Fowler & Hoyle (1964) was employed. The expansion is assumed to occur on the hydrodynamic timescale¹

$$\tau_{HD} = (24\pi G\rho_i)^{-1/2} = 446\rho_6^{-1/2} \text{ ms}, \quad (4.1)$$

where ρ_i is the initial density. This yeilds timescales of 10 to 100 millisceonds for supernova conditions. The density and temperature of the radiation dominated gas

¹The time it would take the star to collapse by the force of gravity if all the pressure support were suddenly removed.

($\gamma = 4/3$) are then given by

$$\rho(t) = \rho_i \exp\left(\frac{-t}{\tau_{HD}}\right) \quad (4.2)$$

$$T_9(t) = T_{9i} \exp\left(\frac{-t}{3\tau_{HD}}\right). \quad (4.3)$$

Both full and QSE-reduced networks use the same LU decomposition routines to find the inverse of the Jacobian matrix given in Equation 2.14. In both networks the method of calculating the new trial time step is based on abundance changes in the previous time step. After the initial time step a trial time step is calculated by

$$\Delta t = \frac{\Delta t_{\text{old}}}{10} \frac{\vec{Y}}{|\vec{Y} - \vec{Y}_{\text{old}}|} \quad (4.4)$$

Where Δt_{old} is the previous time step and $\vec{Y}$ and $\vec{Y}_{\text{old}}$ are the current and previous abundance of the isotope with the largest fractional change in abundance. Abundances smaller than 10^{-7} are not considered in the time step calculation.

Two sets of nuclei were tested, one containing 299 nuclides up to germanium 78 and another containing 200 nuclides up to krypton 86. The large set was chosen because its diversity of isotopes allows for most nuclear reaction paths to be represented. The smaller set was chosen because it was used by Calder et al (2007) in self-heating simulations to calibrate the energetics and timescales of their FLASH-based three stage flame model and we wish to ultimately reproduce simpler cases of their calculations using the QSE-reduced network.

In order to find the number and membership of QSE groups that optimized network speed and accuracy for each set of test conditions, the QSE-reduced network was run with one, two, and three QSE groups configurations for each trial. Figures 4.1 through 4.4 show the QSE group membership of the 1-group, 2-group, 3-group, and 3*-group configurations for the largest set of nuclei. The 1-group network assumes

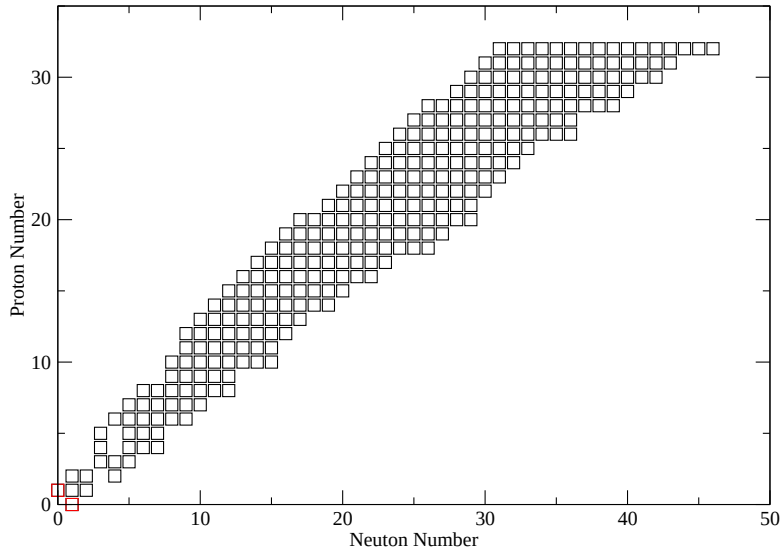


Figure 4.1 This shows the 1-group network configuration, where the evolution of all the species shown in black is followed by the two species, protons and neutrons, shown in red.

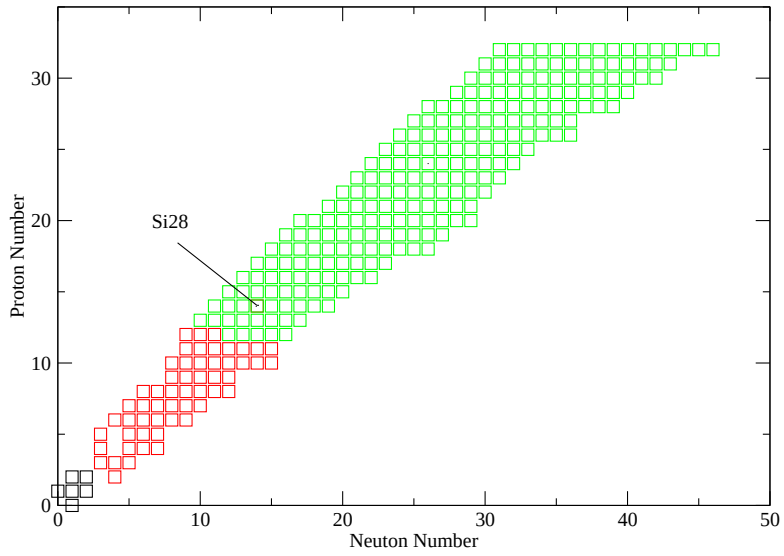


Figure 4.2 This shows the 2-group QSE-reduced network configuration. Independent species are shown in red. The large QSE group, stretching from magnesium to germanium, is shown in green, and the light QSE group is shown in black.

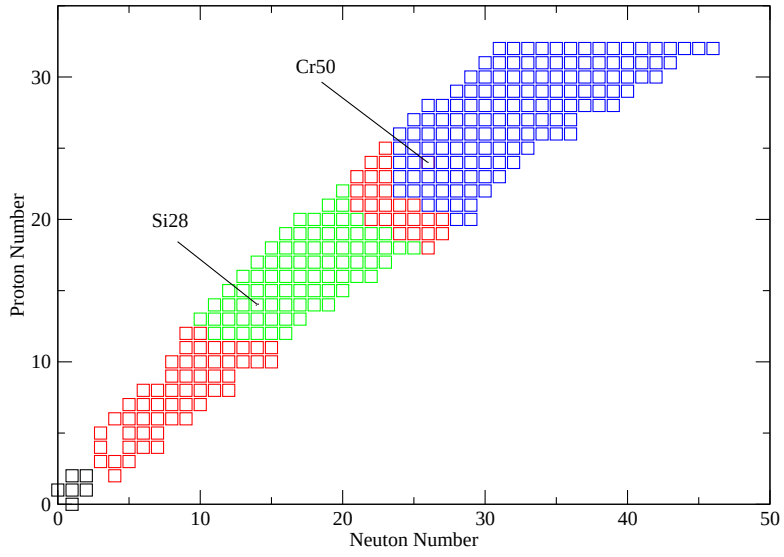


Figure 4.3 This shows the 3-group QSE-reduced network configuration. Independent species are shown in red. The silicon QSE group is shown in green, the iron-peak QSE group is shown in blue, and the light QSE group is shown in black.

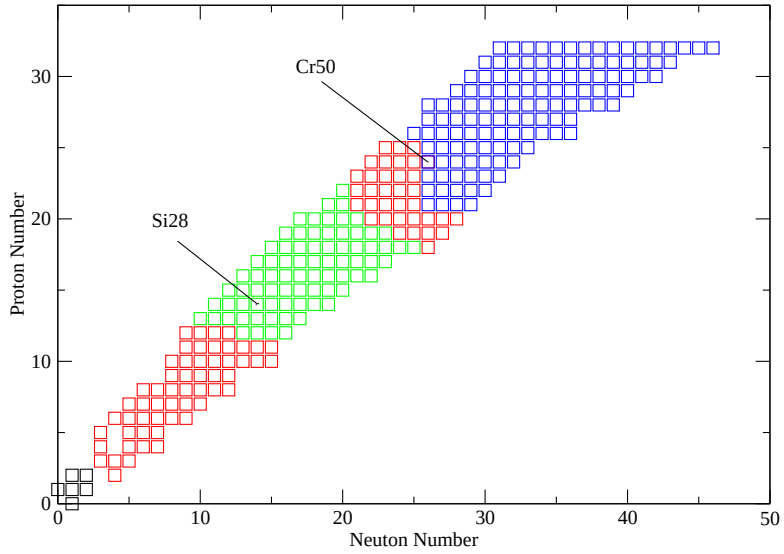


Figure 4.4 This shows the 3*-group QSE-reduced network configuration. Independent species are shown in red. The silicon QSE group is shown in green, the iron-peak QSE group is shown in blue, and the light QSE group is shown in black.

that the composition is in NSE and therefore only needs to follow 2 independent variables to evolve the 299 nuclide composition as the temperatures changes. The two independent variables are described by the upper two expressions in equation 3.5, representing the group abundances of protons and neutrons, to evolve the 299 nuclide composition as the temperatures changes. However, this network is limited to temperature and timescales where NSE is well established. The 2-group configuration uses 57 independent variables consisting of the independent nuclei, the proton and neutron group abundances, and one group abundance for its large QSE group, to follow the composition. The 3-group configuration follows the evolution with 82 independent variables, making it under a third as large as the network it replaces. The 3*-group network increases the number of independent variables to 93, which is still less than a third the number of independent variable need for the full network.

Similar group boundaries are useful for the smaller 200 nuclei set. Other configurations, which were used for conditions that produce alpha-rich freezeout, will be discussed later.

4.1 Reducing the 299 Nuclide Network

4.1.1 Constant Conditions

Results are shown for a representative case of constant conditions where $Y_e = 0.480$, $T_9 = 4$, and $\rho = 10^7 \text{ g cm}^{-3}$. Figure 4.5 shows several critical abundances as a function of time with the full network calculation represented by solid lines, the 3-group QSE-reduced network calculation represented by circles, and the 2-group QSE-reduced network represented by crosses. After about 10 microseconds, the circle representing the 3-group QSE-reduced network have merged with the sold lines of the full network showing that QSE has been established in the silicon and iron-peak groups of the 3-group network. The large QSE group of the 2-group network

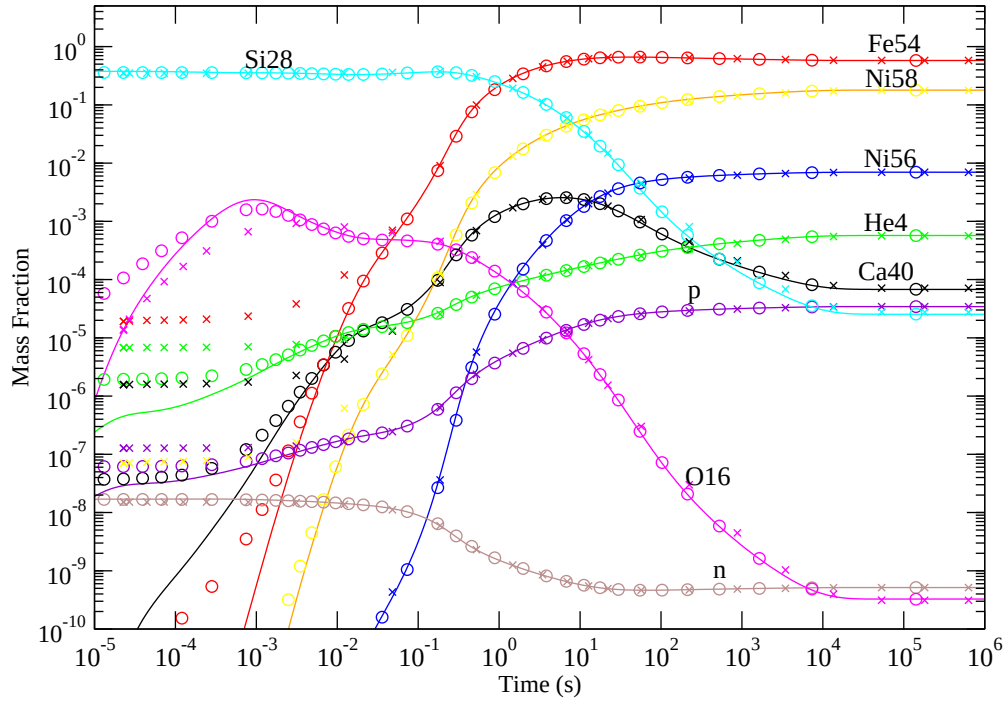


Figure 4.5 A comparison between the full network (solid lines), the 3-group QSE-reduced network (circles), and the 2-group QSE-reduced network (crosses) for constant conditions is shown. A selection of important nuclei is shown.

takes longer to equilibrate as can be seen in Figure 4.5, where the 2-group crosses for ^{40}Ca , ^{16}O , and ^{54}Fe do not join the solid lines of the full network until after approximately 0.05 seconds. From this point forward, both calculations are in good agreement for the most dominant nuclei. By 1 second the abundances of ^{28}Si , and neutrons are diminishing rapidly as the abundances protons, ^4He , ^{54}Fe , ^{58}Ni , and ^{56}Ni , are increasing. The abundance of ^{40}Ca is still increasing at 1 second, but by 10 seconds it begins to diminish. Silicon and its nuclear neighbors are melting through the intermediate mass elements, such as ^{40}Ca , into the iron-peak elements. ^{54}Fe and ^{58}Ni are the dominant products of the equilibrium because their respective ratios of nuclear protons to total nucleons match that global electron fraction of 0.48. Figure 4.6 shows the deviations for all abundances for the 3-group QSE-reduced network at $t = 100$ seconds. The top and bottom panel of the figure show results for this trial using two different versions of the reaction rate library, REACLIB. First, note that the 3-groups network reproduces the abundance pattern of the full network to 10% or better for all species as silicon burning is winding down. The only exception to this is ^{57}Cu , seen in the top panel of 4.6. ^{57}Cu is on the edge of the iron-peak so it is reasonable to assume that does not belong in the iron-peak group. However, in this case, the Q value used to calculate the reaction rate of $^{57}\text{Cu} (\gamma, p) ^{56}\text{Ni}$ from its reverse, -0.767 MeV, differed from the value deduced from the masses in the data file named winvn which accompanies REACLIB. With the $^{57}\text{Cu} (\gamma, p) ^{56}\text{Ni}$ reaction rate recalculated using this correct Q value of -0.694 MeV, the ratio of abundances in the 3-group case between the QSE-reduced network and the full network is 1.0002, as shown in the bottom panel of Figure 4.6. This was not the only Q value mismatch between the networks. Since different rates dominate at different temperatures, no one temperature plot could show all the effects of all the discrepancies. I added a reaction rate checking routine to the network setup that found and corrected 50 of these Q value disagreement among the reactions that used detailed balance to

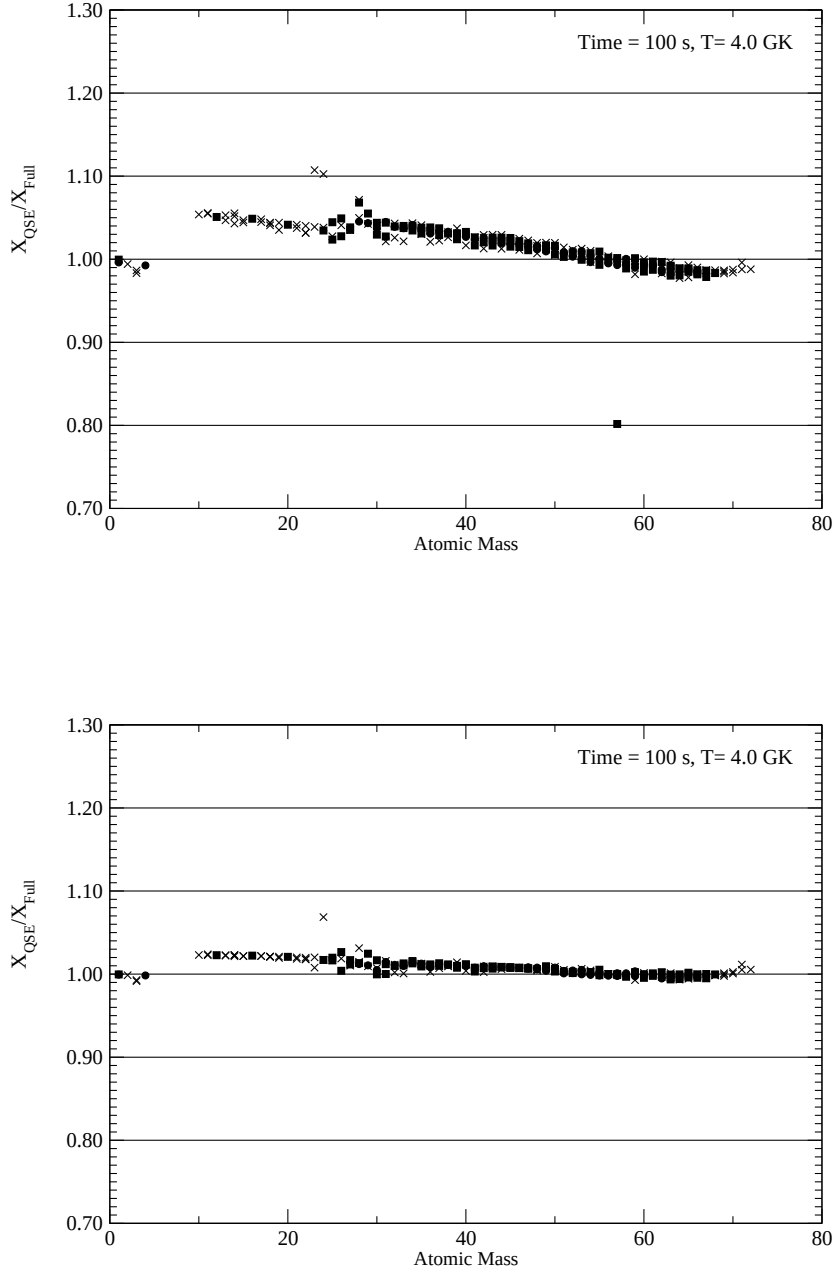


Figure 4.6 Shown here are deviations of the abundances calculated with the 3-group QSE-reduced network from those calculated by the full network. The calculation with the original rate library is shown on the top panel and a calculation using the balanced rate library is shown on the lower panel. The circles are the dominant nuclei with mass fractions larger than 10^{-6} . The squares are mass fractions between 10^{-6} and 10^{-12} . The X's are mass fractions between 10^{-12} and 10^{-20} .

Table 4.1. Network Speed for Constant Conditions

Network	Core Duo			Pentium4		
	cpu time (s)	matrix time (%)	Iteration count	cpu time (s)	matrix time (%)	Iteration count
Vendor Supplied Solver						
3QSE	1.275	42	1170	1.83	27	1084
2QSE	0.54	25	764	0.88	23	736
Full	23.00	60	1545	23.79	84	1556

determine their reverse rates. In addition to inconsistent Q values, we found that several reactions had missing or undefined reverse reactions. Since the QSE-reduced network doesn't use the reaction rates to evolve any of the group abundances, missing rates lead the full network to choose a very different equilibrium than the QSE-reduced network. The missing inverses were calculated and added to the network. The effect of this correction can be seen in the reduced slant of the line formed by abundance ratios in the bottom plot when compared to the top plot. Later examples with different temperatures and densities, will still show a few nuclei that lie outside the trend of the QSE to Xnet ratio plots. These outliers indicate that there are still problems with a few reactions in the reaction rate library. This example illustrates some of the challenges of running networks in equilibrium with the current reaction rate libraries.

Table 4.1 shows the timing comparison for this constant conditions case with the corrected rate library, using a vendor supplied matrix solver. For the 3-group QSE-reduced network the gain in computational speed varies between 13 and 18 times faster than the full network depending on the platform used. The 2-group network runs between 27 and 43 times faster than the full network. The adaptive network runs between 20 and 30 times faster than the full network. Iteration counts for each configuration of the network are also shown in the table. The network usually take 2 to 3 iterations to converge for each time step in the calculation. For

example, the 3-group QSE case, labeled 3QSE in the table, takes 1170 iterations for its 530 time steps. The table shows that the more reduced the network, the fewer the number of iterations required. The reduced networks gain computational speed by both doing fewer iteration and doing each iteration faster.

4.1.2 Explosive Silicon Burning

Explosive silicon burning occurs in both thermonuclear and core collapse supernovae. Depending on the initial density and the peak temperature, three results are possible.

1. *Incomplete Silicon Burning*, where a significant amount of silicon and other intermediate mass elements remain after the freeze out of the charged particle reactions.
2. *Normal Freezeout*, where all the fuel is burned to iron-peak nuclei. This is also referred to as Complete Silicon Burning.
3. *α -rich Freezeout*, where a significant fraction of α -particles remains after freeze-out due to the low density during the burning process.

Clearly the QSE approximation cannot be correct for low temperatures as sufficient photodisintegrations are necessary to maintain the (partial) equilibrium. Hix & Thielemann (1999a) found that for expansion rates typical of supernovae, the freezeout of photodisintegrations becomes important for temperatures less than 3.5 GK. The accuracy of the QSE-reduced network is highly dependent on charged particle captures that occur after the QSE approximation breaks down. For the special case of the α -network, Hix et al. (1998) found that a QSE-network is applicable for temperatures down to $T_9 = 3.0$ GK and that the QSE abundances at this temperature are in good agreement with the full network abundances for the important nuclei. Within the next subsection we will demonstrate similar results for the general QSE-reduced network.

Incomplete Silicon Burning

Initial conditions of 5 GK coupled with a peak density of 10^9 g cm^{-3} lead to incomplete silicon burning. The initial abundances used for this trial contain most of the mass in the elements near silicon and were set up with an electron fraction of 0.48. As the network progresses this silicon is transformed into iron-peak elements, predominately ^{54}Fe and ^{56}Ni , in this case because the electron fraction is 0.48. However the decline in temperature prevents the total exhaustion of silicon and its nuclear neighbors, leaving rough 10% remaining in silicon as the burning freezes out.

Figure 4.7 shows a selection of the most dominant mass fractions as a function of time. Figure 4.8 shows the energy generation of the full network and the QSE-reduced network as a function of time. From Figure 4.7, it is clear that the 3-group network matches the full network well even at early times. However, the 2-group network's equilibrium initially over estimates the amount of iron formation and, therefore, over estimates the energy generation by a factor of two compared to the full network. While the temperature is hot enough at early times, not enough of the iron-peak elements were populated in the initial abundances to allow the full network to match the equilibrium abundances predicted by the large QSE group of the 2-group network. This matches the previous observation of Woosley et al. (1973) that during the initial phase of silicon burning there is a break in the QSE groups between silicon and iron. The time required to close this break depends of the electron fractions (Hix & Thielemann, 1996).

Also plotted on Figure 4.8 is the energy generation rate of a 14 element alpha network. This network ran under the same conditions as the full and QSE networks, with the exception that an abundance set with an electron fractions of 0.48 is impossible in an alpha network, thus different initial abundance with an electron fraction of 0.50 were used. To obtain the alpha network's initial abundances, it started with pure ^{28}Si . Figure 4.8 shows that the alpha network underestimates the energy gen-

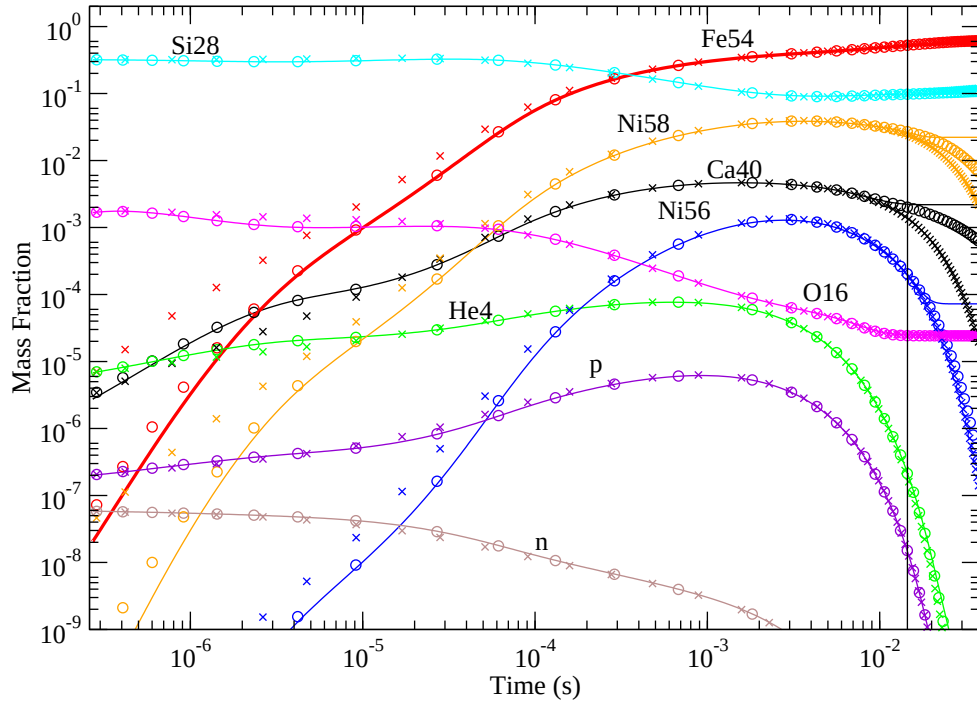


Figure 4.7 An example of incomplete silicon burning is shown. The solid lines represent the full network calculation, the crosses the 2-group QSE-reduced network and the circles the 3-group QSE-reduced network. A vertical black line marks the time that corresponds to a temperature of 3.5 GK.

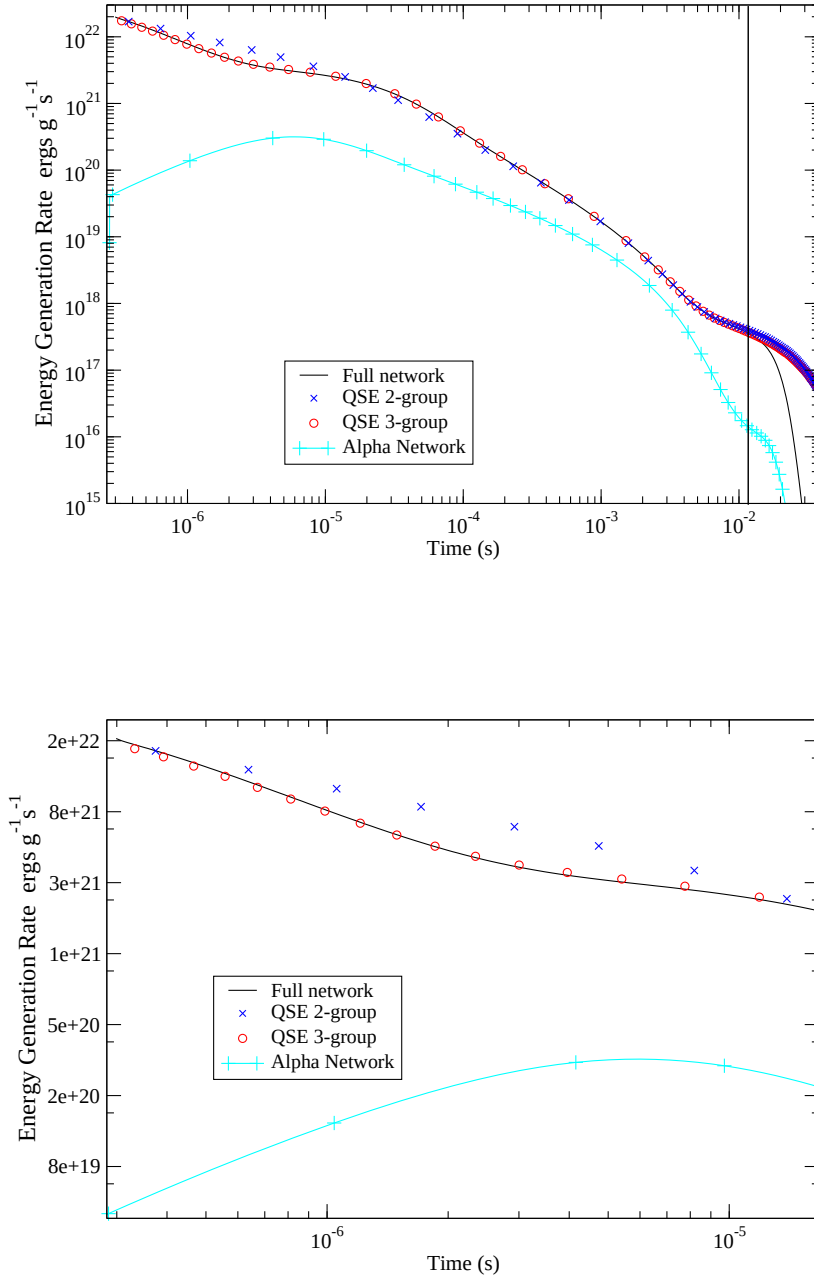


Figure 4.8 A comparison of the energy generation rate of the full network and the QSE-reduced network. The solid lines represent the full network calculation, the crosses the 2-group QSE-reduced network and the circles the 3-group QSE-reduced network. A vertical black line marks the time that corresponds to a temperature of 3.5 GK. The lower plot shows more detail for early times.

eration of the full network by an order of magnitude or more for the duration of the simulation. This under estimation is not surprising because the alpha network lacks many of the reaction channels represented in the full and QSE-reduced networks. The dominantly produced nuclei are those whose ratio of protons to total nucleons match the global electron fraction, in this case 0.48. All of the alpha network's species have equal numbers of protons and neutrons, so the network is locked into following a composition with an electron fraction of 0.5. Thus, the alpha network misses the energy contribution of this trial's most dominantly produced nuclei, such as ^{54}Fe . The 2-group network's early factor of 2 over estimation of the energy generation is made to seem better by the alpha network's under-estimation of a factor well over 10. At 10^{-4} seconds, by which time almost all the silicon is burned, the full network has sufficiently populated the iron-peak so that its abundance predictions match those of the 2-group network.

For temperatures below 3.5 GK, the reactions of the full network freeze out, as can be seen by the leveling out of their mass fractions in Figure 4.7 after the vertical black line marking 3.5 GK. The abundances produced by the QSE-reduced networks continue to drop because the networks assume a false equilibrium for the light particle captures and photodissociations.

Figures 4.9 through 4.11, illustrate how well the 2-group and 3-group QSE-reduced networks reproduce the all the abundances of the full network as the temperature falls. Figure 4.9 confirms that the large QSE group, extending from magnesium to germanium, of the 2-group configuration should be split into two groups, consisting of the silicon and iron-peak groups of the 3-group configuration, until after 10^{-4} seconds. The 2-group configuration's over-production of iron at early time is also well illustrated by the red symbols in top panel of Figure 4.9. Figure 4.10 shows that the large QSE group of 2-group network has again severed in to two groups by 0.012 seconds. This is due to the lower temperatures (3.7 GK) slowing the particle

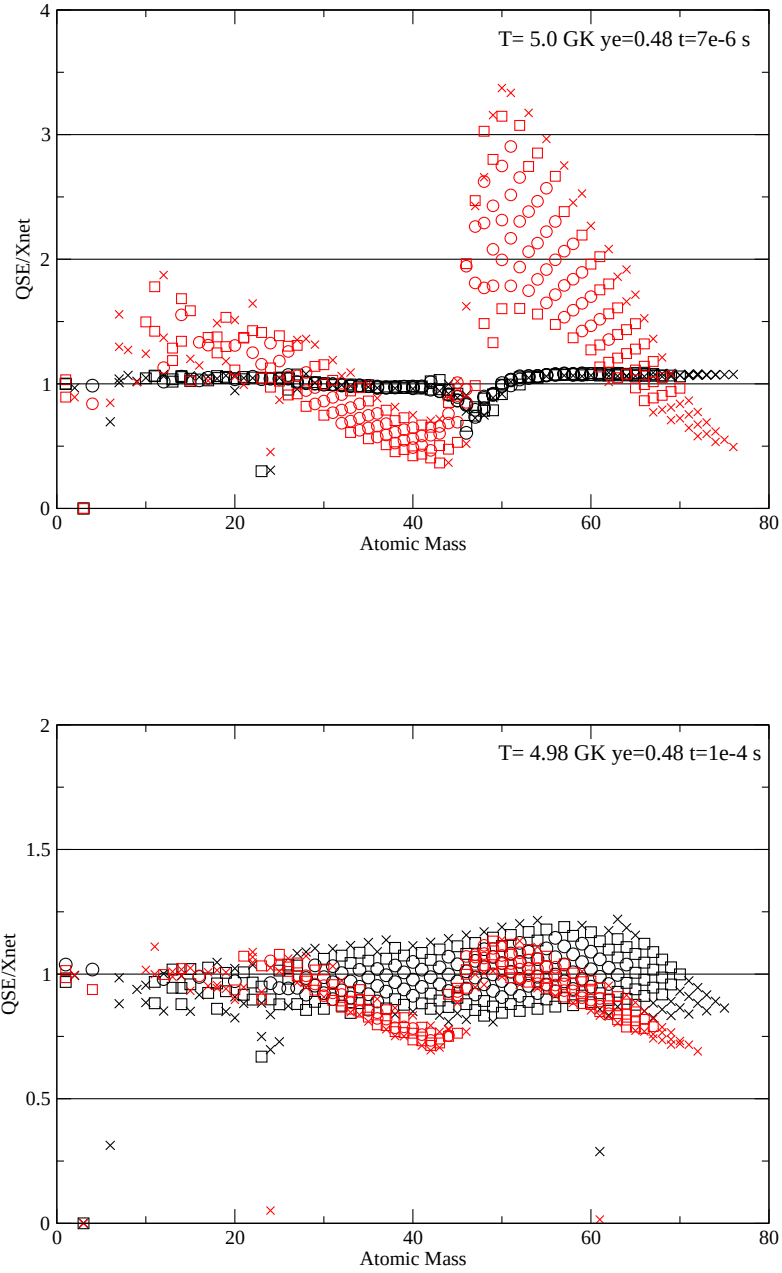


Figure 4.9 Ratios between abundances calculated with the QSE-reduced network and those calculated with the full network are shown for the case of incomplete silicon burning. Black symbols indicate the 3-group network and red symbols indicates the 2-group network. Circles are dominant nuclei with mass fractions greater than 10^{-6} . Squares are mass fractions between 10^{-6} and 10^{-12} and X's are mass fractions between 10^{-12} and 10^{-20} .

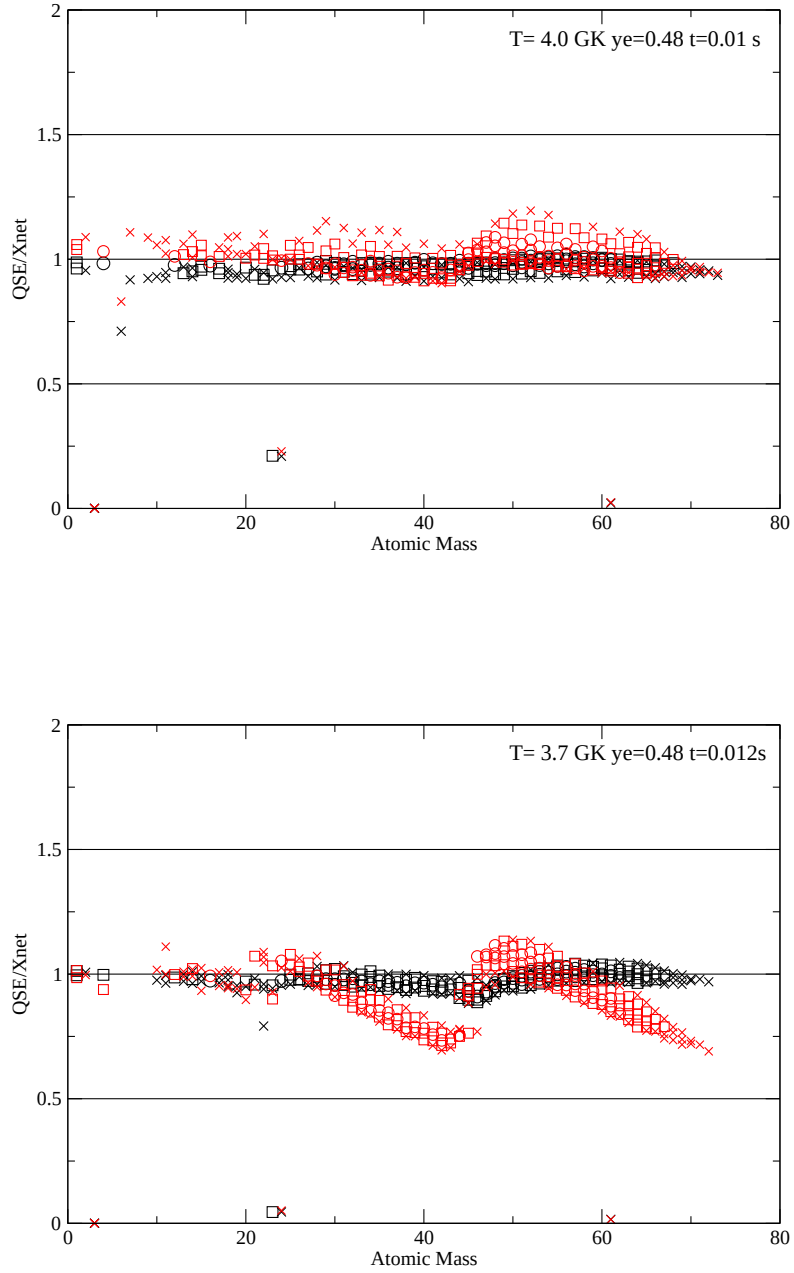


Figure 4.10 Shown here are the ratios between abundances calculated by the QSE-reduced network and those calculated by the full network for incomplete silicon burning at 4 and 3.7 GK. Black symbols indicate 3-group and red symbols indicates 2-group. The 2-group network reproduces the abundances of the full network as the temperature drops to 4GK, but at lower temperatures the 3-group network gives the better match.

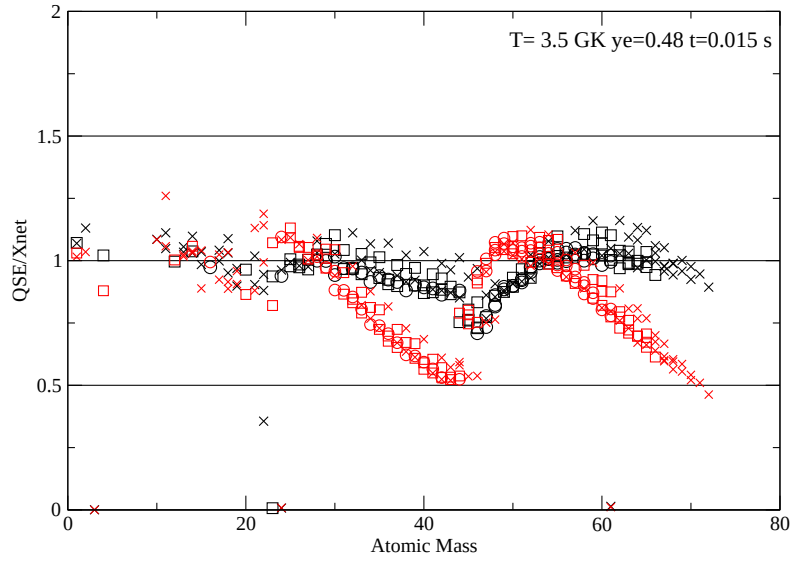


Figure 4.11 Shown here are ratios of abundances calculated with the QSE-reduced network and the full network for the case of incomplete silicon burning at 3.5 GK. Black symbols indicate the 3-group network and red symbols indicates the 2-group network. The 3-group network still matches the full network to 20% or better. Only the most abundant species of the 2-group network still match.

capture rates on the intermediate nuclei such as Ti and Cr. Thus, as Figures 4.10 and 4.11 illustrate, after 4 GK, the 3-group network follows the evolution of full network to 20% or better for most species, but the 2-group network shows larger deviations. The most abundant nuclei such as ^{54}Fe are well followed by both the 2-group and 3-group networks down to 0.015 seconds, where the temperature has fallen to 3.5 GK. That is why the energy generation rate of both QSE-reduced networks, show in Figure 4.8, follows that of the full network between 10^{-4} and 0.015 seconds.

To summarize, the 3-group network reproduces the abundances of the full network for most species to 20% accuracy or better for the duration of the simulation. The majority of the abundances of 2-group network match the full network to 20% or better for temperatures between 5 and 4 GK, but even at lower temperatures the most abundant species such as ^{54}Fe and ^{28}Si match to 20% or better.

This analysis leads to several possible choices for when the adaptive network should switch between QSE group configurations. If the energy generation of the QSE-reduced network were to be closely coupled to a hydrodynamics calculation, the 2-group network's early over estimation of the energy generation could cause an inaccurate initial rise in temperature that would greatly alter the abundances and energy generation for the rest of the simulation.

Figure 4.12 shows how the network switched between the QSE group configuration for 4 different adaptive runs.

To maximize network speed as well as the network's energy generation accuracy, the first run of the adaptive network, called Adaptive-1, starts the simulation with the 3-group configuration and runs for 10^{-4} seconds before switching to the 2-group QSE configuration. Figure 4.13 shows that the Adaptive-1 trial's energy generation matches the full network's down to 3.5 GK. However, by 3.5 GK, Figure 4.14 shows that while many of the most abundant species match the full network to 20 % or better, the overall abundance pattern is a poor match. Table 4.2 shows that

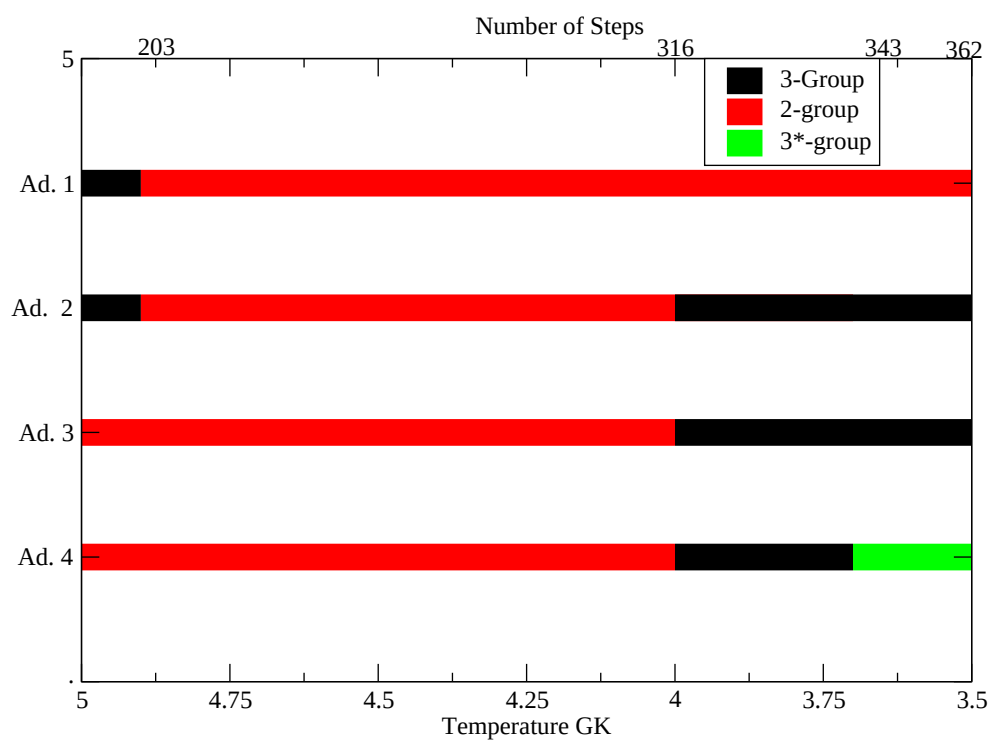


Figure 4.12 Shown are four variations for how the Adaptive QSE-reduced network can be tuned to switch between QSE group configurations during incomplete silicon burning.

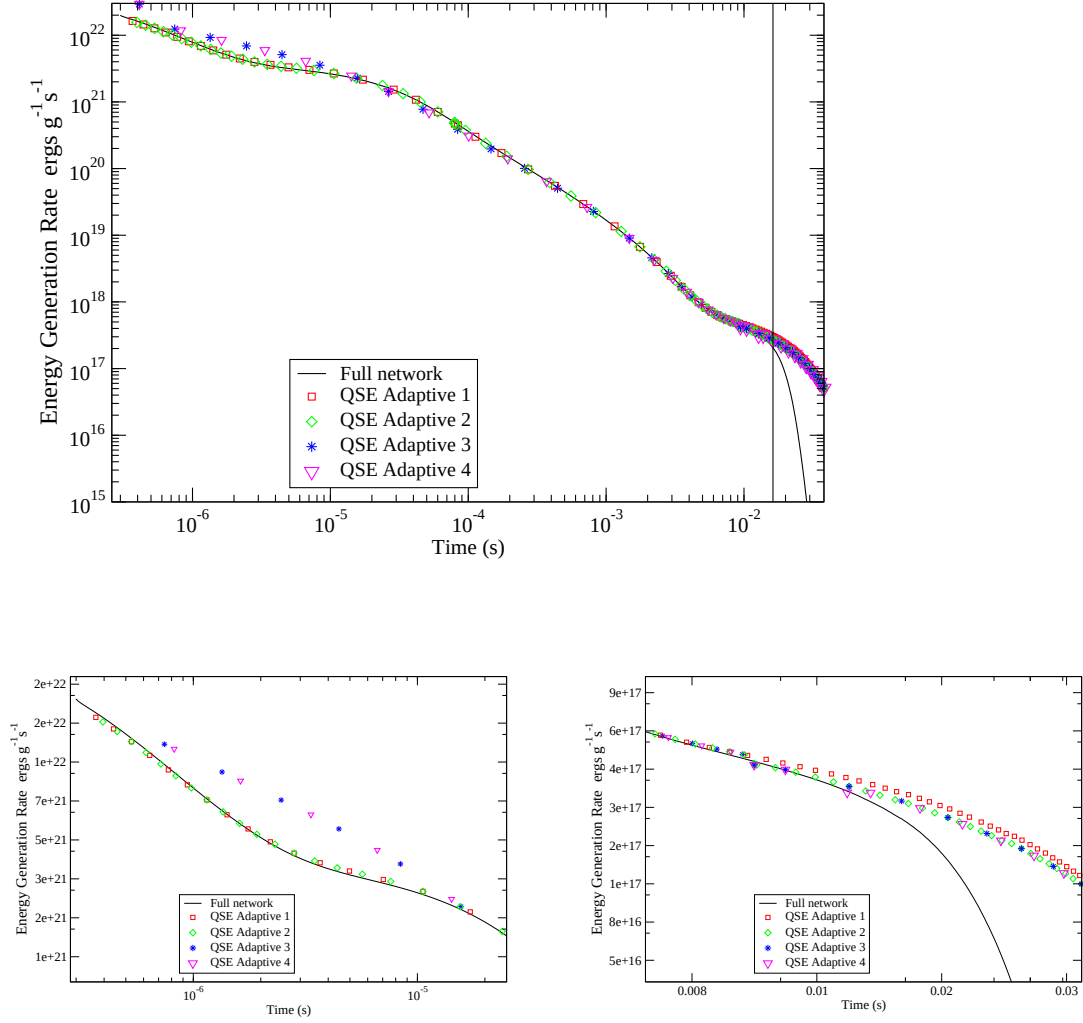


Figure 4.13 Shown here is a comparison of the energy generation rate of the full network and the QSE-reduced network for incomplete silicon burning. A vertical black line marks the time that corresponds to a temperature of 3.5 GK. The lower plots show more detail for early and late times.

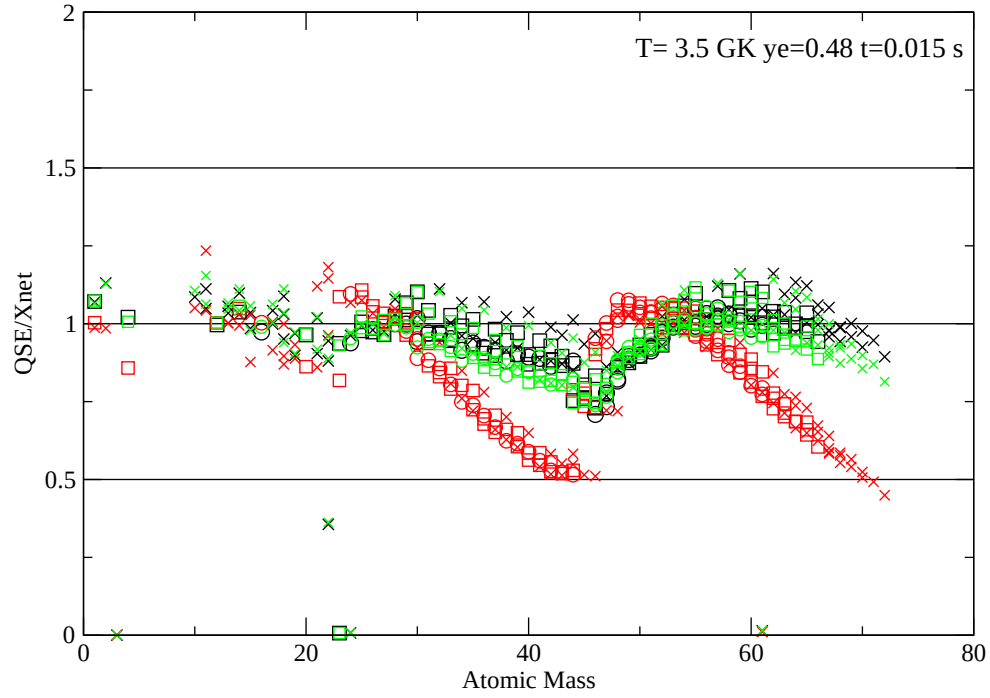


Figure 4.14 Shown here are the ratios between abundances calculated with the adaptive QSE-reduced network and those calculated by the full network for incomplete silicon burning. Black symbols indicate the 3-group network, red symbols indicate the Adaptive-1 run, and green symbols indicate the Adaptive-2 run. The shapes of the symbols have the same meaning as Figure 4.9.

Table 4.2. Network Speed for Incomplete Silicon Burning

Network	Core Duo			Pentium4		
	cpu time (s)	matrix time (%)	Iteration count	cpu time (s)	matrix time (%)	Iteration count
Vendor Supplied Solver						
3QSE	1.07	45	1066	1.56	29	1065
2QSE	0.56	27	831	0.82	23	831
Ad.1	0.83	30	991	1.12	28	950
Ad.2	1.05	32	1035	1.46	28	985
Ad.3	0.78	30	933	1.04	23	864
Ad.4	0.95	30	978	1.25	22	921
Full	17.36	83	1155	18.48	82	1280

the Adaptive-1 network is faster than the 3-group network by virtue of the phase where the 2-group configuration is used. The Adaptive-2 run follows the same early behavior as the Adaptive-1 run but recaptures the abundance accuracy of the 3-group network by switching from the 2-group to 3-group configuration at 10^{-3} seconds (4 GK). However, time is lost in each network switch. Table 4.2 shows that at 17 times faster than the full network, the Adaptive-2 configuration is only negligibly faster than running the 3-group network for the whole simulation.

Given that the 2-group network is more accurate than the alpha network at reproducing the energy generation of the full network, its initial inaccuracy may not be a problem for some applications. Figure 4.12 shows that the network spends over half of its 362 time steps in this initial high temperature period. To gain speed, the adaptive network could start in the 2-group configuration, which runs each iteration faster and uses less iterations per time step during this initial hot phase. The Adaptive-3 run starts with the 2-group configuration and then switches to a 3-group configuration to run from 4 GK to the end at 3.5 GK. Table 4.2 shows that the Adaptive-3 run is significantly faster than the fixed 3-group network and Figure 4.15 shows that it recaptures the 3-group network's accuracy after 10^{-4} seconds.

The Adaptive-4 run demonstrates that the adaptive network can also adjust the

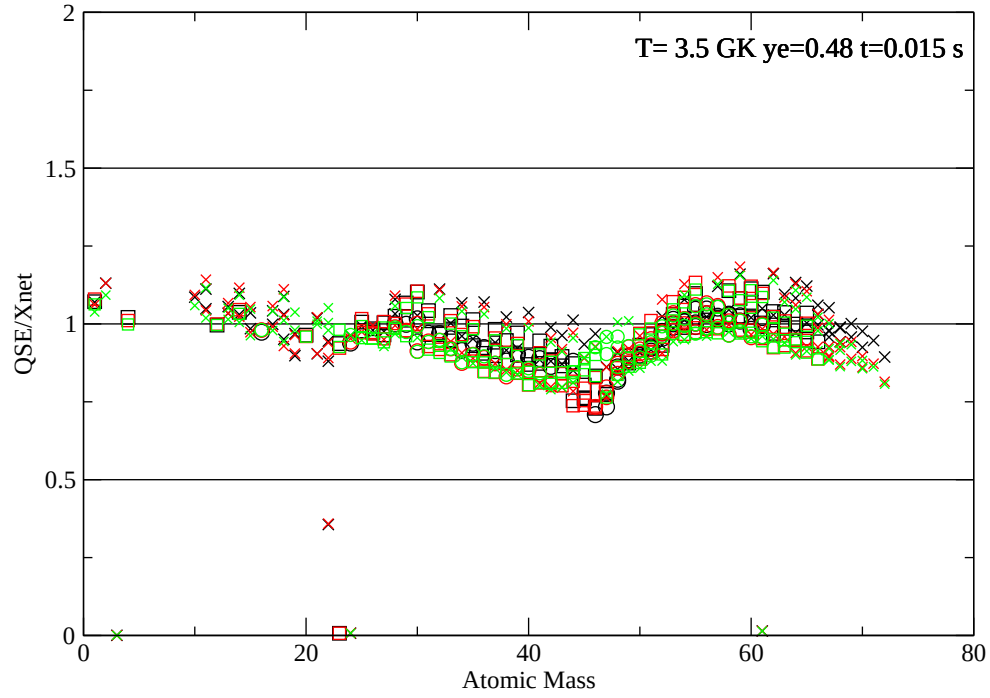


Figure 4.15 Shown here are the ratios between abundances calculated with the adaptive QSE-reduced network and the full network for incomplete silicon burning. Black symbols indicate the 3-group network, red symbols indicate the Adaptive-3 run, and green symbols indicate the Adaptive-4 run.

membership of the groups as well as the number of groups. The Adaptive-3 run shown in red in Figure 4.15 has several isotopes of calcium further out of equilibrium than the rest of the abundance. This "fraying" of the iron group begins at 3.7 GK. Of these outliers, only ^{48}Ca and ^{49}Ca are in the iron-peak group. If these nuclei are cut free of the QSE group and evolved independently, they bring their close isotopic neighbors into a better match with the full network as well. Any over or under population in the network pulls on its neighbors in a similar fashion.

This run repeats the configuration of the Adaptive-3 run but after 3.7 GK (0.012s) it allows ^{48}Ca and 10 other iron group members to evolve independently. The green plot in Figure 4.15 shows the better endpoint abundances accuracy of this run and Table 4.2 shows that it is still faster than the fixed 3-group network.

Table 4.2 shows that all QSE-reduced network configurations performed at least 10 times faster than the full network for this study of explosive incomplete silicon burning, making them good candidates for use in hydrodynamic simulations. The alpha network ran over 1000 times faster than the full network, explaining its pervasive use by hydrodynamists, but as Figure 4.8 demonstrates, its energy generation rate was often more than a factor of 10 different from that of the full network. At over 20 times faster than the full network with an energy generation rate that agrees to better than factor of two, the speed, accuracy, and simplicity of fixed 2-group QSE may make it the best initial candidate to replace the alpha network in hydrodynamic simulations where the conditions for QSE apply.

Complete Silicon Burning

Initial conditions of 7 GK coupled with a peak density of 10^9 g cm^{-3} lead to complete silicon burning. Due to the very high temperatures and densities, NSE is established after only 10^{-8} seconds. For an electron fraction of 0.48, this NSE is dominated by ^{54}Fe and ^{58}Ni with a few percent of ^4He . Figure 4.16 illustrates that as the temper-

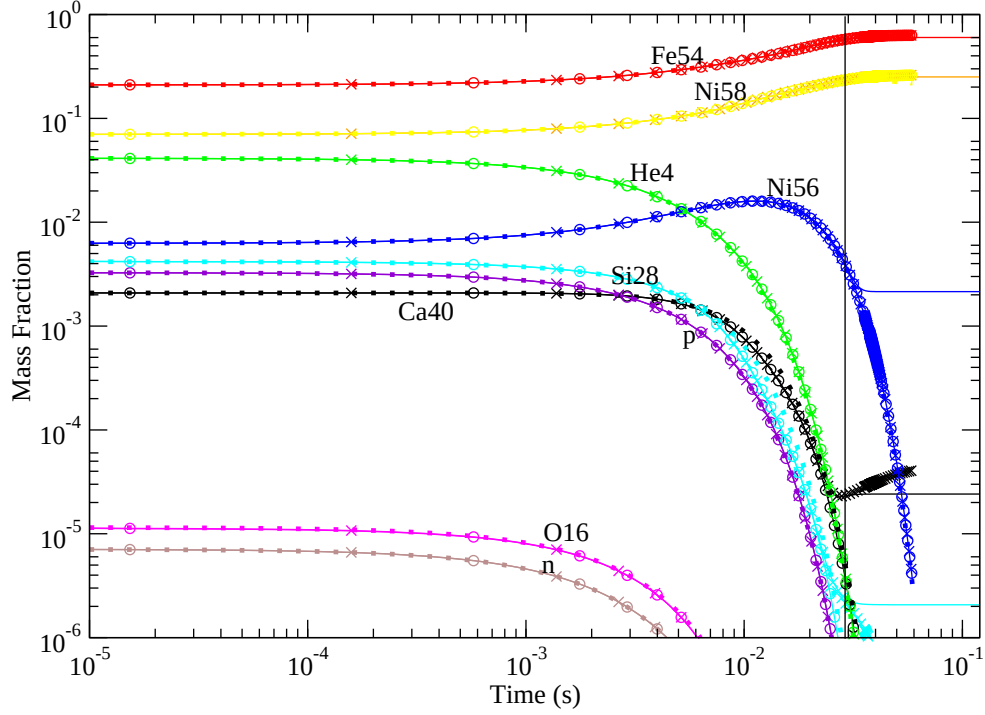


Figure 4.16 An example of complete silicon burning is shown. The solid lines represent the full network calculation, the circles the QSE 3-group network, the crosses the QSE 2-group network, and the dotted lines the QSE 1-group network.

ature falls, those ${}^4\text{He}$ are incorporated into the iron-peak nuclei such as ${}^{54}\text{Fe}$, ${}^{56}\text{Ni}$, and ${}^{48}\text{Ni}$. Finally as the temperature drops below 5 GK, the abundances distribution concentrates on ${}^{54}\text{Fe}$ and ${}^{58}\text{Fe}$ at the expense of other iron-peak nuclei and lighter species.

The early achievement of NSE makes the early phase of this trial a good test for the 1-group QSE-reduced network. Figures 4.17 through 4.19 show the comparison of the 1-group, 2-group, and 3-group QSE-reduced networks as the temperature declines. The green QSE/Xnet abundance ratio symbols for the 1-group network show that this equilibrium, with a maximum abundance error of 10 % at 6 GK, holds until the temperature falls below 6 GK. After this time the evolution is better

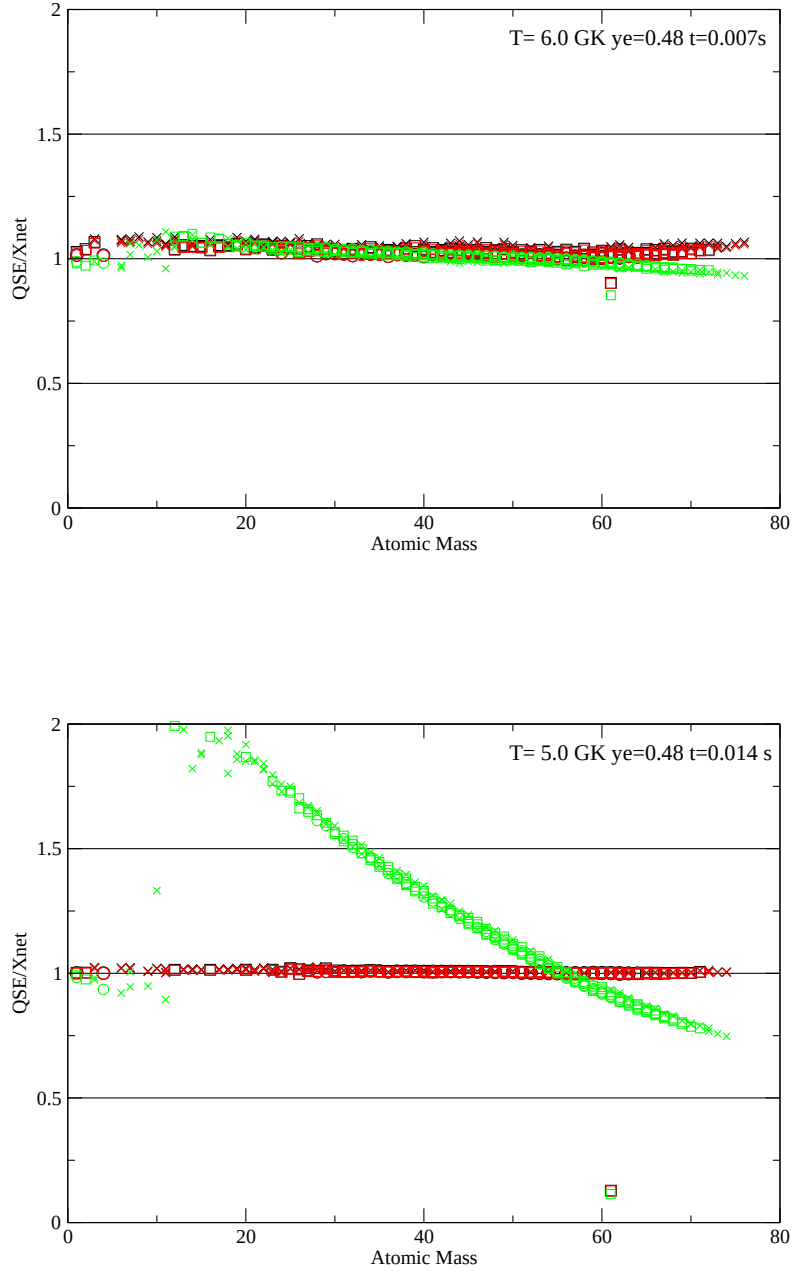


Figure 4.17 Shown here are the ratios of QSE-reduced to full network abundances for the case of complete silicon burning at early times. Here black symbols represent the 3-group network, red symbols represent the 2-group network, and green symbols represent the 1-group network.

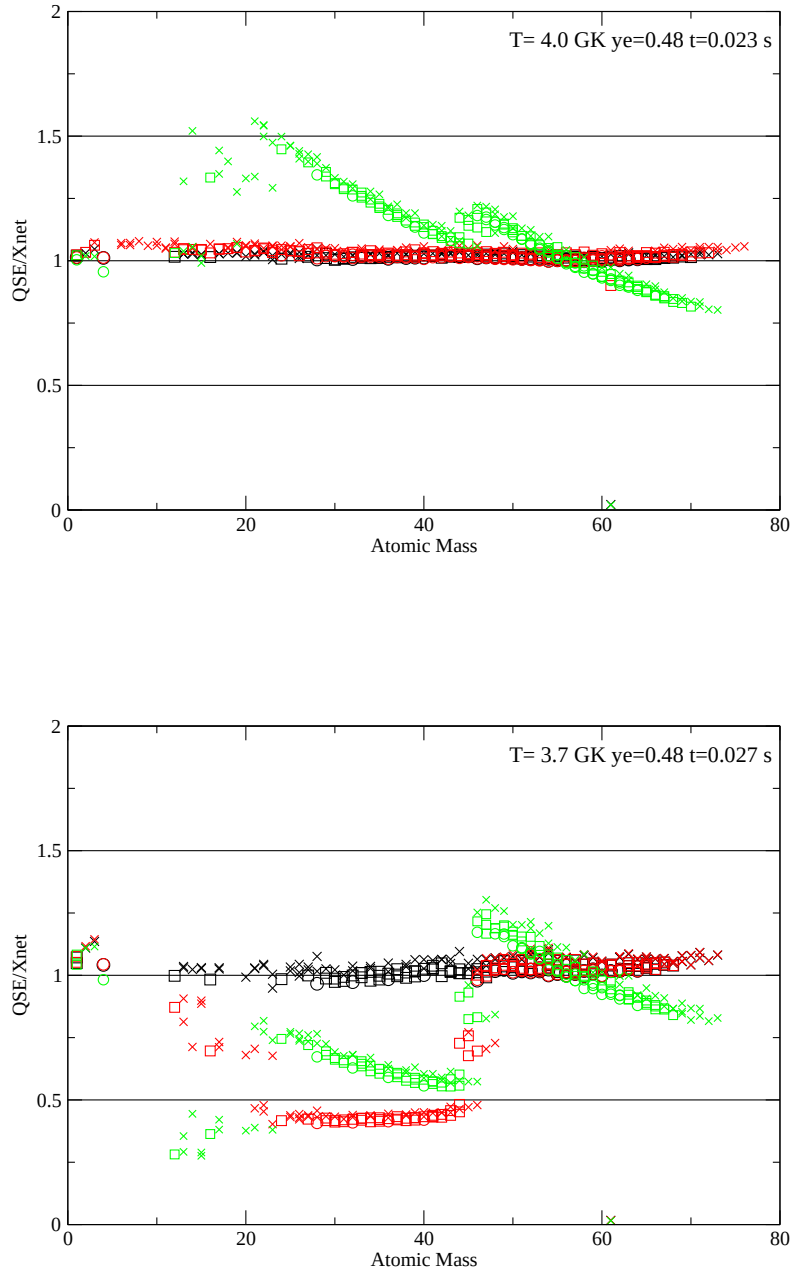


Figure 4.18 Shown here are the ratios of QSE to full network abundances for the case of complete silicon burning at different times and temperatures. Black symbols represent the 3-group network, red symbols represent the 2-group network, and green symbols represent the 1-group network.

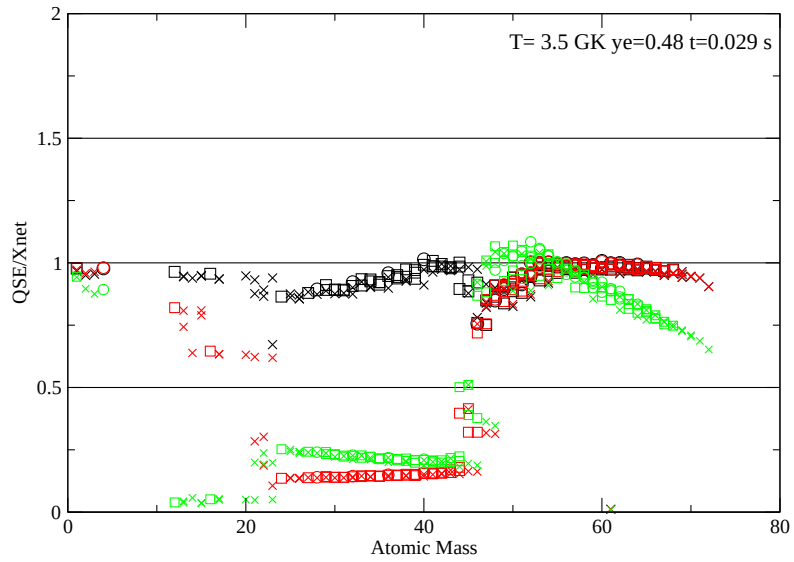


Figure 4.19 Ratio of the QSE-reduced to full network abundances for the case of complete silicon burning at 3.5 GK, where QSE is still valid. Black symbols represent the 3-group network, red symbols represent the 2-group network, and green symbols represent the 1-group network.

followed by the 2-group network, shown in red, until the temperature falls below 4.0 GK. The maximum error for the 2-group network is less than 10% at 4 GK. The evolution down to 3.5 GK is well followed by the 3-group network shown in black in Figure 4.19.

As the temperature continues to drop, the particle capture reactions freeze out. This can be seen in the leveling out of the mass fraction versus time of the full network (solid lines) in Figure 4.16. While the QSE abundances of most species drop precipitously beyond this point, the most abundant nuclei, such as ^{58}Ni and ^{54}Fe , match the full network even at temperatures well below 3.5 GK. The largest changes for each of these abundances occurred at higher temperatures where QSE was a valid assumption and the subsequent changes at lower temperatures were proportionally insignificant relative to the large abundance of each of these species.

The energy generation rate shown in Figure 4.20 as a function of time is based on the binding energies of the nuclei and the change in their abundances over small increments of time. Since the largest abundances represent most of the total mass and match their analogs in the full network throughout the evolution, the energy generation rate of the full network is well reproduced by all but the 1-group set of the QSE-reduced networks down to temperatures of 3.5 GK. The 1-group network fails because its assumption of NSE becomes incorrect at temperatures that are still high enough for significant evolution to occur for large abundances such as ^{28}Si . The dotted line in Figure 4.16 for the 1-group mass fractions of ^{28}Si can be seen diverging from the full network at 10^{-2}s , which corresponds to a temperature of 5 GK.

The adaptive QSE-reduced network was tuned to switch from the 1-group to the 2-group configuration at 6 GK and then to the 3-group configuration at 4 GK and the evolution was repeated. Figure 4.20 shows that the adaptive network matched the energy generation of the full network until the temperature fell below 3.5 GK.

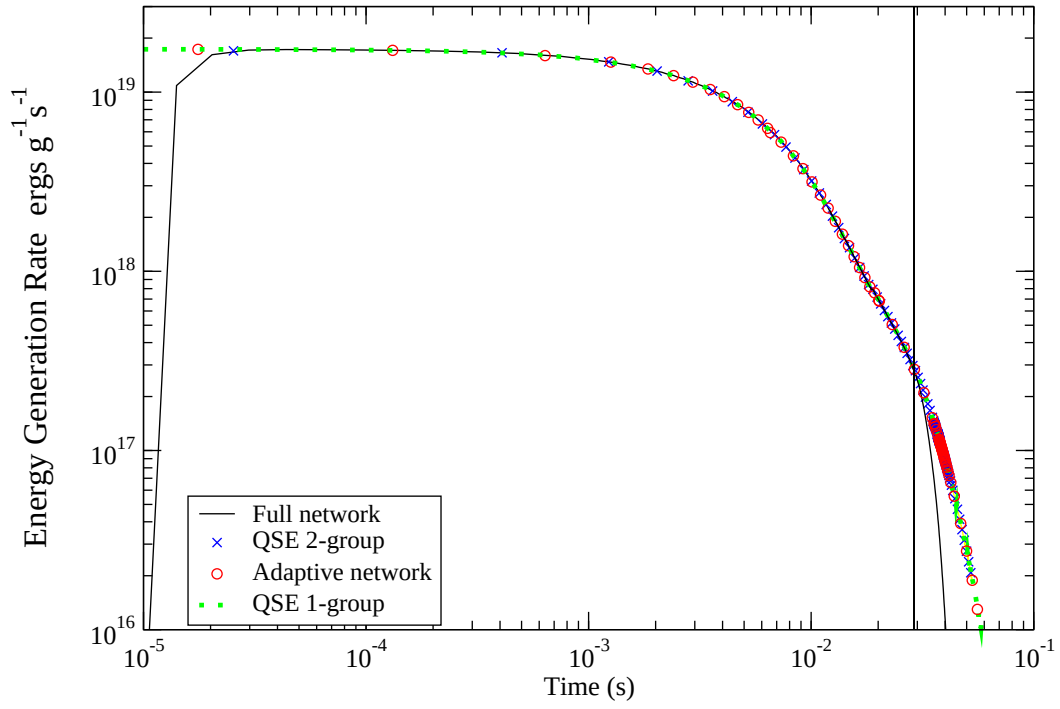


Figure 4.20 Shown here is a comparison of the energy generation rate of the full network, the 2-group network, and the adaptive QSE-reduced network. A vertical black line marks the time that corresponds to a temperature of 3.5 GK on both plots.

Table 4.3. Network Speed for Complete Silicon Burning

Network	Core Duo			Pentium4		
	cpu time (s)	matrix time (%)	Iteration count	cpu time (s)	matrix time (%)	Iteration count
Vendor Supplied Solver						
3QSE	1.51	40	1362	2.05	28	1065
2QSE	0.89	27	831	0.82	22	831
1QSE	0.13	0.01	271	1.12	1.4	950
Ad.1	1.02	30	996	1.63	23	1194
Full	18.90	84	1047	106	86	3582

As shown in Figure 4.21, at the 3.5 GK endpoint of the run, the abundances of the adaptive network match full network as well as those of the 3-group network, but as Table 4.3 shows, the adaptive network accomplished this in two-thirds the time of the 3 group network, making it almost 19 times faster than the full network. In Figure 4.21, most of the nuclei agree to within 12% for temperatures down to $T=3.5$ GK for both adaptive and 3-group QSE-reduced networks.

Table 4.3 shows that, in all cases, the QSE-reduced network was at least an order a magnitude faster than the full network. The Pentium4 struggles with the large matrix solve of the full network during conditions that produce equilibrium because the small changes in abundance over each time step cause the matrix to become nearly singular. (The particular Pentium4 cluster used for this trial literally catches on fire when you try to run complete silicon burning inside a hydrodynamics code such as FLASH with a full network.) This deficiency leads to the unusually long running time for the full network shown on the bottom right of Table 4.3. Newer platforms with larger cache memory and better math libraries have less of this problem. However, for students attempting to avoid the batch queues of modern supercomputers by developing their methods for hydrodynamics on ancient computers, the QSE method is faster (and less incendiary) because it reduces the matrix solve from 86% of the calculation to 40% or less.

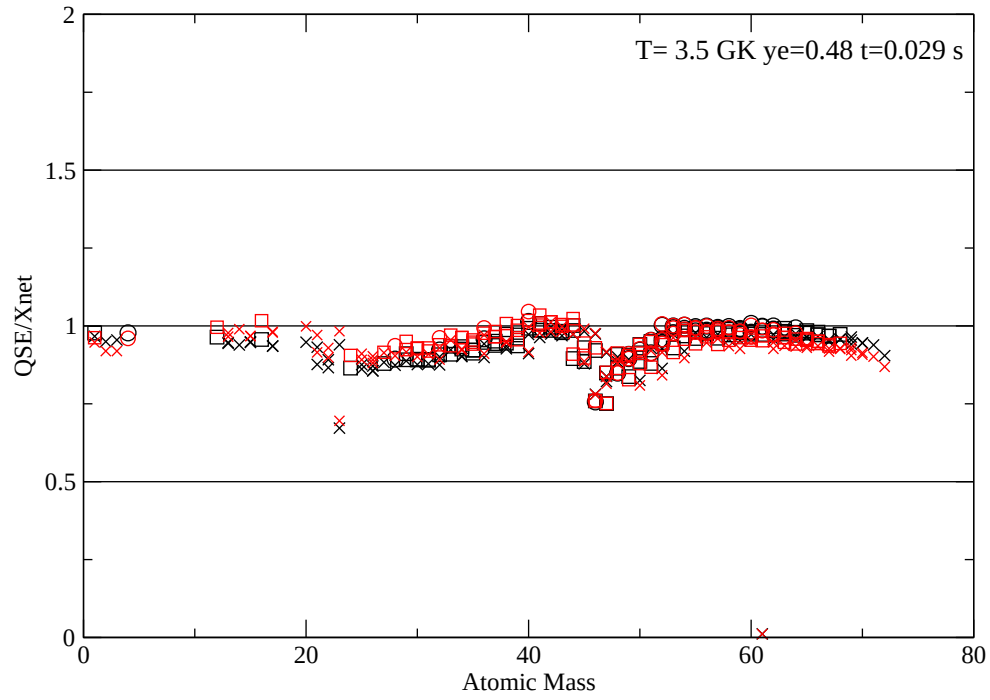


Figure 4.21 Shown here are the ratios of the abundances produced by the QSE-reduced networks to those produced by the full network for the case of complete silicon burning. Black symbols represent the 3-group network and red symbols represent the adaptive network. The two networks garner the same abundance results

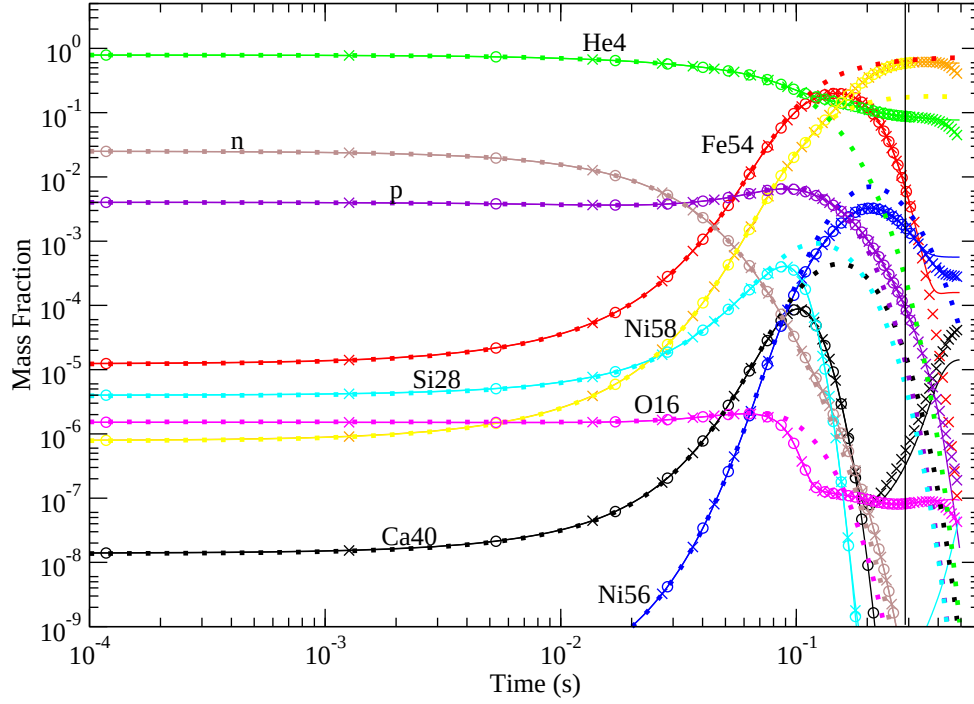


Figure 4.22 An example of silicon burning with an α -rich freezeout is shown. The solid lines represent the full network calculation, the circles the 3-group QSE-reduced network, the crosses the 2-group QSE-reduced network, and the dotted lines the 1-group QSE-reduced network.

Silicon Burning with α -rich Freezeout

A peak temperature of 7 GK coupled with a peak density of 10^7 g cm^{-3} produces an α -rich freezeout. Figure 4.22 shows the mass fraction for some of the most dominant nuclei as a function of time as the temperature falls. Under these conditions, NSE is rapidly established and dominated by α -particles and free nucleons. Between 0.65 and 0.14 seconds ^4He and other lighter nuclei, such as ^{16}O , rapidly transmute into the iron-peak nuclei and the more dominant silicon group abundances which are growing rapidly as the temperature falls from 6 to 5 GK. The 2-group and 3-group networks follow the evolution of these dominant species, such as stable ^{40}Ca , well

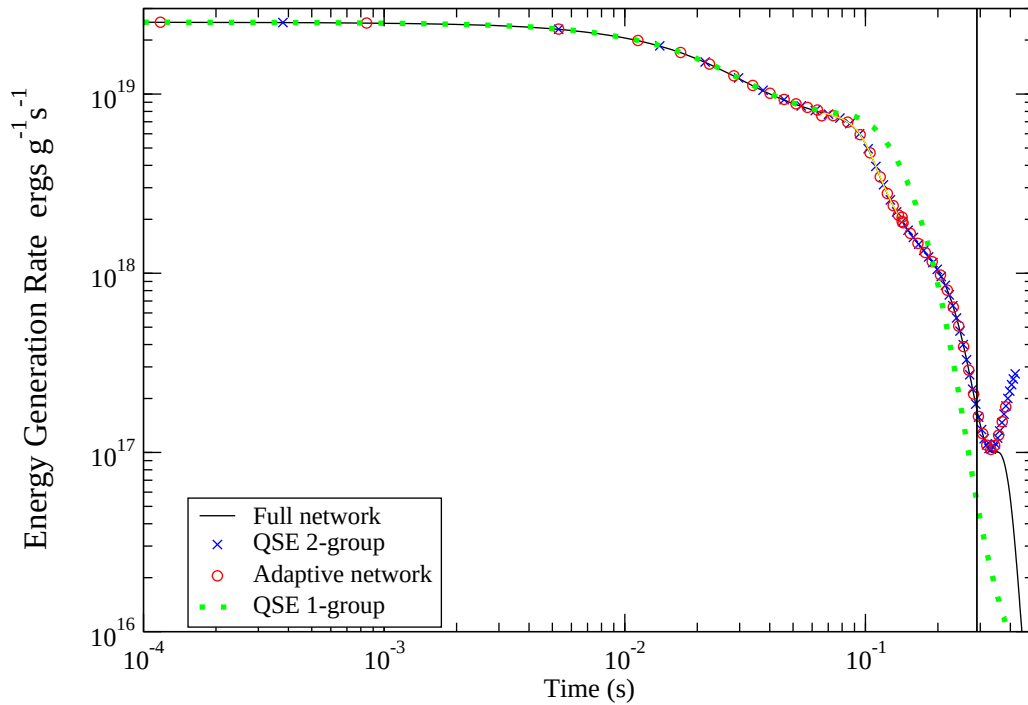


Figure 4.23 An example of silicon burning with an α -rich freeze out. A comparison of the energy generation rate during α -rich freeze out is shown. A vertical black line marks 3.5 GK.

in this region even as the silicon QSE group breaks up. The QSE assumption only fails for the lesser abundant species. Therefore, as Figure 4.23 illustrates, the 2-group and 3-group networks follow the energy generation of the full network until the reactions freeze out. If the QSE composition is frozen at .038 seconds (3.0 GK), the abundances of its most dominant species would match those of the full network for the remainder of the evolution.

The case is more difficult for the 1-group network's assumption of NSE; It fails while the dominant species are still growing rapidly, leading NSE to over estimate the energy generation after 0.065 seconds, as Figure 4.23 demonstrates. Thus, there is no way to obtain accurate results from the 1-group network at the lower temper-

Table 4.4. Network Speed for Silicon Burning α -rich Freezeout

Network	Core Duo			Pentium4		
	cpu time (s)	matrix time (%)	Iteration count	cpu time (s)	matrix time (%)	Iteration count
Vendor Supplied Solver						
3QSE	1.61	40	1471	2.02	30	1343
2QSE	1.04	23	1357	1.18	23	1242
1QSE	0.13	0.02	322	0.13	1.2	271
Ad.1	3.95	80	1457	4.46	58	1087
Full	22.00	84	1047	27.10	84	1583

atures. This error in the energy generation rate would be particularly detrimental if the 1-group network was closely coupled to a hydrodynamics code. The inaccurate extra energy generation could change the temperature and density, carrying the composition's evolution increasingly away from that of the full network.

Figures 4.24 and 4.25 show the comparison of the 1-group, 2-group, and 3-group QSE-reduced networks as the temperature declines. The 2-group and 3-group networks' abundances for iron-peak nuclei, proton, neutrons, and ^4He agree to 20% or better with the full network down to a temperature of 3.5 GK. However, alpha-rich freezeout conditions are the most challenging for QSE-reduced networks, due to small abundances in the region around silicon and the resulting breakdown in this QSE group.

Table 4.4 shows that the various groupings in the nonadaptive QSE-reduced network run between 10 and 150 times faster than the full network. At 20 times faster, with a descent reproduction of the energy generation of the full network, the 2-group configuration may have the best compromise between speed and accuracy for inclusion in hydrodynamics codes for the conditions presented here.

The QSE-reduced network could also be useful, in the absence of coupling to a hydrodynamics code, to speed up post-processing for large networks containing thousand of species. In this case, the accuracy of the total abundances pattern

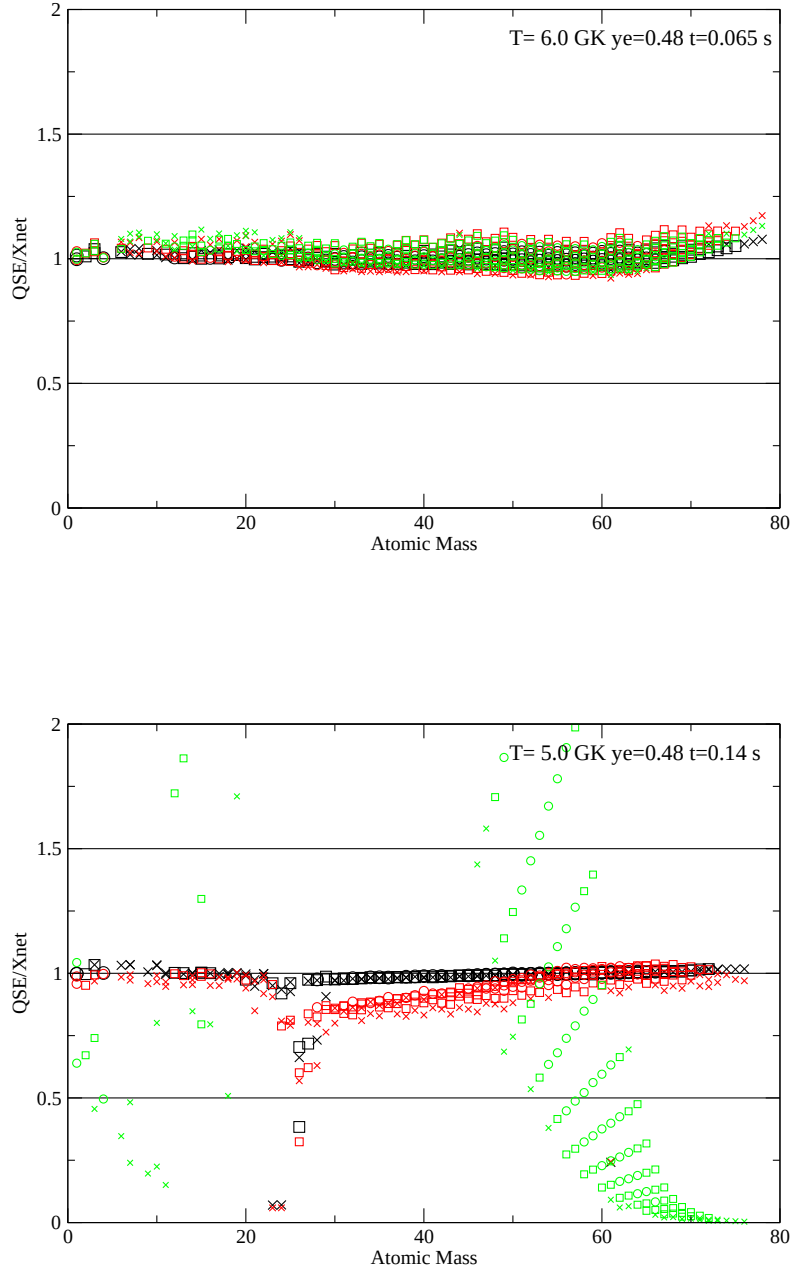


Figure 4.24 Comparison of the QSE and the full network abundances for the case of silicon burning with an α -rich freezeout for early times and temperatures is shown. Black symbols represent the 3-group network, red symbols represent the 2-group network, and green symbols represent the 1-group network.

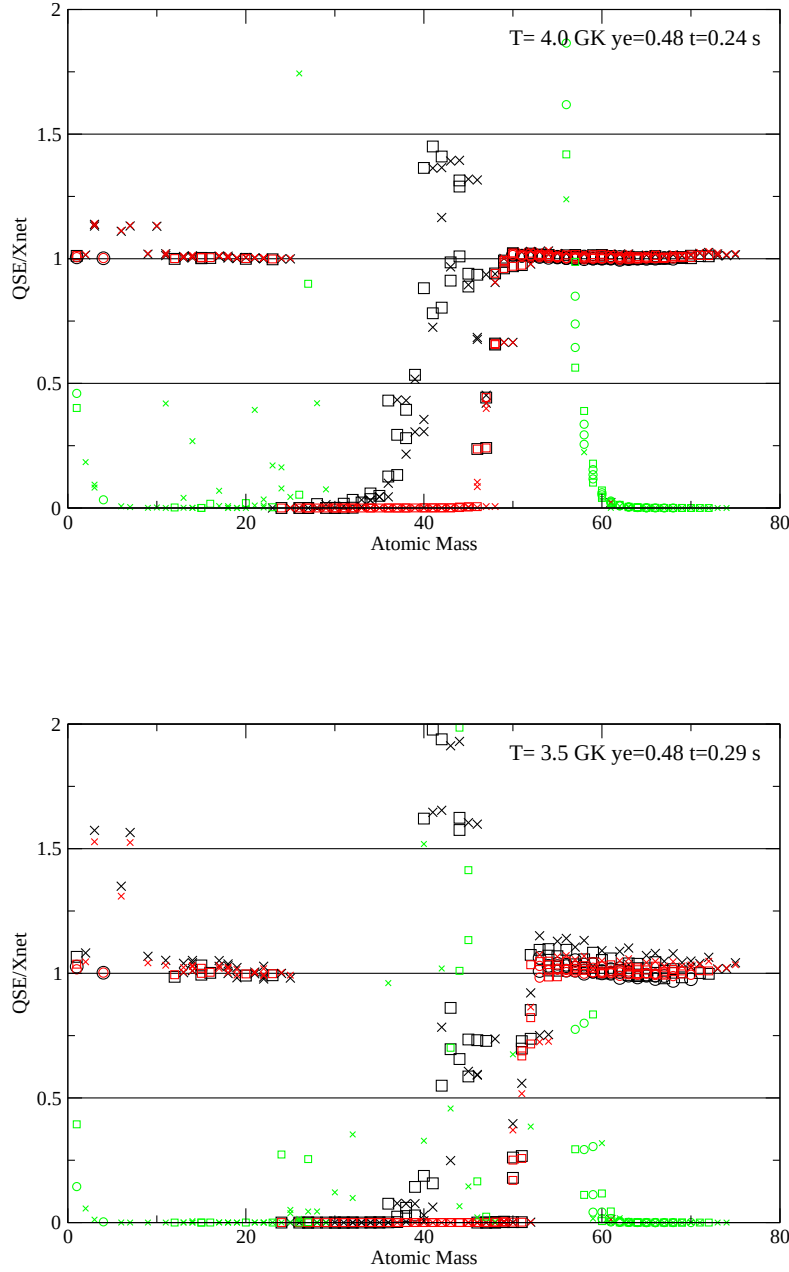


Figure 4.25 Comparison of the QSE-reduced and the full network abundances for the case of silicon burning with an α -rich freezeout at different times and temperatures is shown. Black symbols represent the 3-group network, red symbols represent the 2-group network, and green symbols represent the 1-group network.

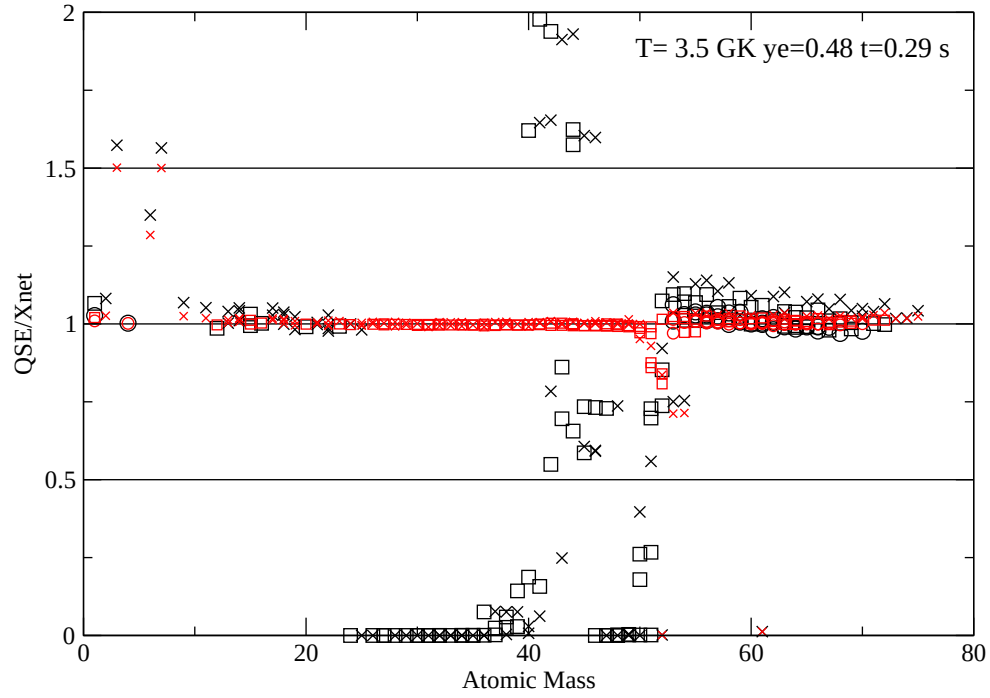


Figure 4.26 Ratios of the Adaptive and 3-group QSE-reduced network abundances to those of the full network abundances for the case of silicon burning with an α -rich freeze out at 3.5 GK are shown. Black symbols represent the 3-group network and red symbols represent the adaptive network.

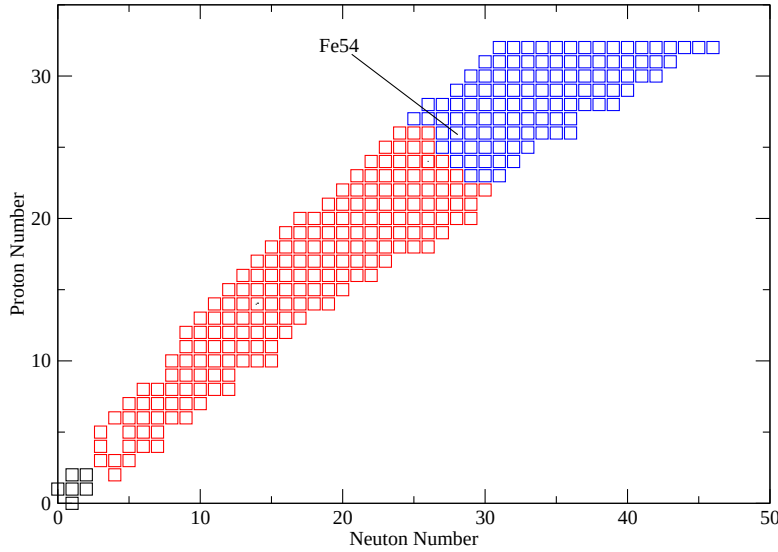


Figure 4.27 This shows the 2*-group network configuration, where only two independent variables are used to follow the chemical evolution.

would be just as important as the accuracy of the energy generation. To maximize the accurate reproduction of even the smallest abundances, the adaptive network has been utilized in a different way for this problem. The species from mass 23 to mass 42 are split off into their own QSE group at 6 GK. This is the same configuration as the 3-group network. This configuration only holds until 5 GK, where the silicon group begins falling out of equilibrium with the rest of the network. After 5 GK, all the silicon group members are evolved independently and only the iron and light groups maintain QSE. Pictured in Figure 4.27, is the 2*-groups configuration. The red curve in Figure 4.25 shows that this adaptation allows agreement for most species to within 20% or better of the full network. Both the adaptive and fixed networks reproduce the energy generation of the full network.

Table 4.4 shows that the adaptive network is only 5 times faster than the full network when used in this fashion. About 80% of the adaptive network's time is spent in 2-groups configuration, evolving the abundances from 5 to 3.5 GK. This final

configuration uses 188 variables to evolve the 299 species in the network. The initial configuration and the fixed 2-group QSE-reduced network use only 56 variables. Since the fixed network is faster and reproduces the energy generation of the full network, it or a simpler adaptive scheme that remains in the 3-group configuration from 5 to 3.5 GK may be the better choices for running in situ in a hydrodynamics model. Then the detailed abundance composition of the silicon group members could be recovered later by post processing.

This illustrates the flexibility of the QSE-reduced network for alpha-rich freezeout. Depending on the application, one may choose to achieve a factor of 20 speedup and get the largest abundances and the energy generation correct or one may choose a factor of 5 speedup if the detailed accuracy of all abundances is needed.

4.2 Conclusion

I have demonstrated the ability of QSE to greatly reduce the number of independent nuclear species that need to be evolved to accurately track nucleosynthesis during silicon burning. I have written and developed a QSE-reduced nuclear reaction network, based on these studies, which can be run with a fixed QSE group configuration or tuned to adaptive adjust the number of QSE groups and QSE group membership to fit the changing thermodynamic conditions. This network is compatible with Xnet and will become incorporated as a feature in future version of Xnet.

A network reduced in this fashion provides a reasonable estimate of the nuclear energy generation and elemental production even in cases where thermodynamic variations result in incomplete silicon burning or α -rich freezeout. The smaller number of variables resulting from the use of QSE groups allows a smaller matrix build and solve in the nuclear reaction network calculation, in this case, speeding up the calculation by a factor of 10 or greater. The reduction in the number of nuclei traced

also will reduce the number of equations which must be solved within an encompassing hydrodynamic model. By adapting the number and membership of the QSE groups, even better agreement with the abundances of the full network and/or further reduced computational cost can be achieved with the QSE-reduced network. The choice of how to apply this improvement will vary with the application. For many burning stages, where a single QSE group stretching from Si-Fe is present, use of adaptivity allowAs a result,e QSE-reduced network to run 20 times faster than the full network. For more complex behavior, like that seen during alpha-rich freezeout, varying degrees of adaptivity can allow sufficient accuracy for the dominant species and energy generation with a large (15-20x) improvement in speed, or a high degree of accuracy even for trace species with a more modest improvement (5x) in speed. Decisions on how best to apply adaptivity to the QSE-reduced network within a hydrodynamic model also influence the treatment of advection and mixing. With dynamic QSE group allocation, the meaning of each group abundance can be different between adjoining hydrodynamic zones or mass elements, thus the hydrodynamic evolution can not take advantage of the reduction in the number of evolved abundances and must evolve the full abundance set. As a result, the use of QSE-group adaptivity should be cost-effective for models where the thermonuclear evolution dominates the computational cost, but fixed groups may be the proper choice for models which more closely balance the thermonuclear and hydrodynamic costs.

When this network is successfully incorporated into self-consistent hydrodynamic models of supernovae, it will lead to the most accurate modeling of the nucleosynthesis and nuclear energy generation associated with iron formation to date, while remaining as cost effective as possible. Therefore, its estimate of the nucleosynthesis contributions to individual core-collapse supernovae and Type Ia supernovae will allow for better comparison to past and future observations. This will improve our

understanding of the different supernovae mechanisms and give us a clearer picture of our chemical origins.

4.3 Postlude

As a first practical application of the QSE-reduced network, much of the past few months have been devoted to installing Xnet (the full network), the QSE-reduced network described in this dissertation, and an Xnet-based alpha network inside the FLASH hydrodynamics code, in order to conduct studies toward understanding the role that nucleosynthesis plays in Type 1a supernovae. While much of the ground-work is complete for this installation, efforts continue to validate our installation of both the full network and the QSE-reduced network against the existing small networks in FLASH. All three codes will run to the completion in a simple 64-zone self-heating calculation in FLASH, but among the three networks and the alpha network originally used by Calder et al (2007), the amount of energy liberated and the timescale of its liberation is inconsistent. Because this is the first time that anyone has attempted to include such detailed networks in FLASH, we are not sure what to expect and much more testing is required. We have demonstrated that the QSE-reduced network is flexible and performs with adequate speed and accuracy under many different hydrodynamic conditions. These studies strongly indicate that QSE would be a useful addition to FLASH and other hydrodynamic models. I hope that our work toward the adaptive QSE-reduced network will continue to grow into a tool that allows more accurate nucleosynthesis to become the standard feature of hydrodynamic supernova models. Since the observed elemental abundances are our best window into the inner workings of a star, accurately modeling them is important for understanding how supernovae produce the elements that make up our world.

Bibliography

Bibliography

Arnett W.D., Bahcall J.N., Kirshner, R.P., Woosley S.E., 1989, *Annu. Rev. Astron. Astrophys.* 27, 629

Arnett, W. 1969, *Ap. Space Sci.*, 5, 280

Arnett, W. D. 1996, *Supernovae and Nucleosynthesis : An Investigation of the History of Matter, from the Big Bang to the Present* (Princeton: Princeton University Press)

Bethe H.A., & Wilson J.R. 1985, *ApJ* 295, 14

Bodansky, D., Clayton, D., & Fowler, W. 1968, *ApJS*, 16, 299

Brachwitz, F., Dean, D., Hix W.R., Koichi, I., Langanke, K., Martinez-Pinedo, G., Nomoto, K., Strayer, M., Thielemann, F.-K., Umeda, H. 2000, *ApJ*, 536, 934

Buras, R., Rampp, M., Janka, H.-T., & Kifonidis, K. 2003, *Phys. Rev. Lett.*, 90, 241101

Burrows, A., Hays, J., and, Fryxell, B., 1995, *ApJ*, 450, 830B

Calder, A., Townsley, D., Seitenzahl, I., Peng, F., Messer, O. E. B. Vladimirova, N., Brown, E., Truran, D., Lamb, D. 2007, *ApJ*, 656, 313

Calder, A., Fryxell, B., Plewa, T., Rosner, R., Dursi, L., Weirs, V., Dupont, G., Robey, H., Kane, J., Remington, B., Drake, R., Dimonte, G., Zingale, M., Timmes, F., Olson, K., Ricker, P., MacNeice P., Tufo, H. 2002, *ApJS*, 143, 201

- Clayton, D., *Principles of Stellar Evolution and Nucleosynthesis* University of Chicago Press, Chicago, (1983)
- Chieffi, A., Domìnguez, I., Höflich, P., Limongi, M., Straniero, O. 2003, MNRAS, 345, 1, pp. 111-122
- Fowler, W., Caughlan, G., & Zimmermann, B. 1967, ARA&A, 5, 525
- Fryxell, B., Olson, K., Ricker, P., Timmes, F., Zingale, M., Lamb, D., MacNeice P., Rosner, R., Truran, D., Tufo, H. 2000, ApJS, 131, 273
- Fowler, W., & Hoyle, F. 1964, ApJS, 9, 201
- Hoyle, F., & Fowler, W. 1960, ApJ, 132, 565
- Herant, M., Benz, W, Hix, W.R., Fryer, C.L., & Colgate, S.A. 1994 ApJ, 435, 339
- Hix, W. R. 1995, Ph.D. thesis, Harvard University.
- Hix, W. R., Khokhlov, A. M., Wheeler, J. C., & Thielemann, F.-K. 1998, ApJ, 503, 332
- Hamuy M., Phillips, M. M., Maza J. Suntzeff N.B., Schrommer R.A., Aviles R. 1995, ApJ, 109, 1669
- Hix, W. R., & Thielemann, F.-K. 1996, ApJ, 460, 869
- Hix, W. R., & Thielemann, F.-K. 1996, ApJ, 511, 862
- Hix, W. R., Parete-Koon, S., Freiburghaus, C., Thielemann, F-K, 2007, ApJ, 667, 467
- Hix, W. R., & Thielemann, F.-K. 1999a, J. Comp. Appl. Math, 109, 321
- Höflich P., Khokhlov A., Wheeler J.C., Hamuy M., Philips M. M., Suntzeff N.B. 1996, ApJ.472 L81-L84
- Iben I. Jr.,& Tutukov A.V. 1984, ApJS, 54, 335
- Janka, H.-T. & Müller,E. 1995 A&A, 306, 167
- Käppeler,F., Thielemann,F.-K., Wiescher, M., Annu. Rev. Nucl. Part. Sci. 48 (1998) 175–251.
- Khokhlov, A. M. 1991, A&A, 245, 114
- Khokhlov, A. M. 1991, ApJ, 449, 695
- Kifonidis, K., Plewa, T., Janka, H.-T., & Müller, E. 2003, A&A, 408, 621K
- Kippenhann, R. & Weigert, A. *Stellar Structure and Evolution*, Springer-Verlag, Berlin, (1990)
- Meyer, B. S., Krishnan, T. D., & Clayton, D. D. 1998, ApJ, 498, 808
- Mezzacappa, A., Calder, A.C., Bruenn S.W., Blondin, J.M., Guidry M.W., Strayer, M.R., Umar, A.S. 1998 ApJ 495,911
- Mezzacappa, A., Liebendörfer, M., Messer,O., Hix,W.R., Thielemann, F.-K., & Bruenn S. 2001, Phys. Rev. Lett., 86, 1935

- Nadyozhin D.K. 1994, ApJS, 92, 527N
- Nagataki, S., Shimizu, T. M., & Sato, K. 1998, ApJ, 495, 413
- Nomoto 1980 IAU-Sym. 93, eds. D. Sugimoto. D.Q. Lamb & D. Schramm, Dordrecht, D. Reidel Publ. Comp., p. 295
- Nomoto K., Sugimoto D., Neo S. 1977, PASJ, 29, 765
- Nomoto K., Sugimoto D., Neo S. 1976, ApSS, 39, 137
- Phillips M.M., 1993 ApJ, 413L, 105
- Press, W., Teukolsky, S., Vetterling, W., & Flannery, B. 1992, Numerical Recipes ((Cambridge:Cambridge Univ.)), second edition
- Rampp, M., & Janka, H.-T. 2000, ApJ, 539, L33
- Reiss, A.G., Press, W.H., & Kirshner, R.P. 1996, ApJ, 473, 88R
- Reinecke, M., Hillebrandt, W., & Niemeyer, J. C. 2002, A&A, 386, 936
- Rols C.E. & Rodney W.S. Cauldrons in the Cosmos, University of Chicago Press, 1988
- Schramm, D.N., Arnett, W.D. 1975, Mercury, vol. 4, May-June, p. 16-22
- Shigeyama, T., Nomoto, K., and Hashimoto, M. 1988, Astr. Ap., 196, 141
- Thielemann, F., & Arnett, W. 1985, ApJ, 295, 604
- Thielemann, F.-K., Hashimoto, M. & Nomoto, K., M. 1990, ApJ, 349, 222
- Thielemann, F.-K., Nomoto, K., & Hashimoto, M. 1996, ApJ, 460, 408
- Thielemann, F.-K., Brachwitz, F., Höflich, P., Martinez-Pinedo, G & Nomoto, K. 2004, New Astronomy Review, 48, pp. 605-610.
- Thielemann F-K, Nomoto K. 1990, ApJ, 34, 222
- Thielemann F-K, Nomoto K., Yokoi, K. 1986, Astron. Astrophys., 158, 17-33
- Thompson T.A., Burrows A. & Pinto P.A., 2003 ApJ, 592, 434
- Timmes, F. X., Hoffman, R. D., & Woosley, S. E. 2000, ApJS, 129, 377
- Timmes, F. X. & Woosley, S. E. 1992, ApJ, 396, 649
- Tutukov, A.V., Yungelson L.R. 1982, IAU colloquium 70, D. Reidel Publ. Comp., p238
- Webbink, R.F. 1984, ApJ 277, 355
- Woosley, S. E., Arnett, W. D., & Clayton, D. D. 1973, ApJS, 26, 231
- Woosley, S. E., & Weaver, T. A. 1995, ApJS, 101, 181
- Woosley, S. E., & Weaver, T. A. 1986, Ann. Rev. Astr. Ap. 24, 205
- Woosley, S. E., Taam R.E., & Weaver, 1980 in :Type I Supernovae, eds, C.Wheeler, Austin U. Texas, 96

Vita

Suzanne Parete-Koon was born in 1974, in Oswego, New York. She received a Bachelor of Arts degree in 1997 from Bluffton College in Bluffton, Ohio where she majored in Physics and Chemistry. She received a Masters degree in Physics from the University of Tennessee at Knoxville in December of 2001. She expects to complete a PhD in astrophysics at the University of Tennessee in August 2008. She will begin an American Institute of Physics Diplomacy Fellowship at the US State Department in September of 2008.