REACTION RATE CALCULATIONS IN DENSE STELLAR MATTER

A Dissertation

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An interesting question in nuclear astrophysics is the fate of X-ray burst ashes as they descend under gravity to the deep layers of an accreting neutron star crust. As the ashes sink, they are subject to a range of nuclear reactions which transmute the nuclei. The primary of these reaction mechanisms are electron capture reactions, which are activated for different isotopes depending on the electron Fermi energy. At sufficiently high mass densities ($\rho = 2.1 \times 10^9 \text{ g cm}^{-3} \text{ for } ^{12}\text{C} + ^{12}\text{C} \text{ and } \rho = 3.2 \times 10^{12} \text{ g cm}^{-3} \text{ for } ^{40}\text{Mg} + ^{40}\text{Mg}$), density induced fusion reactions, known as pycnonuclear reactions, begin to occur.

By combining existing electron capture formalism and a phenomenological expression for pycnonuclear reactions (specifically developed for a multi component plasma environment) with a network solver, the fate of the X-ray burst ashes have been addressed. In this context it has been found that with increasing mass density, the rigid Coulomb lattice of the neutron star crust dissolves into the isotopes $^{40}\text{Mg}$ and $^{46}\text{Si}$, with an integrated energy release of between $\sim 1.8 \text{ MeV/u}$ and $\sim 2.4 \text{ MeV/u}$, depending on lattice models. This result is fairly insensitive to the initial abundance distribution. The production of $^{46}\text{Si}$ is determined to be the result of a cyclical pycnonuclear fusion, electron capture process.

The magnitude of the pycnonuclear reactions have been found to be dependent on the mass fraction contained in the nuclei, and consequently to drop off quickly
at mass densities greater than the neutron drip density. To large effect this halts the production cycle of $^{46}\text{Si}$. 

For My Parents
CONTENTS

FIGURES ................................................................. v

TABLES ................................................................. xi

ACKNOWLEDGMENTS ................................................... xii

CHAPTER 1: INTRODUCTION ........................................... 1
  1.1 Neutron Star Formation ........................................ 2
  1.2 Interior Structure ............................................. 6
  1.3 Binary Neutron Stars ........................................... 9
    1.3.1 X-Ray Bursts ........................................... 9
    1.3.2 The Fate of the RP-Process Ashes ....................... 11
  1.4 Why Study Neutron Stars? .................................... 13
  1.5 Goals of This Work ........................................... 14

CHAPTER 2: HEAVY ION FUSION ..................................... 16
  2.1 Scenario Relevant Nuclei .................................... 17
  2.2 The Barrier Penetration Model ............................... 20
  2.3 The Effective Potential ...................................... 22
    2.3.1 Coulomb Potential ...................................... 22
    2.3.2 Nuclear Potential - The São Paulo Potential .......... 24
    2.3.3 Angular Potential ...................................... 25
    2.3.4 Folding Potential ...................................... 25
  2.4 The Astrophysical $S(E)$ Factor ............................. 26
  2.5 Applicability of Calculated $S(E)$ Factors ................ 27
    2.5.1 Stable Nuclei ........................................... 27
    2.5.2 Unstable Nuclei ....................................... 30

CHAPTER 3: ASTROPHYSICAL $S(E)$ FACTORS FOR FUSION REACTIONS INVOLVING C, O, Ne AND Mg ISOTOPES ........................................ 35
  3.1 Analytical Approximation of $S(E)$ Factors ................ 36
    3.1.1 Physical Meanings of the Fit Parameters ............... 37
    3.1.2 Evaluating the Fits ................................... 38
3.2 $S(E)$ Factors at Zero Energy ........................................ 42

CHAPTER 4: DENSE MATTER NUCLEOSYNTHESIS ....................... 54
4.1 The Extremes of Stellar Burning ...................................... 56
4.1.1 General Reaction Rate Formalism ................................. 57
4.2 Physical Conditions .................................................... 63
4.2.1 Classical Thermonuclear Regime ................................. 66
4.2.2 $T=0$ Kelvin Pycnonuclear Regime .............................. 69
4.2.3 Thermonuclear Burning with Strong Electron Screening ....... 69
4.2.4 Thermo-pycnonuclear Regime .................................. 70
4.2.5 Thermally Enhanced Pycnonuclear Regime ..................... 70
4.3 Lattice Considerations ............................................... 71
4.4 Formulation of Pycnonuclear Reactions ............................. 72
4.4.1 One Component Plasmas ......................................... 72
4.4.2 Multi Component Plasma ....................................... 74
4.5 $T=0$ Pycnonuclear Rate Calculations .............................. 79
4.6 Single Analytic Approximation .................................... 82
4.7 $T$-$\rho$ Nuclear Burning ............................................ 87

CHAPTER 5: CRUST ISOTOPIC EVOLUTION ............................. 92
5.1 Crust Reaction Channels ............................................. 92
5.1.1 EC Calculations ................................................ 93
5.1.2 Neutron Capture ................................................. 95
5.1.3 Nuclear Masses .................................................. 98
5.2 Equation of State .................................................... 100
5.3 The Reaction Network Code ....................................... 102

CHAPTER 6: RESULTS OF NETWORK CALCULATIONS ................... 105
6.1 Pure $^{56}$Fe Matter ................................................ 105
6.1.1 Analysis of Reaction Flows ....................................... 105
6.1.2 Production of $^{40}$Mg ............................................ 109
6.1.3 Flows at Higher Densities ....................................... 111
6.1.4 Integrated Energy Generation ................................. 117
6.1.5 Error in the Pycnonuclear Rate ................................ 121
6.2 Other Pure Stable Nuclei Compositions ............................. 123
6.3 Realistic X-Ray Burst Ash Composition .......................... 127

CHAPTER 7: DISCUSSION AND CONCLUSIONS ......................... 137
7.0.1 How Could We Detect Pycnonuclear Reactions? ............... 140

BIBLIOGRAPHY .......................................................... 143
FIGURES

1.1 Comparative plot of mass densities stretching from water, to two orders of magnitude greater than nuclear density. A heavy ion fusion reaction rate formalism has been developed for this thesis which can calculate reaction rates from main sequence stellar densities to beyond the neutron drip density. .................

1.2 The internal structure of a neutron star, showing the five main regions. As the density increases from the crust ($\rho \sim \times 10^6$ g cm$^{-3}$) inward towards the core ($\rho \sim \times 10^{14-15}$ g cm$^{-3}$) nuclei melt into nucleons, which are twisted into shapes by the interplay of short range attraction and Coulomb repulsion. At the very center of the neutron star a pion condensate may exist. .......................

1.3 The theoretical abundance distribution of ashes after the thermonuclear runaway, taken from [87]. Enhancement at the N=Z waiting points of A=64,68,72, and 104 can be clearly seen. The result of the thermonuclear burning is to push the abundance distribution from that composed of the secondary star, towards the neutron deficient line, populating many more isotopes than were originally present. .

1.4 Reaction paths for the X-ray burst ashes: EC lead to lower Z material, and after the neutron dip line has been reached, also lower N material. Pycnonuclear reactions can occur between the lighter (Z = 6 - 12) nuclei which are formed from EC induced neutron emission.

2.1 The effective potential barrier $V_{eff,\ell}$ as a function of angular momentum, $\ell$. The classical turning points are located at $r_1$ and $r_2$. The lowest potential barrier comes from the contribution where there is no angular momentum barrier, $\ell = 0$. .........................

2.2 Charge density distribution descriptions, $\rho_1$ and $\rho_2$, of ions taking part in the nuclear reaction. As the nuclei are of a comparable size and are interacting at very close range, neither can be approximated by a point charge, and so the Coulomb potential between the nuclei cannot be described simply. Instead a more realistic Fermi shape must be used. The distance between the centers of the nuclei is given by $r$, radii of nucleus 1 and 2 is given by $r_{o1}$ and $r_{o2}$ respectively. 22
2.3 Experimentally measured $S(E)$ factors for three reactions compared to $S(E)$ factors calculated with the BPM and the São Paulo potential. Experimental data is represented by symbols, lines give calculations. Figure from [32].

2.4 Experimentally measured $S(E)$ factor for the reaction $^{16}\text{O}+^{16}\text{O}$, symbols refer to individual data sets. Solid line represents the BPM calculation, the dotted line is the CC formalism.

2.5 $S(E)$ factors for the reactions $^{20}\text{O}+^{20}\text{O}$, $^{20}\text{O}+^{26}\text{Ne}$, $^{20}\text{O}+^{32}\text{Mg}$, $^{26}\text{Ne}+^{26}\text{Ne}$, $^{26}\text{Ne}+^{32}\text{Mg}$. Solid lines are the BPM calculations, solid circles represent the CC calculations.

3.1 Analytic approximations of $S(E)$ calculated using Eq. 3.1 for C+C reactions. The curves from bottom to top refer to $(A_1, A_2)$ = (10,10), (12,12), (12,16), (12,20), (16,16), (12,24), (16,20), (16,24), (20,20), (20,24), and (24,24) reactions. Solid curves show the 9-parameter approximation (3.1); dashed curves (plotted at $E \leq E_C + 0.3 \text{ MeV}$) show the 3-parameter approximation (3.4). Filled dots are where $E = E_C$.

3.2 Analytic approximation (3.1) of $S(E)$ for 36 C+C reactions, 112 C+Mg reactions, and 105 Mg+Mg reactions (Table 2.1). The curves for each reaction type are enclosed by the (thick) curves for the (indicated) reactions involving lightest and heaviest isotopes. Filled dots are where $E = E_C$.

3.3 Top: Analytic approximations of $S(E)$ for the $^{20}\text{Ne}+^{24}\text{Mg}$ reaction. The solid and dashed lines are, respectively, the 9- and 3-parameter approximations (3.1) and (3.4). The filled dot refers to $E = E_C$. Bottom: Relative errors of these approximations with respect to computed data. The dotted line shows zero error to guide the eye.

3.4 Nucleus - nucleus potential, $U(r)$, as a function of separation, $r$, for the reaction $^{18}\text{Ne}+^{20}\text{Mg}$. The blue line is the Coulomb potential for separations greater than the nuclear potential. The pink line shows the behavior of the Coulomb potential in the limit $r \rightarrow 0$. The green line shows a parabolic model for the short range attractive nuclear potential. The peak of $U(r)$ has an energy $E_C \sim 21 \text{ MeV}$. This occurs either at $r = R_C \sim 8.0 \text{fm}$ or $r = R_C \sim 8.2 \text{fm}$ depending on the form of the short range potential. The difference of these values characterizes the width of the potential peak, $\delta$.

3.5 Effective potential $U(r)$ versus radius for four different values of $\delta$ for the specific case of $^{18}\text{Ne}+^{20}\text{Mg}$. Increasing $\delta$ widens the peak of the potential, producing a less attractive short range potential (red line). Decreasing $\delta$ significantly sharpens the attractive potential.
3.6 Log of \( S(E) \) factor against center of mass energy for the fusion reaction \( ^{18}\text{Ne}+^{20}\text{Mg} \), calculated using Eq.3.15 with five different values of potential width parameter \( \delta \).

3.7 Log of \( S(E) \) factor against center of mass energy for the fusion reactions \( ^{12}\text{C}+^{12}\text{C} \) and \( ^{12}\text{C}+^{16}\text{O} \), calculated using Eq.3.15 with five different values of potential width parameter \( \delta \). Also plotted are the same experimental data used in fig. 2.3.

4.1 Log temperature - log density plane for pure \( ^{12}\text{C} \) matter. The upper and lower lines refer to \( ^{12}\text{C} \) burning times of 1 second, and \( \times 10^9 \) years respectively. \( T_L, T_P \) and \( T_m \) refer to the points at which the stellar matter can be regarded as a Coulomb liquid, plasma, and solid Coulomb lattice. \( T_F \) is the electron degeneracy temperature. Hatched areas represent the five possible stellar burning regimes.

4.2 Dependence of the reaction cross section for charged particles as a function of energy, taken from ref. [84]. The left curve shows the Maxwell-Boltzmann distribution, the right curve shows the probability to tunnel through the Coulomb barrier. The sum of these to curves give the central line, which defines the effective burning window. The peak of this curve is \( E_{ij}^{pk} \).

4.3 Top Nuclei in the thermonuclear regime move freely as an ideal gas. Bottom With increasing \( \Gamma_{ij} \) ions are frozen out into an electrostatic lattice. Vibrations of either excited state or ground state ions, depending on the value of \( \Gamma_{ij} \), cause nuclear wave-function overlap, and give rise to pycnonuclear reactions.

4.4 Calculation of the \( T=0 \) pycnonuclear reaction rate for three reactions, plotted on a log mass density - log reaction rate scale. The calculation was performed using eq.4.45 where model parameters were taken from table 4.1. The \( S(E) \) factors were determined from sec. 3.1.

4.5 Calculation of the \( T=0 \) pycnonuclear reaction rate for some \( \text{C}+\text{C}, \text{C}+\text{O}, \text{O}+\text{O} \) (left pane), \( \text{Ne}+\text{Ne}, \text{Ne}+\text{Mg} \) and \( \text{Mg}+\text{Mg} \) (right pane) fusion systems. Calculations were performed using model 1 of tab. 4.1 and eq.4.45.

4.6 Reaction cross section as a function of temperature for the reactions \( ^{12}\text{C}+^{12}\text{C}, ^{12}\text{C}+^{16}\text{O} \) and \( ^{16}\text{O}+^{16}\text{O} \), calculated using eq.4.58 with model parameters from table 4.1.

4.7 Reaction rate as a function of temperature and density for the reactions \( ^{12}\text{C}+^{12}\text{C}, ^{12}\text{C}+^{16}\text{O} \) and \( ^{16}\text{O}+^{16}\text{O} \), calculated using model 1 of table 4.1 and eq.4.58.
4.8 Reaction rate as a function of temperature and density for the neutron rich reaction \(^{40}\text{Ne} + ^{46}\text{Mg}\), calculated using model 1 of table 4.1 and eq.4.58.

5.1 Electron capture by nucleus \((Z,N)\) happens when the electron Fermi energy is equal to the mass difference between parent and daughter. Odd-odd daughter nucleus \((Z-1,N+1)\) will EC to a granddaughter state, which may have an excitation level beneath Fermi energy. Neutrons may be emitted too, if the separation energy is less than the excitation energy of the state.

5.2 Nuclear masses used in the crust abundance simulations. Where possible the FRDM mass model was used. Where this was not possible, the Hilf mass model was used instead.

5.3 Temperature and mass density profile used to model star. This was not obtained self consistently, but from [35].

6.1 Initial (top) and final (bottom) abundance distributions for a pure \(^{56}\text{Fe}\) simulation. At the end of the simulation the initial \(^{56}\text{Fe}\) composition has been evolved to a mixture of predominantly free neutrons \((Y_n = 0.934)\) and \(^{40}\text{Mg}\) \((Y_{40\text{Mg}} = 1.156 \times 10^{-3})\), with a trace amount of \(^{46}\text{Si}\) \((Y_{46\text{Si}} = 8.514 \times 10^{-11})\).

6.2 Plot of the abundance as a function of time for the \(A=56\) chain. The simulation was performed assuming an initial composition of \(X_{^{56}\text{Fe}} = 1, Y_{^{56}\text{Fe}} = 0.0179\).

6.3 Plot of the fluxes for a simulation assuming an initial composition of \(X_{^{56}\text{Fe}} = 1\) at three different times. Neutron number is given along the bottom, proton number up the side. Grey squares mark the valley of stability. Red lines represent flows from lower \(N\) to higher \(N\), green from higher \(N\) to lower \(N\). Dashed lines represent flows between \(1 \times 10^{-5}\) and \(1 \times 10^{-6}\).

6.4 Density induced fusion rates as a function of mass density for the reactions \(^{18,20}\text{C} + ^{18,20}\text{C}\) and \(^{18,20}\text{C} + ^{32}\text{Ne}\).

6.5 Thermonuclear neutron capture rates and heavy ion fusion rates (calculated using model 1 of table 4.1 and eq.4.58) for the isotopes \(^{36}\text{Mg}, ^{38}\text{Mg}\) and \(^{40}\text{Mg}\). Fluctuations in the heavy ion rates at high densities reflect dynamic changes in electron abundance and number density in the network simulation. At low densities structure reflects changes in \(<Z>\).
6.6 Plot of the fluxes for a simulation assuming an initial composition of $X_{56Fe} = 1$ at three different times. Neutron number is given along the bottom, proton number up the side. Grey squares mark the valley of stability. Red lines represent flows from lower N to higher N, green from higher N to lower N. Dashed lines represent flows between $1 \times 10^{-5}$ and $1 \times 10^{-6}$.

6.7 Abundance as a function of time for $^{20,22}C$, $^{40,44}Mg$, $^{60,62,64}Ar$ and $^{46}Si$. The $^{40}Mg$ is formed initially through neutron capture on $^{36}Mg$, then at later times by the heavy ion fusion of $^{20}C$. The formation of $^{62}Ar$ follows neutron capture on $^{60}Ar$, formed by $^{20}C^{+40}Mg$. After the initial formation of $^{46}Si$ via EC on $^{62}Ar$, a cycle of $^{46}Si$ production is set up, where pycnonuclear reactions between C and Mg isotopes lead to isotopes of Ar, which in turn EC to $^{46}Si$, which EC back to lighter elements, releasing energy.

6.8 Average mass, proton number, and the mass fraction contained in the nucleus as a function of mass density, for a $X_{56Fe} = 1$ simulation. At $\sim 9 \times 10^{11}$ g cm$^{-3}$ $X_N < 1$. This marks the the neutron drip point.

6.9 Integrated energy deposited into the crust as a function of mass density, assuming an initial $X_{56Fe} = 1$ composition. The red line is the simulation with no pycnonuclear reactions included, the green line is with pycnonuclear reactions, calculated using eq. 4.58.

6.10 Impact of the uncertainty in the pycnonuclear reaction rate formalism on the stellar reaction rate (top) and integrated energy generation curve (bottom) for the reaction $^{40}Mg + ^{40}Mg$. The 7 models plotted represent BCC lattice types, and are taken from table 4.1.

6.11 Average mass number (top), proton number (middle) and neutron number (bottom) for 11 different starting compositions, as a function of mass density.

6.12 Stellar reaction rate as a function of mass density for 5 different values of $X_N$. At mass densities greater than the neutron drip, $X_N < 1$. Since the pycnonuclear reaction rate depends exponentially on $X_N$, reduction in $X_N$ translates into a many order of magnitude decrease in the reaction rate.

6.13 Initial (top) and final (bottom) abundance distributions for a network simulation involving realistic x-ray burst ashes. Similar to the previous examples studied, the final abundance distribution is composed of free neutrons ($Y_n = 0.9483$), $^{40}Mg$ ($Y_{40Mg} = 1.292 \times 10^{-3}$), and a smaller amount of $^{46}Si$ ($Y_{46Si} = 3.21 \times 10^{-7}$).
6.14 Plot of the fluxes for a simulation assuming a composition of realistic X-ray burst ashes. Neutron number is given along the bottom, proton number up the side. Grey squares mark the valley of stability. Red lines represent flows from lower N to higher N, green from higher N to lower N. Dashed lines represent flows less than $1 \times 10^{-5}$ of the maximum flow.

6.15 The abundance evolution of the initial $^{12}$C as a function of time. At a Fermi energy of 4.7 MeV, the Carbon begins to fuse forming $^{24}$Mg. This nucleus is unstable against EC at 6.81 MeV, and so $^{24}$Ne is rapidly formed at greater crust depths.

6.16 Zoomed section of fig. 6.14, showing nuclei of relevance to pycnonuclear reactions.

6.17 Average mass number, proton number and neutron number, as a function of density, for an abundance vector composed of x-ray burst ashes.

6.18 Integrated energy deposited in the crust as a function of mass density. The feature at ~ $3.9 \times 10^{11}$ g cm$^{-3}$ is a model artifact, and corresponds to the switch between FRDM masses and Hilf masses.
TABLES

2.1 HEAVY ION FUSION REACTIONS \((A_1, Z_1) + (A_2, Z_2)\) WHICH HAVE BEEN CONSIDERED IN THIS THESIS.

2.2 LOW ENERGY EXCITED STATES (QUOTED IN MEV, PROVIDED IN PARENTHESES) ALLOWED IN THE CC CALCULATIONS FOR THE NUCLEI OF INTEREST.

4.1 COEFFICIENTS USED IN PYCNONUCLEAR REACTION RATE FORMALISM
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CHAPTER 1

INTRODUCTION

The purpose of this dissertation is to understand the role of density induced heavy ion fusion reactions in high density stellar environments. This nucleosynthesis process is thought to be of particular importance in the deep crust of neutron stars, and the cores of white dwarf stars [89], [88]. By understanding this burning mechanism one can estimate energy production within these stellar sites.

For this thesis a new formalism for calculating density induced heavy ion fusion reaction rates has been developed. The framework for calculating the rates has involved producing state of the art cross section calculations for both stable and neutron rich nuclei, as well as developing a reaction rate formalism which can be applied to a spectrum of stellar temperature and density conditions. The reaction rate formalism has been particularly developed to address the technicalities associated with fusion in dense stellar environments. In this context, a dense environment is one where the mass density is between $\times 10^6$ g cm$^{-3}$ and $\times 10^{13}$ g cm$^{-3}$. Contrast this with the density of a main sequence star like the Sun, fig. 1.1. Thermonuclear stellar environments are hot and composed of fully stripped nuclei moving in a bath of free electrons. Nuclear fusion in this sort of environment occurs between nuclei which are energetic (owing to the thermal energy) and able to tunnel through the mutual repulsive barrier which scales proportionally as a function of nuclei charge, and inversely as the square of the nuclei separation. In contrast to the thermonuclear conditions, dense stellar environments are composed of largely bound nuclei
surrounded by highly degenerate electrons. Fusion reactions under these conditions occur mostly between neighboring nuclei. Presented in this thesis is a reaction rate formalism which can be used to calculated heavy ion fusion reactions from thermonuclear to dense matter conditions.

Once developed, the fusion reaction formalism has been applied in the context of neutron stars. Following a general introduction to neutron stars, the motivation for understanding these stellar objects is examined.

1.1 Neutron Star Formation

Stars produce energy in response to gravitation pressure from with out. Each nuclear reaction produces energy which keeps the star in hydrostatic equilibrium; with out this mechanism the gas from which the star is composed would collapse under gravitational pressure altogether. It is energetically favorable to expend as little energy as possible counteracting gravity, and so nuclei with low proton number are preferentially fused first. In the main sequence, this involves fusion of hydrogen to produce helium. For stars with masses below $\sim 1.5 \, M_\odot$ this is done via the $p+p$ reactions, for more massive stars it is done via $p$ capture on Carbon, Nitrogen and Oxygen isotopes, in a process known as the CNO cycle. As the star begins to exhaust the H fuel it contracts under gravity, raising the core temperature. The thermal increase translates into H shell burning, which in turn results in yet more $^4\text{He}$ deposited in the stellar core. As the core temperature and mass rises $^4\text{He}$ isotopes fuse, producing $^{12}\text{C}$. If the star is massive enough (between $8 - 10 \, M_\odot$), once the $^4\text{He}$ core has been consumed the star contracts once more burning $^{12}\text{C}$ to produce the energy to maintain hydrostatic equilibrium. Successive isotopic fuel burning continues, with the exhaustion of each fuel leading to radial contraction, elevated stellar core temperatures and the initiation of a new isotope fuel. With
Figure 1.1. Comparative plot of mass densities stretching from water, to two orders of magnitude greater than nuclear density. A heavy ion fusion reaction rate formalism has been developed for this thesis which can calculate reaction rates from main sequence stellar densities to beyond the neutron drip density.
each new fuel, the time to exhaust that fuel decreases.

Having burned the available nuclear fuel (successive shells of H, He, C, Ne, O and Si) up to the peak of the binding energy curve, $^{56}\text{Ni}$, a pre-supernova star can be thought of as a central iron core enveloped by successively lighter burning shells. Though Si burning (through $\alpha$ capture) results in $^{56}\text{Ni}$, this isotope $\beta^+$ decays with a half life of 6 days to form $^{56}\text{Co}$, which decays in turn (half life of 77 days) to produce $^{56}\text{Fe}$. Fusion with $^{56}\text{Fe}$ results in nuclei with less binding energy per nucleon than $^{56}\text{Fe}$, i.e, it requires energy, it does not produce it. Consequently fusion reactions can no longer produce the energy required to maintain hydrostatic equilibrium. Instead the star is supported by electron degeneracy pressure.

Nuclear burning continues in the shells surrounding the Iron core. The fusion produces nuclear ashes, which add to the core mass. When the mass exceeds 1.4 $M_\odot$ electron degeneracy pressure can no longer support the core, and it collapses inward under gravity. As the core begins to contract, central temperature and density increase with core densities rising to $\rho_c \approx 10^{10} \text{ g cm}^{-3}$ as the external pressure increases. This adds to Fermi energy of the electrons, supplying electrons with sufficient energy to overcome the negative Q-values which prevent electron capture (EC) on the Iron peak nuclei. Enabling EC in the core removes electrons which were providing support against collapse. At the same time, high energy photons begin to break down the $^{56}\text{Fe}$ nuclei into lighter nuclei and neutrons. Both processes remove energy from the star and promote the gravitational collapse.

Core contraction continues, with the outer core falling at nearly 25 per cent of the speed of light $^{[97]}$, until the density reaches $4-8 \times 10^{14} \text{ g cm}^{-3}$. Nuclear density is on the order of $2 \times 10^{14} \text{ g cm}^{-3}$. At 2-4 times this, the short range nuclear potential is highly repulsive. When the in falling material encounters the short range repulsion it is rebounded and sent outward from the core, where it...
interacts with material still in free fall towards the core. This effect produces a shock wave moving outward from the center. Initially the shock wave losses energy via photo interaction with the Iron peak nuclei and neutrino emission (from EC capture on Iron peak, other nuclei and \( p + e \rightarrow n + \nu_e \)) and stalls when it reaches the outer core. It is not certain how the stalled shock wave is revived, nor how it propagates to the outer layers of the star \[94\]. Once it reaches the inner layers of the star however (which are composed of \(^{28}\)Si and \(^{16}\)O) it initiates a round of explosive nuclear burning, forming more Iron peak nuclei.

By the time the shock wave reaches the outer layers of the star, a good deal of the energy has been lost and so the temperature is lower. The outer layers are ejected into space. Depending on the energy of the initial shock wave, the highly processed inner (Iron peak) layers can fall back on the stellar core \[98\]. What is left at the center of the former star is the neutron degenerate proto neutron star. It is composed of the remnant of the original Iron peak core, neutrons (from photo dissociation of heavy nuclei and EC by protons), and additional Iron and Nickel which was formed from explosive nuclear burning of the inner layers which fell back towards the compact object after the shock wave had passed through. Observations suggest that the object is surrounded by a thin atmosphere composed of H and \(^4\)He, which came from spallation of heavier elements from the inner layers, and fell back towards the core.

The proto-neutron star is formed with a mass of \( \approx 1.2 - 1.6M_\odot \) \[28\], a radius of less than 20 Km \[80\] and a core density of \( \approx 4 - 5 \times 10^{14} \text{ g cm}^{-3} \). This is comparable to every human on Earth being squeezed into a volume of 1 cm\(^3\) \[10\]. Further compression is only halted when neutron degeneracy pressure dominates, stabilizing the core against further contraction.

The process of rapidly converting gravitational binding energy to neutrinos, elec-
tromagnetic radiation, kinetic energy of ejecta and gravitational waves represents a huge energy release, on the order of $3GM^2/5R \approx 10^{53}$ ergs. The process is termed a type II supernova and can be observed on Earth.

1.2 Interior Structure

Following the creation mechanism, a nascent neutron star is initially a hot compact object (perhaps $6 \times 10^{11}$ K \cite{66}), composed of $^{56}$Fe, some $^{56}$Ni, highly degenerate electrons and neutrons. Neutrino loss rapidly acts to cool the neutron star within the first few seconds of creation, as the mean free path of the neutrinos increases and they start to escape the proto neutron star. Though the object is transparent to all flavors of neutrino emission, some heat remains in the crust which cools slowly (on the timescale of years \cite{64}).

The internal structure of a neutron star can be broadly described by five main regions (see Figure \ref{1.2}). The first of these regions is the atmosphere, a thin shell of mass $\approx 10^{-20}$ M$_\odot$ \cite{15} which current X-ray observations indicate is made up of predominately hydrogen and helium for neutron stars younger then $4-5 \times 10^5$ years \cite{77} (see sec \ref{1.1}), with heavier nuclei playing a more important role in older neutron stars \cite{78}. The atmosphere is thought to evolve due to H and He diffusion; temperatures and density at the top of the atmosphere is not sufficient to initiate fusion, but beneath the atmosphere it is. Therefore light elements which diffuse down are rapidly captured, depleting the original atmosphere.

Beneath the atmosphere is the envelope, a region composed largely of hydrogen and helium. With a thickness of typically 1-2 Km, the crust is mostly made up of fully ionized nuclei with a proton number strongly coupled to mass density. At the top of the crust the density is over $1 \times 10^6$ g cm$^{-3}$. As such the electron wavefunctions start to become compressed, rapidly filling the electron phase space. The
density threshold for relativistic Fermi electrons is at \( \rho \sim 1 \times 10^6 \text{ g cm}^{-3} \) and so the crust is typified by bare nuclei submerged in a bath of highly degenerate, relativistic free neutrons. Descending through the crust, the nuclei become neutronised as the electron degeneracy increases causing electron capture (EC) reactions, resulting in lighter \( Z \) nuclei at higher densities. It is this region of the neutron star, and the density dependent reactions which can occur in it, which is of greatest interest to this work. At the interface of the outer core and the crust densities exceed the neutron drip density, \( \rho \approx 4 - 6 \times 10^{11} \text{ g cm}^{-3} \). Since there is a significant free neutron density at this limit, the nucleon-nucleon interaction between free neutrons and nuclei start to reduce the surface energy of the nuclei. As a result, the surface tension of the nuclei starts to decrease and the nuclei begin to melt to a “nucleon soup” [89] [65].

Below the crust lies the inner and outer core, a region where the density is greater than \( \sim 2 \times 10^{14} \text{ g cm}^{-3} \). At nuclear densities the length scales for short range attraction and Coulomb repulsion approach each other. This gives rise to complex shape manifestations as the nucleons arrange themselves to the lowest energy configuration possible under spherical-seeking surface tension and the repulsive Coulomb force [46]. These shapes are known as nuclear pasta. At such extremes the calculation for the equation of state (EOS) is severely hampered by two things, finding the correct form for the nucleon-nucleon interaction, and treating the many body problem in a realistic manner [1]. The density of the central core depends sensitively on the choice of EOS (see eg [89], [80]), but is on the order of \( \times 10^{15} \text{ g cm}^{-3} \). This is enough for the mesons between neighboring nucleons to start to overlap, and possibly to leak out to form a pion condensate core.
Figure 1.2. The internal structure of a neutron star, showing the five main regions. As the density increases from the crust ($\rho \sim \times 10^6 \text{ g cm}^{-3}$) inward towards the core ($\rho \sim \times 10^{14-15} \text{ g cm}^{-3}$) nuclei melt into nucleons, which are twisted into shapes by the interplay of short range attraction and Coulomb repulsion. At the very center of the neutron star a pion condensate may exist.
1.3 Binary Neutron Stars

Since roughly half of all stars are not isolated but in a multiple system with one (or more) companion, at least half of all neutron stars are formed as part of a binary system. Providing that less than half of the total binary system mass is ejected in the supernova event, the explosion will not disrupt the binary pair \[10\] and so the objects with continue to orbit each other. If the objects are close enough, there is a possibility for mass transfer, a scenario discussed in the following section.

1.3.1 X-Ray Bursts

Of the observed systems, most are low-mass x-ray binaries [67] [76]. In this scenario, a neutron star (the primary) is in close binary with a star of mass \(1 - 2M_\odot\) (the secondary). The radius of the orbit of the secondary star can decrease in the presence of the neutron star due to a loss of angular momentum propagated by gravitational radiation. This action brings the secondary star inside the inner gravitational equipotential which defines the surface of the Roche lobe. Consequently matter begins to transfer from the secondary star to an accretion disk around the primary. The disk matter is funneled towards the poles by the neutron star’s magnetic field, and is deposited on it’s surface.

The accreted material has the same composition as the secondary star, and is largely made of fully ionized hydrogen and helium. Once on the surface of the neutron star, the material is immediately compressed by the weight of freshly accreted material. A layer of several cm starts to build up. Under the degenerate conditions at \(\rho \geq \times10^6 \text{ g cm}^{-3}\), heating from gravitational compression initiates H fusion on \(^{12}\text{C}, ^{13}\text{N}\) and \(^{14}\text{O}\) in what is known as the hot CNO (HCNO) cycle (hot because the temperature is in the range of 0.1 - 1 Giga Kelvin, GK). Energy release from these reactions heats the material further since the conditions are degenerate.
preventing expansion. An increase in temperature is enough to overcome the He-He Coulomb barrier, and begin the triple α process (the conversion of three $^4$He into a $^{12}$C), providing yet more Carbon fuel for the HCNO cycle. As a result, the temperature increases further, allowing enough energy for the reaction $^{15}$O$(\alpha,\gamma)$, which represents a break out from the HCNO cycle [3], [58], [63] and allows the α-p process to set in.

The α-p process is characterized by a sequence of $(\alpha,p)$, $(p,\gamma)$ reactions which breakout via the reaction $^{15}$O$(\alpha,\gamma)$ and the chain $^{14}$O$(\alpha,p)^{17}$F$(p,\gamma)^{18}$Ne$(\alpha,p)^{21}$Na [96]. The temperature sensitive α-p process is a dominant nucleosynthesis mechanism until the Coulomb barrier starts to inhibit fusion due to the an increasing proton number. This occurs at about $^{34}$Ar, $^{38}$Ca [63] (depending on the temperature).

Beyond this point, the thermonuclear explosion is propagated by the rp-process. This is the rapid capture of protons with the emission of γs typified by $(p,\gamma)$. Rapid proton captures compete with $\beta^+$ decays, such that after a proton capture a nucleus either $\beta^+$ decays back towards the valley of stability, or else rapidly captures another proton before decay is possible. The result of this competition is that the rp-process closely follows the proton drip line, while efficiently processes the HCNO ashes into the mass range beyond $^{56}$Fe and $^{56}$Ni. The rp-process finally stalls out in the region of $^{107}$Te, $^{108}$Te where Schatz has demonstrated that $(\gamma,\alpha)$ reactions stop the flow proceeding [87]. The results of Schatz et al were obtained using a simple one zone, post processing model (see sec 5.3 for a definition of post processing), but were later confirmed by the more sophisticated model of Woosley et al [99].

Ashes from the burst are enriched at A=64,68,72 and 104 corresponding to the N=Z waiting point nuclei, $^{64}$Ge, $^{68}$Se, $^{72}$Kr, $^{104}$Sn [91]. This nuclide distribution is plotted in Figure 1.3.

The energy release from the thermonuclear explosion peaks at X-ray wave-
1.3.2 The Fate of the RP-Process Ashes

Following the X-ray burst, the ashes of the rp-process sink into the crust of the neutron star under the weight of freshly accreted material experiencing a continual increase in density accompanied by a continual increase in Fermi energy. For completely degenerate electrons the Fermi energy is given by

\[ E_F = \frac{\hbar}{2m_e} \cdot (3\pi^2 N_A)^{2/3} \cdot (\rho Y_e)^{2/3}, \]  

(1.1)

where \( N_A \) is Avogadro’s number, and \( Y_e \) is the electron fraction.

As a consequence of the elevated Fermi energy there is a ready supply of electrons at the high energy tail which can “switch on” EC reactions that would otherwise be blocked by negative Q values. Progression through the crust is accompanied by EC, resulting in a strong tendency towards neutronization represented by the green
arrow in fig. 1.4. This process eventually evolves the initial isotopic abundance
distribution towards the neutron drip line, creating highly neutron rich nuclei such
as $^{40}$Mg \cite{38}. It is interesting to note that the EC reactions proceed in a manner
which minimizes the energy such that odd-odd nuclei are quickly processed by an
electron capture into even-even nuclei \cite{38}. At the neutron drip line ($\rho = 6.6 \times 10^{11}$
g cm$^{-3}$) further EC lead to neutron emission as the neutron decay channel opens
up, shown by the blue arrows in fig. 1.4. Systematically the joint mechanisms of
EC and neutron emission set about processing the rp-process ashes from the proton
drip line, to the neutron drip line, producing nuclei with either very low, or even
negative, neutron binding energy. Produced are a spectrum of low, even Z, neutron
rich isotopes in the range of $^{16-24}$C, $^{18-28}$O, $^{30-40}$Ne and $^{34-46}$Mg.

![Diagram of reaction paths](image)

Figure 1.4. Reaction paths for the X-ray burst ashes: EC lead to lower Z
material, and after the neutron dip line has been reached, also lower N
material. Pycnonuclear reactions can occur between the lighter ($Z = 6 -
12$) nuclei which are formed from EC induced neutron emission.
The processed ashes constitute a dense bound lattice, where frozen nuclei are embedded in a sea of free degenerate electrons. The electrons shield the neighboring nuclei from the repulsive Coulomb force from the protons, whilst the increasing compression forces the nuclei closer together. These effects result in the significant reduction of distance between the nuclei. In the presence of the electron gas the nuclear wave functions begin to overlap, promoting reactions between adjacent nuclei which are enhanced due to the reduced electrostatic barrier [86], [9], [19], [60]. Such reactions occur in very compact conditions, and are highly sensitive to density, thus they are known as pycnonuclear reactions (the root “pycnos” being Greek for dense, or thick). Pycnomuclear reactions occur between the neutron rich nuclei of the crust, and can lead to exotic fusion products, such as $^{58}\text{Ar}$, shown in pink in fig. 1.4.

1.4 Why Study Neutron Stars?

Though fascinating in themselves, neutron stars do not significantly offer any enrichment to the interstellar medium since the surface gravity is typically so large that nothing will escape (for 1.4M$_\odot$ star of radius 10 Km, surface gravity is given by $1.86 \times 10^{14}$ cm s$^{-2}$ [10]). In this sense, understanding neutron stars and their particular fusion mechanisms add very little to our understanding of elemental compositions (one of the questions of the National Research Council’s Committee of Physics of the Universe [75]). There are other ways however that neutron stars can contribute to our understanding of the Universe.

Normal nuclear matter has nearly equal fractions of protons and neutrons. Since neutron star matter has only a few per cent protons (due to the reaction $p^+ + e \rightarrow n + \nu_e$) it represents an exotic form of matter. It is relevant to study such a system because neutron stars represent essentially infinite nuclear matter [75]. Viewed like
this, a neutron star can be thought of as a gigantic nucleus with mass number $A \approx 10^{57}$ for mass $1.4M_\odot$ [10]. Understanding neutron stars can give us insight into the nuclear EOS. Since exceedingly unusual terrestrially unbound nuclei can exist on neutron stars, they provide a unique laboratory for not only probing nuclei at extremes, but also for studying new reaction mechanisms unobtainable on Earth. As such, neutron stars provide rich information not only for testing theories related to dense matter physics and nuclear theory, but also for providing a connection between the inter-disciplines of astrophysics, nuclear physics, high energy physics and statistical physics [65], [64], [89] [66], [34].

1.5 Goals of This Work

The focus of this work is to understand the role of density induced heavy ion fusion processes in a dense stellar environment. This is desirable since these reactions may provide an energy source in the neutron star crust. A detailed knowledge of energy production can contribute towards a global understanding of the physical properties of neutron stars. This in turn can be used to shed light on the microscopic nucleon-nucleon interaction, revealing something more fundamental about the nuclear equation of state (EOS).

A potentially critical source of crust heating comes from pycnonuclear reactions. These reactions are a remarkable type of fusion in that they are highly density dependent, and somewhat temperature insensitive. This combination of features is very alien to the normal ideas of thermonuclear fusion, but means that reactions are taking place in the crust even when the temperature is comparatively low (less then $\approx 10^7$ K). It has been suggested by [38] and [56] that pycnonuclear reactions could represent a significant source of deep crust heating.

One of the goals of this work is to improve on previous treatments of pycnonu-
clear reactions. Previous work has focused on calculating fusion rates in stellar plasmas composed of either one, or two isotopes. Most of the previous studies have specifically centered on the reactions $^{12}\text{C} + ^{12}\text{C}$, $^{16}\text{O} + ^{16}\text{O}$ and $^{12}\text{C} + ^{16}\text{O}$, which can occur in the cores of white dwarf stars [8], [86], [88], [74]. Presented here is a formalism which can be used to calculate fusion between different nuclei in a realistic a multi component stellar environment. Developing the formalism required a new mathematical treatment of the problem of fusion in a dense many body environment. In order to treat pycnonuclear reactions in a comprehensive manner, cross sections needed to be estimated for all heavy ion fusions of interest. Estimating cross sections at zero energy is a tricky business, which required a robust treatment of Coulomb barrier tunneling, and finally characterizing the cross sections in a manner which allows easy extrapolation to very low energy. To this aim a set of reaction cross sections were developed, particularly for reactions where no experimental data exists.

A realistic picture of energy production can only be achieved by bringing together nuclear processes which can occur in accreting neutron stars: electron capture, heavy ion fusion and other types of reactions, such as (n, $\gamma$), (p, $\gamma$) and (\alpha, $\gamma$). This required evolving the X-ray burst ash abundance distribution by solving a network of nuclear reactions which could occur from the surface, down through the crust.
In order to study an astrophysically interesting process such as x-ray bursts, a detailed knowledge of nuclear transformation rates over a wide range of densities and temperatures (the mass density of the neutron star crust ranges over 5 orders of magnitude, between $\sim 10^8 \text{ g cm}^{-3}$ and $\sim 10^{13} \text{ g cm}^{-3}$, with increasing depth) is required. For calculating the nucleosynthesis reaction rates, it is necessary to know the reaction cross sections. In the majority of cases, stellar burning takes place at energies of typically less than a few MeV. For reactions rates taking place between the exotic nuclei present in a neutron star crust, there are no hard laboratory cross section data available. The reason for this is that the nuclei involved in the reactions are so neutron rich that they are unstable in the laboratory environment, making beam or target production impossible with the facilities of today. Conversely, for reactions involving stable nuclei, extrapolating measured cross sections from laboratory accessible energy regions down to required regions, is often unreliable. A suitable solution to these dual problems is to express the cross section in terms of the astrophysical $S(E)$ factor. The $S(E)$ factor is a way of expressing the reaction cross section as a product of the Coulomb barrier penetration dependence, the energy dependence and any nuclear structure dependence. This last term should be small for the non-resonant reactions developed here. The mathematical definition is presented in sec. 2.4 but practically speaking it is more reliable to extrapolate $S(E)$ factor down to the necessary energy region than it is the cross section. The
extrapolation has been performed in this thesis by means of a uniform theoretical expression which is applicable for a wide range of nuclear reaction systems.

Presented first is a detailed justification of which heavy ion fusion reactions are relevant in accreting neutron star crusts. Following this is a brief look at the barrier penetration model, which is a convenient approach for calculating fusion cross sections. Though this simple approach to sub barrier fusion does not contain any inherent physics suitable for describing the kind of structure beneath the barrier which has been observed for some reactions, e.g. $^{12}\text{C}+^{12}\text{C}$, it is still a convenient model for obtaining simple fusion cross sections. After having established a framework for producing cross sections, the various required potentials are discussed. The chapter closes with a discussion concerning the relation between the $S(E)$ factor and the cross section.

2.1 Scenario Relevant Nuclei

Once the nucleosynthesis processes associated with the X-ray burst have finished, the nuclei produced are mainly peaked around the N=Z waiting point nuclei, $^{64}\text{Ge}$, $^{68}\text{Se}$, $^{72}\text{Kr}$ and $^{104}\text{Sn}$ shown in fig. [1,3]. Once the Fermi energy has risen, through matter compression, to a threshold at which EC can set in, material is rapidly transitioned from a mix of odd-odd, odd-even and even-even nuclei to predominantly even-even nuclei. The reason for the dominance of even-even nuclei lies in the Pauli pairing of nuclei. Nuclei which have fully paired nucleons are more bound than nuclei with unpaired nucleons. In mass models, e.g. the Weizacker mass formula which models the nucleus as a liquid drop, the pairing term is a parameter which adds binding energy for even-even nuclei and removes it for odd-odd nuclei (the parameter is zero for odd-even nuclei). This gives rise to the odd-even staggering of nuclear binding energies, where odd-odd nuclei are less bound than even-even.
nuclei. Consequently there is a tendency for nuclei to convert the unpaired nucleon to either a proton or a neutron which can pair with the other single nucleon. For EC on an odd-odd nuclei, the unpaired proton captures an electron and is converted into a neutron to pair up with the secondary unpaired neutron.

According to ref. [72], the experimental atomic mass excesses of $^{56}$Fe, $^{56}$Mn and $^{56}$Cr are $\Delta_{56Fe} = -60.60$ MeV, $\Delta_{56Mn} = -56.91$ MeV, and $\Delta_{56Cr} = -55.29$ MeV respectively. The Q-value for the reaction $^{56}$Fe + $e^-$ $\rightarrow$ $^{56}$Mn + $\bar{\nu}_e$ is -3.696 MeV; once the Fermi energy has risen to approximately this threshold an EC is energetically permissible and can take place, beneath this threshold the reaction is blocked by the negative Q-value. The threshold will be reached at a mass density of $\rho = 1.14 \times 10^9$ g cm$^{-3}$. The EC reaction $^{56}$Mn + $e^-$ $\rightarrow$ $^{56}$Cr + $\bar{\nu}_e$ has a negative Q-value of only -1.617 MeV, requiring a density of just $\rho = 1.44 \times 10^8$ g cm$^{-3}$ to “switch on” this reaction. Consequently the threshold density of the $^{56}$Mn + $e^-$ $\rightarrow$ $^{56}$Cr + $\bar{\nu}_e$ reaction has already been exceeded before the creation of $^{56}$Mn through the $^{56}$Fe + $e^-$ $\rightarrow$ $^{56}$Mn + $\bar{\nu}_e$ reaction - the odd-even binding energy staggering favors the stability of even-even nuclei over odd-even nuclei.

Because heavy ion fusion is exponentially suppressed by the presence of the repulsive Coulomb barrier, there are a limited number of nuclei which can appreciable participate in fusion induced burning. For this thesis 946 heavy ion fusion systems have been considered, consisting of 10 reaction types, stretching from the neutron deficient, through the valley of stability, up to, and beyond, the neutron drip line. These are summarized in Table 2.1. Columns 1, 2 and 3 detail the specific nuclei (even nuclei only) for which calculations were performed (see Chapter 3 for an elucidation concerning the calculations). Column 4 states how many heavy ion fusion systems of each type were studied; column 5 gives the maximum energy cutoff for the calculations. Section 3.1 provides a contextual explanation of this last column.
TABLE 2.1

HEAVY ION FUSION REACTIONS \((A_{1}, Z_{1}) + (A_{2}, Z_{2})\) WHICH HAVE BEEN CONSIDERED IN THIS THESIS.

<table>
<thead>
<tr>
<th>REACTION</th>
<th>(A_{1})</th>
<th>(A_{2})</th>
<th>Nr. of CASES</th>
<th>(E_{MAX}) MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>C + C</td>
<td>10–24</td>
<td>10–24</td>
<td>36</td>
<td>17.9</td>
</tr>
<tr>
<td>C + O</td>
<td>10–24</td>
<td>12–28</td>
<td>72</td>
<td>17.9</td>
</tr>
<tr>
<td>C+Ne</td>
<td>10–24</td>
<td>18–40</td>
<td>96</td>
<td>19.9</td>
</tr>
<tr>
<td>C+Mg</td>
<td>10–24</td>
<td>20–46</td>
<td>112</td>
<td>19.9</td>
</tr>
<tr>
<td>O + O</td>
<td>12–28</td>
<td>12–28</td>
<td>45</td>
<td>19.9</td>
</tr>
<tr>
<td>O+Ne</td>
<td>12–28</td>
<td>18–40</td>
<td>108</td>
<td>21.9</td>
</tr>
<tr>
<td>O+Mg</td>
<td>12–28</td>
<td>18–46</td>
<td>126</td>
<td>21.9</td>
</tr>
<tr>
<td>Ne+Ne</td>
<td>18–40</td>
<td>18–40</td>
<td>78</td>
<td>21.9</td>
</tr>
<tr>
<td>Ne+Mg</td>
<td>18–40</td>
<td>20–46</td>
<td>168</td>
<td>24.9</td>
</tr>
<tr>
<td>Mg+Mg</td>
<td>20–46</td>
<td>20–46</td>
<td>105</td>
<td>29.9</td>
</tr>
</tbody>
</table>
2.2 The Barrier Penetration Model

In the simplest framework, heavy ion fusion occurs when two ions tunnel through their mutual Coulomb barrier. Theoretical cross sections for this fusion can be obtained in a variety of ways, however central to most descriptions of heavy ion collisions is the optical model potential. The cross sections here have been calculated for all 946 heavy ion fusion reactions of interest in the context of the barrier penetration model (BPM), which is a purely predictive model with no free parameters. The choice of this model (combined with a parameter free, non-local potential, see Section 2.3) has been justified for nuclei on the valley of stability for a number of fusion systems (see e.g. [30], [14]).

The BPM calculates the fusion cross section using a partial wave ($\ell = 0, 1, 2...$) decomposition. At the heart of the BPM is the association of the fusion cross section $\sigma$, to the partial wave flux transmitted through an effective potential barrier of height $V_{\text{eff},\ell}$. This relation is given by

$$\sigma_{\text{BPM}}(E) = \frac{\pi}{k^2} \sum_{\ell=0}^{\ell_{\text{max}}} (2\ell + 1)T_\ell,$$

where $T_\ell$ are the partial wave transmission coefficients.

When the partial wave $\ell$ has an effective barrier height lower than that of the center of mass energy, the effective potential has been characterized by a parabola with curvature described by ([32], [14]),

$$h\omega = \text{mod} \sqrt{\frac{\hbar^2}{\mu} \frac{d^2V_{\text{eff},\ell}}{dr^2}}.$$  (2.2)

In this case the transmission coefficients in Eq.2.1 are obtained through the
Hill-Wheeler formula \[79\],

\[ T_\ell = \frac{1}{1 + e^{\exp \left( \frac{2\pi (V_{\text{eff},\ell} - E)}{\hbar \omega_\ell} \right)}}. \] \hfill (2.3)

For the case in which the angular momentum waves have effective potential barriers larger than the center of mass energy, the radial dependence of the potential requires the use of the WKB method in order to solve for \( T_\ell \),

\[ T_\ell = \frac{1}{1 + e^{\exp (S_\ell)}}, \] \hfill (2.4)

\[ S_\ell = \int_{r_1}^{r_2} \frac{8\mu}{\hbar^2} \sqrt{V_{\text{eff},\ell}(r, E) - E} \, dr. \] \hfill (2.5)

The integration is performed over the limits \( r_1 \) and \( r_2 \), where \( E = V_{\text{eff},\ell} \). These are known as the classic turning points, and are defined as the radius at which the Coulomb potential equals the kinetic energy of the relative motion, and at which point an incident nucleus would classically be retarded.

The region above the barrier, using the Hill-Wheeler approach of Eq.2.3 and below the barrier, using the WKB method given in Eq.2.5 are linked by a parabolic curve described by,

\[ \hbar \omega_\ell = \frac{2\pi (V_{\text{eff},\ell} - E)}{S_\ell}. \] \hfill (2.6)

The sum in Eq.2.1 is performed up to the greatest value of angular momentum, \( \ell \), which produces a pocket in the effective potential (see Fig. 2.1). Fusion induced burning between nuclei of charge range \( Z=6 - 12 \) is typically dominated by the s-wave however; since the Coulomb barrier already suppresses the reaction an additional angular momentum barrier would further suppress the rate.
2.3 The Effective Potential

The calculation of the fusion cross sections (and subsequently the $S(E)$ factor) requires that the BPM be used in tandem with an effective potential, defined as the sum of the Coulomb ($V_C(r)$), nuclear ($V_N(r, E)$) and centrifugal terms ($V_{ang}(\ell, r)$),

$$V_{eff}(r, E) = V_C(r) + V_N(r, E) + V_{ang}(\ell, r).$$

(2.7)

2.3.1 Coulomb Potential

The Coulomb term, which represents the deflective electrostatic potential which exists between nuclei of charge and mass $Z_1, A_1$ and $Z_2, A_2$ and originates from the protons, can be represented as

$$V_C(r) = \frac{e^2 Z_1 Z_2}{r},$$

(2.8)
where $r$ is minimum when $r = r_{min} = 1.2(A_1^{1/3} + A_2^{1/3})$. This expression holds in the limit that the nuclei are treated as point charges.

Figure 2.2. Charge density distribution descriptions, $\rho_1$ and $\rho_2$, of ions taking part in the nuclear reaction. As the nuclei are of a comparable size and are interacting at very close range, neither can be approximated by a point charge, and so the Coulomb potential between the nuclei cannot be described simply. Instead a more realistic Fermi shape must be used. The distance between the centers of the nuclei is given by $r$, radii of nucleus 1 and 2 is given by $r_{o1}$ and $r_{o2}$ respectively.

The fusing nuclei considered in this thesis however all have similar mass and radii, with interactions taking place at very small separations. In this case it is more suitable to model the nuclei not as point charges, but as having charge density distributions, $\rho_i(r_{oi})$ represented by Fermi distributions, see fig. 2.2 [21].

In this case $V_C(r)$ can be obtained by integrating the product of $\rho_1(r_{o1})$ and $\rho_2(r_{o2})$ over the volume of the nuclei,

$$V_C(r) = \int \int \frac{e^2 \rho_1(r_{o1})\rho_2(r_{o2})}{\|\mathbf{r} - \mathbf{r}_{o1} + \mathbf{r}_{o2}\|} dV_1 dV_2, \quad (2.9)$$

where $|\mathbf{r} - \mathbf{r}_{o1} + \mathbf{r}_{o2}|$ represents the interaction radius between the two elements.
This assumes however that the nuclei are spherical and so any effects from deformation are neglected.

2.3.2 Nuclear Potential - The São Paulo Potential

The nuclear potential adopted in this thesis is the parameter-free non-local São Paulo (SP) potential [11,83,12,13]. An ingredient in the SP potential is the interaction potential between nucleons in the context of the Pauli exclusion principle. This principle forbids nucleons from possessing the same quantum numbers, and only allows nucleons to be in the same state if they have opposite spins, i.e, there cannot be more than two protons or two neutrons in a given state. When a nuclear fusion occurs the compound nucleus must order its nucleons according to the Pauli exclusion principle, there cannot be a continuum state for the nucleons to occupy.

The São Paulo potential takes into account the exchange of nucleons between the fusing nuclei as the compound nucleus is formed. Since the model has been developed to be reliable at both low and high energies [2], it is sufficient to globally describe the nuclear potential at the exceedingly low energies of astrophysical interest.

In the context of the SP potential, the real part of the nuclear interaction is associated with the folding potential, \( V_f \) (to be discussed in sec 2.3.4), through the relation

\[
V_{SP}(r, E) = V_f(r) \cdot \exp \left( \frac{-4v(r, E)^2}{c^2} \right),
\]  

(2.10)

where \( c \) is the speed of light. The physical meaning of the exponential term in Eq.(2.10) is that it contains the Pauli exclusion principle. The relative velocity \( v(r, E) \)
of the nuclei at a given separation $r$ is

$$v^2(r, E) = \frac{2}{\mu} (E - V_C(r) - V_{SP}(r, E)). \quad (2.11)$$

2.3.3 Angular Potential

Incident particles can have an orbital angular momentum given by $\ell$. The barrier is determined by,

$$V_{ang}(\ell, r) = \frac{\hbar^2 \ell (\ell + 1)}{2\mu r^2}, \quad (2.12)$$

where $\mu$ is the reduced mass of the system given by $\mu = \frac{A_1 A_2}{A_1 + A_2}$.

2.3.4 Folding Potential

The folding potential, $V_f$ in eq. [2.10], is convoluted over the (globally, yet consistently determined, theoretical) mass densities of the nuclei involved in the fusion and the nucleon-nucleon potential. Analytically this can be represented as,

$$V_f(r) = \int \rho_1(\mathbf{r}_{o1}) \rho_2(\mathbf{r}_{o2}) V_0 \delta(\mathbf{r} - \mathbf{r}_{o1} + \mathbf{r}_{o2}) \, d\mathbf{r}_{o1} \, d\mathbf{r}_{o2}, \quad (2.13)$$

where $\mathbf{r}_{o1}$, $\rho_1$ and $\mathbf{r}_{o2}$, $\rho_2$ are the vector positions of constituent nucleons and densities of nucleus 1 and 2 respectively, $V_0$ $\delta$ can be regarded as the nucleon-nucleon potential, equal to $-456$ MeV fm$^3$, and $\mathbf{r}$ is the vector connecting the nuclei centers of mass.

There are two ways of obtaining the densities to solve for $V_f(r)$. The first approach takes the nucleon densities of the reacting ions, and solves the folding potential using an appropriate form for the nucleon-nucleon interaction which occurs between the target and projectile nuclei. The second approach (and the one adopted
is to use the mass distributions of the nuclei. This model does not treat the nucleons as point size particles, instead it considers the finite size of the protons and neutrons.

2.4 The Astrophysical $S(E)$ Factor

The cross section for a charged reaction such as, $(A_1,Z_1) + (A_2,Z_2)$, occurring with center-of-mass reaction energy $E$, is directly and exponentially proportional to the probability of a reactant nuclei tunneling through the Coulomb barrier. When the classical turning point is much greater than the nuclear radius [84], the cross section can be written as

$$
\sigma = \frac{S(E)}{E} \cdot \exp(-2\pi\eta) = \frac{S(E)}{E} \cdot \exp \left( -\frac{E_G}{E} \right)^{1/2}.
$$

Eq. 2.14

In Eq. 2.14 the term $\exp(-2\pi\eta)$ represents the probability of quantum mechanically tunneling through the Coulomb barrier, whereas the factor $1/E$ represents the De Broglie energy dependence of the cross section, in units MeV$^{-1}$. The parameter $E_G$ is the Gamow energy, to be defined in sec. 4.1.1.

The quantity $S(E)$ in eq. 2.14 is the astrophysical factor. It is a function of center-of-mass energy, and has units MeV b. The parameter $\eta$ is the Sommerfeld parameter, given by $\eta = \frac{Z_1 Z_2 e^2}{\hbar v}$. It contains $v$, the relative velocity between the reacting nuclei, which depends on reduced mass, $\mu$, and is given by $v = \sqrt{2E/\mu}$. Expressed in this form, the tunneling contribution to the cross section has been separated from the nuclear contribution, which defines the meaning of the $S(E)$ factor - $\sigma(E)$ is completely defined by $S(E)$. For non-resonant reactions, $S(E)$ is a slowly varying. It is therefore considered more reliable to extrapolate $S(E)$ to very low energies than it is reaction cross section, which contains an exponential term.
2.5 Applicability of Calculated $S(E)$ Factors

$S(E)$ factors were calculated for all of the heavy in systems listed in Table 2.1 using Eq.2.14, where the cross sections were obtained using the São Paulo potential in the context of the prescription given above. Since the reaction cross section, characterized as the astrophysical $S(E)$ factor, is a major ingredient to heavy ion burning rates, it is important to establish confidence in using the method outlined above. The nuclei listed in Table 2.1 fall broadly into two categories, stable and unstable nuclei. For the cases of stable nuclei fusion, there are some experimental data in existence which the theoretically calculated data can be compared to. This is done for $^{12}$C+$^{12}$C, $^{12}$C+$^{16}$O and $^{16}$O+$^{16}$O fusion. These three reactions are of key importance in nuclear astrophysics; carbon burning is the first heavy ion to fuse in late stellar evolution. The most important reaction in carbon burning is $^{12}$C+$^{12}$C \[5\], but depending on the abundance of $^{16}$O, carbon-oxygen burning can also be of great importance. Carbon burning is of specific importance for type Ia supernovae (explosions driven by carbon ignition in the carbon oxygen cores of accreting white dwarf stars \[44\]), where the $^{12}$C+$^{12}$C fusion rate defines the timescale of the ignition \[100\] \[4\]. This is possibly contributed to by the $^{12}$C+$^{16}$O and $^{16}$O+$^{16}$O reaction rates \[31\].

2.5.1 Stable Nuclei

For the cases of $^{12}$C+$^{12}$C, $^{12}$C+$^{16}$O and $^{16}$O+$^{16}$O, the calculated fusion cross sections were compared to experimental data, shown in Figure 2.3 (taken from \[32\]). Over the last few decades, there has been a significant effort to measure these three fusion cross sections. In Figure 2.3 the experimentally determined $S(E)$-factors are shown as symbols, where as the theoretically determined data is represented by a thick line. Experimental data for $^{12}$C+$^{12}$C comes from Refs \[50\], \[68\], \[69\], \[85\], \[59\].
and [37] respectively. Experimental data for \(^{12}\)C\(^+\)
\(^{16}\)O is from [16] and [18]. Experimental data shown for \(^{16}\)O\(^+\)
\(^{16}\)O is from [29], [62], [101], [61], and [92].

The experimentally determined \(^{12}\)C\(^+\)\(^{12}\)C shows pronounced sub-barrier
structure at \(E \lesssim 6\) MeV Similar structure is seen in the measured \(^{12}\)C\(^+\)
\(^{16}\)O cross section at \(E \lesssim 7.7\) MeV. The structure has been described as the result of shape resonant
states in the compound nucleus [24], referred to as quasi-molecular doorway states
since it produces cross section enhancement normally characteristic of resonance
structure. The reaction cross section for \(^{16}\)O\(^+\)\(^{16}\)O exhibits no such behavior, resulting
in a smoother cross section at sub-barrier energies (\(\sim 9\) MeV).

Figure 2.3 clearly highlights the simplicity of the BPM approach. The formalism
outlined in the BPM does not contain nuclear structure effects, as a result the model
is not able to explain the sub-Coulomb structure observed experimentally. However
the experimental data sets are not always in good agreement either; the C+O data
reveals that at sub-barrier energy, there is a factor of \(\sim 2\) disagreement between the
two experimental data sets. The same disagreement can be observed in the C+C
plot. In the case of O+O there is a disagreement of a factor of 3.

However the BPM model does provide an average description of heavy ion fusion
at energies above and below the Coulomb barrier. The agreement between the
theoretical data and the experimental data is within \(\sim 50\%\) for the case of C+O
and \(\sim 30\%\) for the cases of O+O and C+C. The BPM does not contain any free
parameters and is not a fit to experimental data, instead it is a predictive tool. Since
the BMP used with the São Paulo potential provides a satisfactory parameter-free
description of the energy dependence of the \(S\) factor, it can be regarded safely as a
useful tool for predicting average nonresonant low energy cross sections for stable
nuclei.

The majority of the nuclei listed in Table 2.1 however, such as \(^{20−24}\)C, \(^{22,24}\)O,
Figure 2.3: Experimentally measured $S(E)$ factors for three reactions compared to $S(E)$ factors calculated with the BPM and the São Paulo potential. Experimental data is represented by symbols, lines give calculations. Figure from [32].
36–40Ne and 38–46Mg, are very far from stability. Since there is no experimental
data regarding the fusion cross sections of unstable or exotic nuclei, there is no
direct way to test the validity of the BPM for these reactions. Instead fusion cross
section obtained through the S˜ ao Paulo and BPM can be compared to other, more
elaborate theoretical prescriptions. This is done in the following sub section.

2.5.2 Unstable Nuclei

In order to justify the use of the BPM and S˜ ao Paulo potential, and test the
consistency of the model predictions for neutron rich nuclei, calculations were tested
against another form of theoretical model, specifically coupled channel (CC) calcu-
lations.

It is necessary to validate this collection of isotopes separately from stable ones
because very neutron rich nuclei fusion can have different nuclear aspects. For in-
stance, an extended neutron halo may lower the Coulomb barrier (because neutrons
are charge neutral, a thick neutron skin could allow the nuclei to “touch” while still
maintaining an equilibrium distance between the repulsive protons of the nuclei).
This would result in a fusion enhancement at low energy. On the other hand, a
loosely bound neutron halo could break up when exposed to the electromagnetic
field of the other nucleus. This could suppress fusion compared to the previous sce-
nario, since there would be a loss of neutrons in the reaction channel [48], [25], [20].

$S(E)$ factor calculations for seven reactions were compared to CC calculations as
discussed in Gasques et al [32]. The reactions were $^{16}$O+$^{16}$O, $^{20}$O+$^{20}$O, $^{20}$O+$^{26}$Ne,
$^{20}$O+$^{32}$Mg, $^{26}$Ne+$^{26}$Ne, $^{26}$Ne+$^{32}$Mg, and $^{32}$Mg+$^{32}$Mg. The reaction $^{16}$O+$^{16}$O was
previously discussed in Section 2.5.1, but is presented again for CC calculations
against experimental data for the sake of completeness. The other six reactions
were selected because not only have they been identified as relevant (Table 2.1) but
TABLE 2.2

LOW ENERGY EXCITED STATES (QUOTED IN MEV, PROVIDED IN PARENTHESES) ALLOWED IN THE CC CALCULATIONS FOR THE NUCLEI OF INTEREST.

<table>
<thead>
<tr>
<th></th>
<th>$^{16}$O</th>
<th>$^{20}$O</th>
<th>$^{26}$Ne</th>
<th>$^{32}$Mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>0$^+$</td>
<td>(0.000)</td>
<td>0$^+$ (0.000)</td>
<td>0$^+$ (0.000)</td>
<td>0$^+$ (0.000)</td>
</tr>
<tr>
<td>3$^-$</td>
<td>(6.130)</td>
<td>2$^+$ (1.673)</td>
<td>2$^+$ (2.018)</td>
<td>2$^+$ (0.885)</td>
</tr>
<tr>
<td>2$^+$</td>
<td>(6.619)</td>
<td>4$^+$ (3.570)</td>
<td></td>
<td>2$^+$ (4.072)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0$^+$ (4.456)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3$^+$ (5.614)</td>
<td></td>
</tr>
</tbody>
</table>

they are also unbound systems for which some experimental energy level structure exists. This data is required in order to perform a CC calculation. The CC reactions were carried out using the computer code FRESCO [93]. In CC theory, couplings between inelastic (excitation) channels and the fusion channel are accounted for in the total cross section. In this context, the BPM represents a single (fusion) channel approach. Table 2.2 details the low energy inelastic excited states included in the CC calculations. To maintain consistency, São Paulo potential was used as the nuclear potential for the calculations.

Figure 2.4, taken from [32], plots the $S(E)$ factor obtained for the BPM (solid line) against that obtained for the CC (dotted line) for the reaction $^{16}$O$+^{16}$O. As in Figure 2.3, experimental $S(E)$ factor data were taken from [29], [62], [101], [61], and [92]. At $E < E_C$, $\sim 9$ MeV, there is satisfactory agreement between the BPM
and the CC calculation. Maximum disagreement is on the order of a factor of 4, at E=0 MeV. Since the BPM does not contain any fitting parameters, and so represents a true prediction, this can be considered an acceptable result.

![Graph showing experimental measurements and BPM/CC calculations](image)

Figure 2.4. Experimentally measured $S(E)$ factor for the reaction $^{16}\text{O}+^{16}\text{O}$, symbols refer to individual data sets. Solid line represents the BPM calculation, the dotted line is the CC formalism.

Displayed in Figure 2.5 (also taken from [32]) are BPM calculations (lines) plotted against CC calculations (filled circles) for the six reactions $^{20}\text{O}+^{20}\text{O}, {^{20}\text{O}+^{26}\text{Ne},$
$^{20}\text{O}+^{32}\text{Mg}$, $^{26}\text{Ne}+^{26}\text{Ne}$, $^{26}\text{Ne}+^{32}\text{Mg}$, and $^{32}\text{Mg}+^{32}\text{Mg}$. Including coupled channel effects only affects the energy region below the Coulomb barrier. Above the barrier the effects of CC are not seen since heavy ion collisions result in fusion, rather than inelastic excitations. Beneath the barrier, at $E = 0$ MeV, there is approximately 1 order of magnitude difference between the CC and BPM calculations for four of the reactions. This is not the case for $^{20}\text{O}+^{20}\text{O}$, where there is very good agreement over the entire energy range, indicating that the inelastic channels do not play a large role for this fusion reaction. Conversely the reaction $^{26}\text{Ne}+^{32}\text{Mg}$ exhibits a 2 order of magnitude discrepancy between the BPM and CC calculations, suggesting a strong effect of coupling at sub barrier energies.

The maximum discrepancy of 2 orders of magnitude does affect the region of greatest interest for heavy ion fusion in a neutron star crust and could affect density induced heavy ion nuclear fusion rates calculated with the BPM cross sections versus some more complicated procedure. Potentially this becomes an additional uncertainty in the rate calculation. However the uncertainties associated with using the BPM are less significant when compared to other sources of error which arise from the neutron star crust environment. Such sources of error are discussed in sec 4.3 but include uncertainties in lattice structure, plasma potentials, and inter ion separations.

Given the simplicity of the BPM and the comparative complexity of the CC calculations, what the BPM looses in accuracy it gains in durability. The BPM can reliably produce a uniform set of cross section data with no reaction dependent fine tune parameters, which makes it perfect for this application.
Figure 2.5. $S(E)$ factors for the reactions $^{20}\text{O}+^{20}\text{O}$, $^{20}\text{O}+^{26}\text{Ne}$, $^{20}\text{O}+^{32}\text{Mg}$, $^{26}\text{Ne}+^{26}\text{Ne}$, $^{26}\text{Ne}+^{32}\text{Mg}$. Solid lines are the BPM calculations, solid circles represent the CC calculations.
The need for a reliable method to obtain $S(E)$ factors was highlighted in Section 2.4. Theoretical $S(E)$ factors were calculated in Chapter 2 using the BPM in conjunction with the São Paulo potential. The calculations were performed for 946 heavy ion fusion reactions involving different isotopes of C, O, Ne, and Mg (between the valley of stability and the neutron drip line).

The calculations were performed from 2 MeV up to $\sim18$–$30$ MeV (covering a range of energies below and above the Coulomb barrier). The choice of the isotopes studied was motivated by identifying likely ashes left over after the X-ray burst and subsequent ash processing through EC. Due to pairing effects there is thought to be a predominance of even $Z$ even $A$ nuclei, which are expected to be more stable in the accreting neutron star crust. Heavy ion fusion in a neutron star crust can take place at energies less than 2 MeV however. Due to uncertainties associated with calculating fusion at zero center-of-mass energy, the $S(E)$ factors were not determined at energies less than 2 MeV. Instead the calculations were fitted with an analytical fit expression (containing nine parameters), and then extrapolated from $E = 2$ MeV $\rightarrow 0$.

After presenting the nine parameter analytic approximation of the astrophysical $S(E)$ factors, an assessment is given of the quality of the fits of the calculations compared to the calculations themselves. The discussion of the $S(E)$ factor
parametrization presented here closely follows the arguments set out in [6].

Having discussed the fit parameters, a suggestion is proposed to explain why the \( S(0) \) factor can be many orders of magnitude for some systems.

3.1 Analytical Approximation of \( S(E) \) Factors

All \( S(E) \) factors were first calculated by means of the São Paulo potential in the context of the BPM (see Sections 2.2 and 2.3.2 for details). The \( S(E) \) factors were computed between an energy range of 2 MeV up to some maximum value, which was chosen to be well above the Coulomb barrier for that particular heavy ion fusion system. Column 5 in Table 2.1 details the maximum energy value. Calculations were performed in energy steps of 0.1 MeV, producing a dense energy grid for each reaction. Once calculated, the \( S(E) \) factors were then approximated by the analytic expression

\[
S(E) = \exp \left\{ B_1 + B_2E + B_3E^2 + \frac{C_1 + C_2E + C_3E^2 + C_4E^3}{1 + \exp [(E_C - E)/D]} \right\} \text{ MeV b,} \quad (3.1)
\]

which was used to fit the calculated \( S(E) \) data for each reaction. In this expression, \( E \) is a center-of-mass energy of reacting nuclei expressed in MeV, and \( E_C, D; B_1, B_2, B_3; C_1, C_2, C_3, \) and \( C_4 \) are the nine fit parameters for each of the reactions listed in Table 2.1.

Since there are a great many fit parameters, (9 for each of the 946 heavy ion fusion systems yields 8514 fit parameters), as well as evaluated errors for each fit, the tables of fit parameters are not reproduced here, but can be found in ref. [6]
3.1.1 Physical Meanings of the Fit Parameters

The high number of fit parameters reflects the fact that many fusion systems had to be described by one general, uniform expression. The advantage of fitting all of the $S(E)$ factors with one uniform expression is clear: it allows for easy implementation in to computer codes. This is of use since it means that relevant $S(E)$ factors can be obtained quickly in a dynamic nuclear reaction network code where it is easier to solve a fit expression to extract an $S(E)$ factor rather than to calculate it from first principles each time - this would be very burdensome for computing time.

Most of the fit parameters in eq. 3.1 can be interpreted with physical meaning:

- $E_C$ has units of MeV. It is approximately equal to the height of the Coulomb barrier, and divides the energy range into that below the barrier ($E \lesssim E_C$) and that above the barrier ($E \gtrsim E_C$). This effectively separates the $S(E)$ curve into two regions, where is exhibits distinctly different behaviors.

- $D$ is in units of MeV, and describes the width ($D \sim 1$ MeV) of the region at $E \approx E_C$. This is the point at which the energy region transitions from that below the Coulomb barrier, to that above the Coulomb barrier. This transition is governed by a Fermi-Dirac function

$$\frac{1}{1 + \exp((E_C - E)/D)},$$

(3.2)

(which tends to 0 below the barrier and tends to 1 above the barrier), and can be seen in the second half of Eq. 3.1. As such, beneath the barrier the second half of Eq. 3.1 does not contribute at all, and so at $E \leq E_C$ the $S(E)$ factors are given by just three parameters, $B_1$, $B_2$, and $B_3$.

- $B_1$ is expressed in units of MeV b, and, since it contains no energy dependence,
determines the value of $S(E)$ at zero energy, $S(0)$:

$$S(0) = \exp(B_1) \text{ MeV b.} \quad (3.3)$$

- $B_2$, which has units of MeV$^{-1}$, and $B_3$, in units of MeV$^{-2}$ specify the energy dependence of $S(E)$ at $E \lesssim E_C$,

$$S(E) = S(0) \exp(B_2 E + B_3 E^2) \text{ MeV b.} \quad (3.4)$$

- Since the Fermi-Dirac function of Eq. 3.1 tends to 1 above the barrier, the parameters $C_1$, which is dimensionless, $C_2$, expressed in MeV$^{-1}$, $C_3$, units in MeV$^{-2}$, and $C_4$ with units in MeV$^{-3}$ (together with $B_1$, $B_2$, and $B_3$), specify the $S(E)$ dependence at $E \gtrsim E_C$. This can be written as:

$$S(E) = S(0) \exp[C_1 + (B_2 + C_2) E + (C_3 + B_3) E^2 + C_4 E^3] \text{ MeV b.} \quad (3.5)$$

3.1.2 Evaluating the Fits

The quality of the fitted data was evaluated primarily by finding the percentage difference, at each energy grid point, between the calculated value of the $S$ factor, $S(E)_{\text{calc}}$ and that yielded by the fit approximation, $S(E)_{\text{fit}}$, defined by Eq. 3.1

$$\Delta = \left| \frac{S(E)_{\text{calc}} - S(E)_{\text{fit}}}{S(E)_{\text{calc}}} \times 100 \right| \%.$$

(3.6)

For the fit to be classed as “good” not only did the maximum percentage fit error (the maximum $\Delta$) have to be below 10%, the root mean squared (rms) fit error also had to be on the order of $1 - 2\%$. The rms error is used as a measure of the
mean squared error. It is a useful tool that effectively highlights where a predicted value differs greatly from a “desired” value by exaggerating the mean square error in such cases. Labelling the “desired” value, \( S(E)_{\text{calc}} \), as \( y \), and the predicted value from the fit, \( S(E)_{\text{fit}} \), as \( x \), the rms error can be found from

\[
rms_{\text{err}} = \sqrt{\frac{\sum_{i=1}^{n} (x_i - y_i)^2}{n}},
\]

where the sum is performed over the number of energy points in the grid, \( n \).

This quantity is dependent on the reaction system and is related to the maximum calculation energy cutoff, column 5 in Table 2.1, through the simple relation

\[
n = \frac{E_{\text{max}} - 2\text{MeV}}{\text{stepsize}},
\]

where \( \text{stepsize} = 0.1 \). The number of energy points ranged from \( n = 159 \) for C+C systems, up to \( n = 279 \) for Mg+Mg systems.

It is helpful to slightly rearrange Eq. 3.7, expressing it as

\[
rms_{\text{err}} = \sqrt{\frac{\sum_{i=1}^{n} y_i^2 \left( \frac{x_i}{y_i} - 1 \right)^2}{n}}.
\]

Since the \( S(E) \) factors are typically of many orders of magnitude, the rms errors given by Eq. 3.8 are also of many orders of magnitude. In order to preserve the usefulness of the rms error approach for detecting unsuitable fits, Eq. 3.8 is normalized to value of \( S(E)_{\text{calc}} \) at each energy point. This yields the following expression for the rms error,

\[
rms_{\text{err}} = \sqrt{\frac{\sum_{i=1}^{n} \left( \frac{x_i}{y_i} - 1 \right)^2}{n}}.
\]

Displayed in Figure 3.1 are the analytic approximations of \( S(E)_{\text{fit}} \) for 11 C+C reactions. Solid lines refer to fits performed with Eq. 3.1. These lines practically correspond to \( S(E)_{\text{calc}} \) on a log-scale, and so to keep the figure from becoming cluttered, the calculated values are not given. Figure 3.1 is not only the fit over the
energy range from $E = 2$ MeV to $E = 17.9$ MeV, but also the extrapolation from $E = 2$ MeV down to zero energy, and from $E = 17.9$ MeV up to $E = 20$ MeV.

For energies at which $E \lesssim E_C$, it is possible to describe the $S(E)$ factor fits with just three parameters, given by Eq. 3.4 (where $S(0)$ is provided by Eq. 3.3). This is displayed in Figure 3.1 as the red dashed line. It can immediately be seen that at the Coulomb barrier, distinguished on each curve by a black dot, the curves exhibit strikingly different behavior in regions above and below the barrier. As expected from Eq. 3.2, the transition region is very narrow. At the Coulomb barrier the 3 parameter fit given by Eq. 3.4 starts to diverge from $S(E)_{calc}$, becoming increasingly inaccurate. With increasing isotope mass number Coulomb barrier decreases. This is because as A increases, so does radius, $r$ (since $r$ scales with $A^{1/3}$) and as the Coulomb barrier scales with $1/r$, increasing $r$ decreases the Coulomb barrier.

Shown in Figure 3.2 is the analytical approximation of $S(E)$ (obtained using Eq. 3.1) for all 36 C+C reactions (shown in black), 112 C+Mg reactions (shown in blue), and 105 Mg+Mg (shown in red) fusion reactions listed in Table 2.1. As in fig. 3.1, the Coulomb barrier is marked by solid dots. Also like the previous figure, analytical approximations only are shown, and in all cases the $S(E)$ factors have been extrapolated to $E=0$ MeV. The most striking feature of this plot is that the magnitude of the $S(E)$ factors for the different systems covers an amazing 70 orders of magnitude. Heavier ion fusion systems, with larger reduced mass, have much greater order of magnitude $S(E)$-factors than lighter ion systems, for example, $^{46}$Mg+$^{46}$Mg has an $S(0)$ of order $10^{85}$ MeV b, whereas $^{20}$Mg+$^{20}$Mg has a more modest $S(0)$ of order $10^{45}$ MeV b. The reason for this come from $\eta$ in eq. 2.14, which scales as the square root of the reduced mass. Smaller reduced mass means that the exponent in eq. 2.14 ($\exp[2\pi \eta]$) is smaller which results in smaller $S(E)$ factors for those systems.
Figure 3.1. Analytic approximations of $S(E)$ calculated using Eq. 3.1 for C+C reactions. The curves from bottom to top refer to $(A_1, A_2) = (10,10), (12,12), (12,16), (12,20), (16,16), (12,24), (16,20), (16,24), (20,20), (20,24), \text{ and } (24,24)$ reactions. Solid curves show the 9-parameter approximation (3.1); dashed curves (plotted at $E \leq E_C + 0.3$ MeV) show the 3-parameter approximation (3.4). Filled dots are where $E = E_C$. 

41
However Figure 3.2 also highlights the general uniformity of the energy dependence of the $S(E)$ factors for many different systems over a range of energies, since the curves all exhibit the same essential features.

The decrease in accuracy of the 3 parameter fit, Eq. 3.4 when $E \gtrsim E_C$ compared to the nine parameter fit of Eq.3.1 can best be seen through a specific example. The $S(E)$ dependence for the $^{20}\text{Ne}+^{24}\text{Mg}$ reaction is plotted in the upper panel of Figure 3.3. The solid and dashed lines are the 9- and 3-parameter fits, respectively. The lower panel shows relative errors of fitted values of $S(E)$ [not of log $S(E)$] with respect to the calculated values. It can be seen that the 9-parameter fit is accurate over the entire energy range. The maximum fit error of given by eq. 3.6 is $\approx 1.2\%$ and occurs at $E = 15.8$ MeV (and the root-mean-square fit error over all grid points is $\approx 0.6$). The three-parameter fit, eq. (3.4), stays highly accurate below the Coulomb barrier but diverges when $E$ exceeds $E_C$. For instance, at $E = 25$ MeV it overestimates $S(E)$ by more than two orders of magnitude.

Tables 1-10 in [6] detail both the fit parameter set and the maximum error for each nuclear system considered. The maximum fit error for all of the systems does not exceed 10\%. From this it can be concluded that using fits to obtain heavy ion $S(E)$ factors, rather than calculating the $S(E)$ factors directly, does not represent any significant source of error in the reaction rate.

3.2 $S(E)$ Factors at Zero Energy

The probability of penetrating the Coulomb barrier is simplistically determined by assuming firstly that there is no orbital angular momentum, and secondly that the Coulomb barrier extends to $r \to 0$. The last point is equivalent to requiring that the classical turning point be much larger than the nuclear radius. This is the case for point like particles and with this assumption one arrives at eq. 2.14.
Figure 3.2. Analytic approximation (3.1) of $S(E)$ for 36 C+C reactions, 112 C+Mg reactions, and 105 Mg+Mg reactions (Table 2.1). The curves for each reaction type are enclosed by the (thick) curves for the (indicated) reactions involving lightest and heaviest isotopes. Filled dots are where $E = E_C$. 

43
Figure 3.3.  *Top:* Analytic approximations of $S(E)$ for the $^{20}\text{Ne}+^{24}\text{Mg}$ reaction. The solid and dashed lines are, respectively, the 9- and 3-parameter approximations (3.1) and (3.4). The filled dot refers to $E = E_C$.  *Bottom:* Relative errors of these approximations with respect to computed data. The dotted line shows zero error to guide the eye.
However, as it was discussed in Section 2.3.1, it is not appropriate to treat the nuclei in this manner. In a strict framework nuclei do not behave as point particles. In particular, nuclei exhibit a long range electromagnetic interactions as well as short range attraction. This problem can be treated by writing the cross section in a manner modified slightly from eq. 2.14,

\[
\sigma(E) = \frac{S_0}{E} e^{\phi(E)}
\]  

(3.10)

where \( \phi \) is defined as the integral of the Coulomb potential between the two radial turning points \( r_1 \) and \( r_2 \),

\[
\phi(E) = -\frac{2}{\hbar} \int_{r_1}^{r_2} dr \sqrt{2 \mu (U(r) - E)}.
\]  

(3.11)

The quantity \( S_0 \) is the s wave \( S_\ell \) factor of ref[26]. The \( S_0 \) factor is similar to the usual \( S(E) \) factor in that it contains all of the strictly nuclear quantities (such as reduced mass, nuclear shape effects, nuclear radius and so forth) but it is not energy dependent. It is defined as

\[
S_0 \approx \frac{2\pi \hbar^2}{\mu} \left( \frac{E_C}{40 \text{ MeV}} \right)^{1/2}.
\]  

(3.12)

The physical interpretation of \( U(r) \) in eq.3.11 is the nucleus - nucleus potential. At separations larger than the sum of the radii of the two interacting nuclei, it is entirely dominated by the repulsive Coulomb potential, \( U(r) = Z_1 Z_2 e^2 / r \) (for \( r > 1.2(A_1^{1/3} + A_2^{1/3}) \)). This is plotted as the blue line in fig. 3.4. The Coulomb potential has a physical maximum, equal to \( E_C \) and located at \( R_{C1} \). Solving the Schödinger equation with this potential (assuming large nuclear separations) gives the familiar penetration probability, \( P = e^{-2\pi \eta} \) which is defined by Eq.2.14.

At smaller separations the potential is no longer Coloumbic, it is a short range
attractive nuclear potential, shown as a green line in fig. 3.4. The maximum point of the nucleus - nucleus potential is at the top of the Coulomb barrier, where the potential transitions from repulsive to attractive. If this point is taken to be a sharp transition, then it occurs at a radius of $R_{C1}$. If there is some width to the transition region, then it occurs at some smaller radius, equal to $R_C$. In both scenarios the energy at the peak of $U(r)$ is $E_C$.

The pink line in fig. 3.4 shows the pure Coulomb potential ($U(r) = Z_1 Z_2 e^2 / r$) tending to infinity as $r \to 0$ fm.

Yakovlev et al [102] defined the nucleus - nucleus potential in the regions $r < R_{C1}$ and $r \geq R_{C1}$ as,

$$U(r) = \frac{Z_1 Z_2 e^2}{r} \quad \text{at} \quad r \geq R_{C1}, \quad U(r) = E_C \left[ 1 - \frac{\beta(r-R_C)^2}{R_C^2} \right] \quad \text{at} \quad r < R_{C1}, \quad (3.13)$$

where $\beta$ is defined below by eq.3.14. This formalism allows the transition region to be smooth and possess a physical width, since the short range potential can take a parabolic shape.

Depending on whether one adopts the traditional sharp cut off, or a smooth shape for the transition of Coulomb to attractive potential, the radius which corresponds to the peak of $U(r)$ can occur at different separations. It is convenient to introduce a parameter to characterize the width of the potential peak shown in figure 3.4 given by $\delta = \frac{(R_{C1}-R_C)}{R_C}$. Having defined $\delta$, the meaning of $\beta$ from eq.3.13 is

$$\beta = \frac{1}{\delta(2 + 3\delta)}, \quad (3.14)$$

i.e, the physical meaning of $\beta$ is to produce the tail at $r < R_C$ which arises from the smooth transition. If $\beta$ were equal to zero, there would be no tail and no parabola.
Figure 3.4. Nucleus - nucleus potential, $U(r)$, as a function of separation, $r$, for the reaction $^{18}\text{Ne}+^{20}\text{Mg}$. The blue line is the Coulomb potential for separations greater than the nuclear potential. The pink line shows the behavior of the Coulomb potential in the limit $r \to 0$. The green line shows a parabolic model for the short range attractive nuclear potential.

The peak of $U(r)$ has an energy $E_C \sim 21\ \text{MeV}$. This occurs either at $r = R_C \sim 8.0\ \text{fm}$ or $r = R_{C1} \sim 8.2\ \text{fm}$ depending on the form of the short range potential. The difference of these values characterizes the width of the potential peak, $\delta$. 
at $r < R_C$. Demonstrated in fig. 3.5 is the effect of $\delta$ on $U(r)$. Increasing $\delta$ by say one order of magnitude, is equivalent to smoothing the peak of the transition region, while decreasing the gradient of the attractive slope at $r < R_C$. Conversely decreasing $\delta$ greatly sharpens the peak of the potential, while steepening the slope of the potential at $r < R_C$, reproducing the traditional sharp cut off picture. As expected, at $r > R_C$ the potential is independent of the width of the transition region.

![Figure 3.5](image)

Figure 3.5. Effective potential $U(r)$ verses radius for four different values of $\delta$ for the specific case of $^{18}\text{Ne} + ^{20}\text{Mg}$. Increasing $\delta$ widens the peak of the potential, producing a less attractive short range potential (red line). Decreasing $\delta$ significantly sharpens the attractive potential.
Since the cross section is defined by both Eq.2.14 and Eqs.3.10, 3.11 combining these equations $S(E)$ can be expressed as

$$S(E) = S_0 \exp(2\pi\eta) \exp(\phi(E)) \text{ at } E \leq E_C. \quad (3.15)$$

The nucleus - nucleus potential enters into eq. 3.15 through the variable $\phi$. If the transition region between the Coulomb potential and nuclear potential is taken to be sharp (and so $\delta = 0$) the short range potential is highly attractive. In this case fig. 3.6 (which is valid for the reaction $^{18}\text{Ne}+^{20}\text{Mg}$, but should be representative of all reactions) shows that $S(E)$ increases as $E \to 0$ MeV. Increasing the value of $\delta$ makes the nucleus - nucleus potential of the transition region thicker and less transparent. Shown in figure 3.6 is the effect on the $^{18}\text{Ne}+^{20}\text{Mg}$ $S(E)$ factor of five different values of $\delta$, ranging from $3.39 \times 10^{-4}$ to $3.39 \times 10^0$ in one order of magnitude steps. It is immediately apparent from this figure the significant impact that $\delta$ has on the $S(E)$ factor - a decrease in one order of magnitude between $\delta = 3.39$ and $\delta = 0.339$ produces a thirty order of magnitude change in the $S(0)$ factor, calculated using Eq.3.15. For additional order of magnitude decreases in $\delta$, the resultant increase in $S(0)$ is less dramatic though it is still significant; it is two orders of magnitude between $\delta = 3.39 \times 10^{-3}$ and $\delta = 3.39 \times 10^{-4}$.

Since variation in $\delta$ is manifested by either an enhancement or a suppression of $S(E)$ factor as $E \to 0$, it is possible that this principle could be useful for the explanation of the hindrance of reaction cross section measurements recently proposed by Jiang et al for some sub-barrier heavy ion fusion reactions ([52], [53], [54], [55], [56], [57]). Hindrance of very low energy fusion reaction cross sections would be of critical importance to reactions taking place in the neutron star environment, and would result in a reaction rate decrease of many orders of magnitude. Gasques et al [33] investigated the astrophysical consequences of hindrance...
Figure 3.6. Log of $S(E)$ factor against center of mass energy for the fusion reaction $^{18}\text{Ne}+^{20}\text{Mg}$, calculated using Eq. 3.15 with five different values of potential width parameter $\delta$. 
on carbon and oxygen burning in dense stellar matter. Their findings suggest that the impact of hindrance on low energy $^{12}$C+$^{12}$C fusion is indeed significant, translating into an increase for the carbon ignition temperature for white dwarf stars by a factor of $\approx 1.5$.

Shown in fig. 3.7 is the impact of $\delta$ on the $S(E)$ factor for the reactions $^{12}$C+$^{12}$C (top) and $^{12}$C+$^{16}$O (bottom), plotted against the same experimental data as in fig. 2.3 (sec. 2.5.1). Experimental data for both reactions appears to rule out a large ($> 0.4$) $\delta$. Notably in both cases the experimental data also rules out a very small (or even $\delta = 0$). For the reaction $^{12}$C+$^{12}$C, a $\delta$ of $4 \times 10^{-4}$ overestimates the $S(E)$ factor by $\sim 2$ orders of magnitude at $E = 3.1$ MeV, compared to the data of Patterson et al [50]. For the reaction $^{12}$C+$^{16}$O when $\delta = 4.12 \times 10^{-4}$, there is $\sim 2.5$ order of magnitude overestimation compared to the data of Christensen et al at 4 MeV. The best reproduction for the trend of the data for both reactions is a $\delta$ of 0.04. In both cases however this $\delta$ slightly overestimates the experimental $S(E)$ factors, indicating that the width of the transition region is slightly larger than estimated by that $\delta$.

Without lower energy experimental data it is impossible to say precisely what value $\delta$ should take, and how this value relates to the hindrance effect. The hindrance effect however is not well established, and since there is little hard experimental data to either confirm or contradict this effect, it is impossible at this point to be sure whether the peak broadening effect described above is really a true or complete picture of the phenomena seen by Jiang et al. Instead it can be noted with certainty that the potential of the transition region does not have a sharp cut off shape, it is much more likely to be a smoothed transition. How smooth this transition really is however, and so consequently the degree to which the current method over estimates $S(0)$, is an open question.
Figure 3.7. Log of $S(E)$ factor against center of mass energy for the fusion reactions $^{12}\text{C}+^{12}\text{C}$ and $^{12}\text{C}+^{16}\text{O}$, calculated using Eq. 3.15 with five different values of potential width parameter $\delta$. Also plotted are the same experimental data used in fig. 2.3.
Until more very low energy cross section fusion measurements are made, there is no guidance available on what the peak broadening should look like and consequently what the value of $\delta$ should be. There is also no indication of how the peak broadening might develop with progressively more neutron rich nuclei, though it seems logical to propose that nuclei with a large neutron excess would have a broader peak than stable or proton rich nuclei. Traditionally the peak broadening has been effectively treated as zero, and the potential has been regraded as possessing a sharp cut off with no transitional smoothing. To be consistent with traditional approaches, $\delta$ was treated as zero in the calculation of all fusion cross sections listed in table 2.1. Future measurements at low energies for both stable and neutron rich fusion systems will greatly help to demonstrate if this is a good assumption, and how to improve it if need be.
A full picture of neutron star nucleosynthesis requires a number of things, but in the context of density induced heavy ion reactions, the main requirement is an analytic expression which is valid for the range of temperatures and mass densities thought to reflect the thermal and density profile of an accreting neutron star. Spectra from X-ray burst light-curves suggest that the crust temperature of a neutron star ranges from $\approx 3 \times 10^8 - 3 \times 10^7$ K, decreasing roughly an order of magnitude with increasing column depth \[7\]. The mass density profile of the crust on the other hand ranges over many orders of magnitude, stretching from $\rho \approx \times10^6$ g cm$^{-3}$ on the surface of the star, to $\approx \times10^{14}$ g cm$^{-3}$ at the bottom of the crust (see fig 1.2). This $T - \rho$ range affects the nature of nuclear reactions taking place in that environment, forming domains of characteristic Coulomb barrier penetration, the most extreme of which being pycnonuclear reactions.

Obtaining one analytic approximation valid in this wide $T - \rho$ range translates into a computational advantage for nucleosynthesis applications. Since a single analytic approximation can be calculated quickly, it becomes particularly attractive to applications such as network codes, which essentially evolve the abundance distribution of the star in response to nuclear reactions.

Producing an analytic framework which is valid throughout all of the burning domains has been the main theme of this work. Accomplishing this task required generalizing existing work on exotic matter burning, and then relating this to the
better understood principles of thermonuclear fusion. Documented in the following chapter is the process from which one transitions through different burning environments, from thermonuclear to pycnonuclear. Presented first is a discussion of the types of stellar burning environments that can occur. The environments themselves are an expression of the temperature and mass density dependence of reaction rates, a dependence which ultimately comes from the electromagnetic interaction of the nuclei via the Coulomb barrier. Since so much of this chapter relies on reaction rate formalism, the theory of reaction rates is also discussed, to set the stage for further reaction rate generalizations. Following this is a discussion of physical stellar conditions. This section includes definitions of characterizing properties, such as average ion proton number and mass number, nuclei and electron number densities, charge neutral ion sphere quantities, and a parameter which measures the ratio of electrostatic energy to thermal energy.

Having defined the parameters used to categorize the stellar matter, the different burning regimes are examined, and classified according to those definitions. The strategy here is to recognize that different fusion domains are related by underlying parameters which define the possible heavy ion fusion reactions in that environment. In order to visualize how the regimes relate to each other, first the thermonuclear domain is discussed, then the pycnonuclear regime considered. These two stellar environments represent the extrema in burning conditions, and delimit the ends of the spectra that a single analytical formalism has to cover.

Once the transition from thermonuclear reactions to density sensitive reactions has been made, an examination of the Coulomb lattice which forms the neutron star crust is performed. Following this is a discussion of temperature independent pycnonuclear rates. First to be discussed is the simplest case of a lattice composed of one species of ion. This is then generalized to a discussion of a lattice composed
of a realistic distribution of isotopes. The treatment for the pycnonuclear rates is then extended to include thermal effects. The aim of this last step is to produce a reaction rate expression which is not only analogous to the thermonuclear reaction rate, but can also reproduce the thermonuclear rate at high temperatures and low densities, and yield the thermally independent pycnonuclear rate at high densities and zero temperature.

Following the presentation of a single analytical formalism, it is used to calculate the T-\(\rho\) reaction rate plane for 4 different heavy ion fusion reactions. The plots demonstrate that the formalism is able to reproduce the form of the rates (thermonuclear, pycnonuclear and the transition in between) over a spectrum of temperature and mass density conditions.

4.1 The Extremes of Stellar Burning

It was pointed out by Salpeter and Van Horn in their seminal paper of 1969, [86], that there are in existence five different stellar burning regimes. The distinction between these regimes occurs as a function of environment temperature and mass density, and is mostly manifest in the character of the Coulomb barrier penetration. Qualitatively speaking these regimes are (1) the classical thermonuclear regime; (2) the thermonuclear regime with strong electron screening; (3) a thermopycnonuclear regime; (4) the thermally enhanced pycnonuclear regime; and (5) the zero-temperature pycnonuclear regime.

The T-\(\rho\) domains of these five regimes are plotted schematically in figure 4.1 for the example of pure \(^{12}\)C matter. This particular isotope has been selected because (as discussed in sec 3.2) carbon burning is of particular importance in astrophysics, it is thought to power type Ia supernovae, and has been suggested as a trigger and energy source for super-bursts [19], [90], [17]. The top curve in fig 4.1 corresponds
to a burning time of $\tau = 1$ sec, the bottom to $\tau = 1G$ year. The bisecting lines $T_F$, $T_L$, $T_p$ and $T_m$ represent the temperatures at which the stellar matter is electron degenerate, transitions to a liquid, becomes a plasma, and crystallizes in to a solid.

In the following sections the fusion mechanism of these different domains, and how they relate to each other, will be fully explored.

4.1.1 General Reaction Rate Formalism

The rate of nuclear reactions is dependent on the density of the reactants, the velocity of one reactant relative to another, and the probability of a reaction occurring. Mathematically these ideas can be expressed as,

$$R_{ij}^{th} = N_i N_j v \sigma(v)$$  \hspace{1cm} (4.1)

where $N_i$ and $N_j$ are the number density of ions $i$ and $j$, $v$ is the velocity, and $\sigma(v)$ is the cross section, expressed as a function of velocity rather than energy.

Typical stellar environments are composed of non degenerate, non relativistic nuclei. In this case the velocity of the nuclei $i$ form a distribution which can be described by a Maxwell-Boltzmann function for ideal gases,

$$\phi(v_i) = 4\pi v_i^2 \left( \frac{m_i}{2\pi k_B T} \right)^{3/2} \exp \left( \frac{-m_i v_i^2}{2k_B T} \right),$$  \hspace{1cm} (4.2)

where $k_B T$ is the Maxwell-Boltzmann constant and $m$ is the mass of nucleus $i$.

Folding the velocity distribution of reactants $i$ and $j$, eq. [4.2] with $\sigma(v)$ produces the reaction rate per particle pair,

$$< \sigma v > = \int_0^\infty \int_0^\infty \phi(v_i) \phi(v_j) v \sigma(v) \ dv_i \ dv_j,$$  \hspace{1cm} (4.3)

where the integration limits are $0 \to \infty$ for exothermic reactions, and $v_t \to \infty$ for
Figure 4.1. Log temperature - log density plane for pure $^{12}$C matter. The upper and lower lines refer to $^{12}$C burning times of 1 second, and $\times 10^9$ years respectively. $T_L$, $T_p$ and $T_m$ refer to the points at which the stellar matter can be regarded as a Coulomb liquid, plasma, and solid Coulomb lattice. $T_F$ is the electron degeneracy temperature. Hatched areas represent the five possible stellar burning regimes.
endothermic reactions which require a threshold velocity before the reaction can occur.

Using the reaction rate eq. 4.1 can be re-written as

\[ R_{ij}^{th} = \frac{1}{1 + \delta_{ij}} N_i N_j <\sigma v>, \]  

(4.4)

the \(\delta_{ij}\) function preventing the double counting of identical nuclei.

In the center-of-mass, the reaction has a total mass of \(M\) and a total velocity \(V\) (since \(m_i v_i + m_j v_j = MV\)). Using the reduced mass in atomic mass units (m.u. being equal to \(1.66 \times 10^{24}\) g, or 931.502 MeV/c²),

\[ \mu_{ij} = \text{m.u.} \frac{A_i A_j}{A_i + A_j}, \]  

(4.5)

eq. 4.3 can be re-written as,

\[ <\sigma v> = \int_0^\infty \int_0^\infty \phi(V)\phi(v) v \sigma(v) \, dV \, dv. \]  

(4.6)

Since the normalization condition is

\[ \int_0^\infty \phi(V) dV = 1 \]  

(4.7)

and eq. 4.2 defines \(\phi(v)\), eq. 4.6 can be re-expressed as,

\[ <\sigma v> = 4\pi \left( \frac{\mu_{ij}}{2\pi k_B T} \right)^{3/2} \int_0^\infty v^3 \sigma(v) \exp\left(\frac{-\mu_{ij} v^2}{2 k_B T}\right) \, dv. \]  

(4.8)

Writing this in terms of the center-of-mass energy, \(E = 0.5\mu_{ij} v^2\),

\[ <\sigma v> = \left( \frac{8}{\pi \mu_{ij}} \right)^{1/2} \frac{1}{(k_B T)^{2/3}} \int_0^\infty \sigma(E) E \exp\left(\frac{-E}{k_B T}\right) \, dE. \]  

(4.9)
Reactions can be either resonant or non-resonant. Resonant reactions occur when the compound nucleus \((i+j)\) has an energy state which matches the energy in the entrance channel. Since the energy matching associated with a resonant reaction produces a spike in the cross section, resonances are not smoothly varying with energy. Non resonant reactions on the other hand are smoothly varying with energy, and so are safe to describe with the \(S(E)\) factor formalism of chapter 3.

In stellar environments when heavy ion fusion takes place it typically produces a compound nucleus. In this picture a target and projectile interact, forming an intermediate nucleus which is composed of all of the target and projectile nucleons. The energy from the reaction is distributed evenly over the compound nucleus, producing excitations. The excitations correspond to resonances in the compound state. Typically the resonances form a continuum of energy states, such that all resonances contribute to the cross section. This is a statistical process (discussed in sec. 5.1.2), producing a smooth cross section which is not dominated by any individual resonance. Since the cross section is smooth, substituting eq. 2.14 in to eq. 4.9 the reaction rate per particle pair can be expressed in terms of the astrophysical \(S(E)\) factor,

\[
<\sigma v> = \left(\frac{8}{\pi \mu_{ij}}\right)^{1/2} \frac{1}{(k_B T)^{2/3}} \int_0^\infty S(E) \exp \left(-\frac{E}{k_B T}\right) \exp \left(-\frac{E_G}{E}\right)^{1/2} dE \quad (4.10)
\]

where \(E_G\) is the Gamow energy. Physically \(E_G\) represents the energy required to tunnel through the Coulomb barrier and is given by \(E_G = \sqrt{2\mu_{ij} \pi Z_i Z_j e^2 / \hbar}\). The probability to tunnel through the barrier is proportional to \(\exp(-\sqrt{E_G / E})\).

The product of the Maxwell-Boltzmann distribution and the probability to tunnel through the Coulomb barrier is plotted in fig. 4.2. The peak of the velocity distribution is typically at low energies, corresponding to where the probability of Coulomb barrier tunneling is lowest. At higher energies however the probability of
Coulomb barrier tunneling is much greater, but typically few particles have high velocities. The peak of the products is at an energy of $E_{ij}^{pk} = \left(0.5 \ E_{G}^{1/2} k_B T\right)$.

Figure 4.2. Dependence of the reaction cross section for charged particles as a function of energy, taken from ref.[84]. The left curve shows the Maxwell-Boltzmann distribution, the right curve shows the probability to tunnel through the Coulomb barrier. The sum of these two curves give the central line, which defines the effective burning window. The peak of this curve is $E_{ij}^{pk}$. 
The width of the burning window is given by $\Delta E_{ij}^{pk}$. The width can be approximated by a Gaussian of form,

$$
\exp \left( -\frac{E}{k_B T} \frac{E_{ij}^{1/2}}{E_{ij}^{1/2}} \right) \approx I_{max} \exp \left( -\frac{E - E_{ij}^{pk}}{0.5 \Delta E_{ij}^{pk}} \right)^2,
$$

where $I_{max}$ is the height of the peak,

$$
I_{max} = \exp \left( -\frac{3E_{ij}^{pk}}{k_B T} \right),
$$

and $\Delta E_{ij}^{pk}$ is given by

$$
\Delta E_{ij}^{pk} = \frac{4}{\sqrt{3}} \left( E_{ij}^{pk} k_B T \right)^{1/2}.
$$

The area of the peak is given by roughly the height multiplied by the width,

$$
I_{max} \Delta E_{ij}^{pk} = \frac{4}{\sqrt{3}} \left( E_{ij}^{pk} k_B T \right)^{1/2} \exp \left( -\frac{3E_{ij}^{pk}}{k_B T} \right).
$$

Substituting eq.4.14 as the integral in eq.4.10 the non-resonant thermonuclear reaction rate per particle pair is given by,

$$
< \sigma v > = 4 \sqrt{\frac{2E_{ij}^{pk} S(E_{ij}^{pk})}{3 \mu_{ij}}} \left( E_{ij}^{pk} k_B T \right)^{1/2} \exp \left( -\frac{3E_{ij}^{pk}}{k_B T} \right).
$$

Using eq.4.15 in eq.4.4 the thermonuclear reaction rate can be expressed as,

$$
R_{ij}^{th} = \frac{4n_i n_j}{1 + \delta_{ij}} \left( \frac{2E_{ij}^{pk}}{3 \mu_{ij}} \right)^{1/2} S(E_{ij}^{pk}) \frac{S(E_{ij}^{pk})}{k_B T} e^{-\tau_{ij}}
$$

where $\tau_{ij} = 3E_{ij}^{pk} / (k_B T)$.
4.2 Physical Conditions

Following the definitions laid out in [104] and taking as a starting point stellar matter composed of fully ionized nuclei immersed in a degenerate electron background, the total number density of nuclei (i.e., excluding free neutrons) can be expressed as,

\[ n = \sum_j n_j \] (4.17)

where \( j \) represents a multicomponent matter, composed of ion species \( j = 1, 2, 3, \ldots \), each with mass \( A_j \) and charge \( Z_j \). The number density of each ion species is related to the mass density through the relation

\[ n_j = \rho \frac{N_A X_j}{A_j} = \rho N_A Y_j, \] (4.18)

where \( N_A = 6.02 \times 10^{23} \text{ mol}^{-1} \), \( X_j \) is the mass fraction and \( Y_j \) the abundance of species \( j \). The electron number density is given by

\[ n_e = n < Z >, \] (4.19)

where the mean charge of the nuclei is defined through the fractional number, \( x_j \), as

\[ < Z > = \sum_j x_j Z_j \] (4.20)

and

\[ x_j = \frac{X_j/A_j}{\sum_i X_i/A_i}. \] (4.21)
For completeness, average mass of the ions is defined as,

$$< A > = \sum_j x_j A_j. \quad (4.22)$$

Assuming that all of the nucleons are inside the ions, the total mass density contained with in the ions is,

$$X_N = \sum_j X_j \approx 1. \quad (4.23)$$

This is a good assumption for $\rho \lesssim 6 \times 10^{11} \text{ g cm}^{-3}$, but as the mass density increases beyond the neutron drip density, $X_N < 1$. Practically speaking, $X_N$ can be found by summing the abundances of each ion multiplied by the mass number, then subtracting the abundance of neutrons.

In order to maximize inter-ion separation as $\rho$ increases, the nuclei will arrange themselves in a lattice with sites dictated by the equilibrium between electrostatic repulsion and matter compression. Partitioning the stellar matter into 3-D cells of charge neutrality, a sphere constructed around ion $j$ with charge $Z_j$ has a radius of

$$a_j = \left( \frac{3}{4\pi n_j} \right)^{1/3}, \quad (4.24)$$

since $1/n_j$ is the volume of such a sphere.

The average equilibrium distance between neighboring ion pairs $i$ and $j$ can be approximated by

$$a_{ij} = \frac{a_i + a_j}{2}, \quad (4.25)$$

which means that the total ion number density (in oppose to the species number
density, Eq. [4.18] is

\[ n_{ij} = \frac{3}{4\pi a_{ij}^3}. \]  

(4.26)

It is very helpful to follow other works (for example [89]) and introduce a dimensionless coupling parameter which measures the ratio of the inter-ion electrostatic energy to the thermal energy. In this context \( \Gamma_{ij} \) is defined, where \( k_B = 8.617 \times 10^{-11} \) MeV K\(^{-1} \), as

\[ \Gamma_{ij} = \frac{Z_i Z_j e^2}{a_{ij} k_B T}. \]  

(4.27)

The physical state of the ions can be characterized by the value of \( \Gamma_{ij} \). When \( \Gamma_{ij} << 1 \), temperature effects are dominant and the stellar matter behaves as an ideal Maxwell-Boltzmann gas. Conversely when \( \Gamma_{ij} > 1 \), electrostatic energy is more dominant and the matter can be regarded as a strongly coupled quantum system, manifest as a dense electrostatic lattice.

Transition from thermal to electrostatic domination is smooth, without any phase transitions [104]. The stellar matter transitions from a gas to a Coulomb liquid at a temperature

\[ T_L = \sum_j k_B Z_i Z_j e^2 a_{ij}, \]  

(4.28)

shown in Fig. 4.1. With decreasing temperature (increasing \( \Gamma_{ij} \)) the ions can no longer be considered at classical system. The nuclei form a plasma at the Debye temperature,

\[ T_{ij}^p = \frac{\hbar \omega_{ij}^p}{k_B}, \quad \omega_{ij}^p = \sqrt{\sum_j \frac{4\pi Z_i Z_j e^2 n_{ij}}{2\mu_{ij}}}, \]  

(4.29)

the critical point at which the specific heat of the material is given by nuclei oscillations, of frequency \( \omega_{ij}^p \), rather than from free thermal motion.

Increasing \( \Gamma_{ij} \) further (\( \Gamma_{ij} > 1 \)), by either a reduction in temperature, an increase
in mass density, or both, causes the stellar matter to crystallize into a rigid Coulomb lattice. The solidification temperature needed to realize this is

\[ T_m = \frac{Z_i Z_j e^2}{a_{ij} \Gamma_{ij,m}}, \]  

(4.30)

where \( \Gamma_{ij,m} \approx 175 \) according to ref \[22\].

 Though the nuclei are frozen into a stiff lattice, they still experience zero point motion about their lattice sites with a frequency given by \( \omega_p^p \) and an energy of \( \sim \hbar \omega_p^p \) \[86\]. Since the mass density of the lattice is great, \( \rho \approx \times10^{10} \text{ g cm}^{-3} \) for \(^{12}\text{C}\) according to fig. 4.1, the small zero point oscillations are enough to allow the neighboring nuclear wave-functions to overlap, illustrated in fig 4.3. This action results in a nuclear reaction, which is thermally independent but sensitive to mass density. Such reactions are known as pycnonuclear reactions. This class of heavy ion fusion has the dual characteristics of proceeding under high density, and very low temperature - the specific prescription for deep crusts of neutron stars.

4.2.1 Classical Thermonuclear Regime

Illustrated in fig 4.1 is the effect of temperature and density on the \(^{12}\text{C}+^{12}\text{C}\) reaction rate. At \( \rho \lesssim 10^9 \text{ g cm}^{-3} \) the rate is nearly flat, indicating not only a strong dependence on \( T \), but also an insensitivity to \( \rho \). At higher densities however these dependencies are completely reversed - the sharp knee at \( \rho \lesssim 9.5 - 10.5 \times10^{10} \text{ g cm}^{-3} \) represents the domain in which the reaction rate has almost no temperature dependence, but is acutely affected by density, reflected by the near vertical line at densities greater than this region.

As discussed in the sec. 4.2, the classical thermonuclear regime, pictured in red in fig 4.1 is where \( \Gamma_{ij} \ll 1 \). The nuclei are fully stripped, and there is a small screening effect from the background electron gas. The bulk matter behaves as an
Figure 4.3. Top: Nuclei in the thermonuclear regime move freely as an ideal gas. Bottom: With increasing $\Gamma_{ij}$, ions are frozen out into an electrostatic lattice. Vibrations of either excited state or ground state ions, depending on the value of $\Gamma_{ij}$, cause nuclear wave-function overlap, and give rise to pycnonuclear reactions.
ideal gas [27]. This burning domain is associated with most stellar burning regimes.

Under these conditions heavy ion fusion takes place at an energy given by the peak of sum of the Maxwell - Boltzmann distribution and the Coulomb barrier penetration, shown in fig [4.2] [84]. The non-resonant reaction rate for this process is defined by eq. 4.16.

Since

\[ E_{pk}^{ij} = \left( \frac{\sqrt{E_G k_B T}}{2} \right)^{2/3}, \]

(from sec. 4.1.1), \( \tau_{ij} \) can be rewritten as

\[ \tau_{ij} = \left( \frac{27 \pi^2 \mu_{ij} Z_i^2 Z_j^2 e^4}{2k_B Th^2} \right)^{1/3}. \]

Introducing parameters \( P_{th} \) and \( F_{th} \) defined as

\[ P_{th} = \frac{8\pi^{1/3}}{3^{1/2} 2^{1/3}} \left( \frac{E_G}{k_B T} \right)^{2/3}, \quad F_{th} = e^{-\tau_{ij}} \]

allows Eq [4.16] to be factorized in to the form

\[ R_{th}^{ij} = \frac{n_i n_j}{1 + \delta_{ij}} S(E_{pk}^{ij}) \frac{r_{Bi}}{\hbar} P_{th} F_{th}, \]

where \( r_{Bi} \) is the Bohr radius, expressed as

\[ r_{Bi} = \frac{h^2}{2\mu_{ij} Z_i Z_j e^2} \text{ cm}. \]

For the case when \( i = j \), \( Z_i = Z_j \), \( \mu_{ij} \to \mu_i = (\text{m.u.}A_i)/2 \) and so \( r_{Bi} \to r_{Bi} = h^2/(\text{m.u.}A_i Z_i^2 e^2) \) cm.

The main contribution to the classical thermonuclear reaction rate is from particles with energy greater than \( k_B T \) (see fig. 4.2).
4.2.2 T=0 Kelvin Pycnonuclear Regime

The other end of the stellar environment spectrum occurs when $\Gamma_{ij} >> 1$. Physically this condition is met when thermal energies are negligible compared to electrostatic energies. Generally speaking, $\Gamma_{ij} >> 1$ when $\rho$ is very large, and $T$ is very small such that the lattice crystallizes in to a solid. In this region, displayed in green in fig. 4.1, $T << T_p$. In this domain all nuclei are in the vibrational ground state. Reactions now are possible only between closest pairs, owing to zero point motion. Because these rates have no temperature dependence, they are henceforth referred to T=0 pycnonuclear rates. The form of these reactions are presented in sections 4.4.1 and 4.4.2.

4.2.3 Thermonuclear Burning with Strong Electron Screening

Shown in blue on fig. 4.1 the thermonuclear burning with strong electron screening operates in the temperature domain $T_p \ll T \lesssim T_L$. Coulomb barrier screening between the reacting ions is provided by the degenerate electron background. This region constitutes a colder, denser plasma where the ions are strongly coupled classical Coulomb lattice embedded in a strongly degenerate electron gas ($\Gamma_{ij} \approx 1$). At temperatures greater than $T_L$ the ions are in a liquid phase.

Since most of the nuclei are bound into lattice sites and, generally, $E_{ij}^{pk}$ is greater than the thermal energy, reactions mainly take place between the few unbound, very energetic nuclei. These nuclei are still able to move with relative ease though the lattice. There are however some reactions between nuclei in the lattice, since the electron background, as well as the neighboring spectator nuclei, shield slightly the Coulomb barrier of reacting pairs, enhancing the reaction rate from that given in eq.4.34. The enhancement factor is a function of the plasma potential formed from the ensemble of ions. The plasma potential itself is highly uncertain, and in reality
is not isotropic. Though the exact plasma potential is a thorny subject, Monte Carlo simulations of the plasma sampled for radial pair separation distributions can be used to provide an estimate for the plasma potential \[104\]. This approach assumes that the plasma potential is static and spherically symmetric during a fusion reaction \[23\].

### 4.2.4 Thermo-pycnonuclear Regime

There is a narrow domain in the \(\rho - T\) plane of fig 4.1 which separates the thermonuclear regimes from the pycnonuclear regions. This transitional region is realized at \(\Gamma_{ij} \gtrsim 1\), and occurs at \(T_m \lesssim T \lesssim T_p\).

Much like the strongly screened thermonuclear regime, this intermediate region consists of nuclei embedded in a highly degenerate electron gas. At temperatures greater than \(T_m\), the nuclei form a solid lattice. For pure \(^{12}\)C matter this occurs at \(T \approx 6 \times 10^6\) K, \(\rho \approx 3.1 \times 10^6\) g cm\(^{-3}\).

Reaction rates between nuclei in this region are strongly promoted by the charge screening electron background. Since the vast majority of the nuclei are now bound into deep lattice sites, reactions mostly occur between highly thermally excited bound nuclei, which oscillate with a frequency greater than the plasma frequency, and an energy greater than the zero point energy of \(\approx \hbar \omega_{ij}^p\) (where \(\omega_{ij}^p\) is defined by eq 4.29).

### 4.2.5 Thermally Enhanced Pycnonuclear Regime

When \(\Gamma_{ij} > 1\), all of the nuclei are bound into an electrostatic lattice. Not all nuclei occupy their vibration ground states however, since there is enough thermal energy compared to electrostatic energy to produce some bound highly excited state nuclei. It is reactions occurring between neighboring pairs of these excited ions that
is the major component to the reaction rate.

Though it is possible for the lattice to exist in a liquid state if $T > T_m$, it is most likely a strongly coupled quantum Coulomb lattice in this burning domain.

4.3 Lattice Considerations

An interesting (and open question), is the type of lattice which the nuclei form; specifically whether it is face centered cubic (FCC), body center cubic (BCC), or something else altogether. Recent work by Horowitz [47] using 27,648 nuclei representative of a realistic x-ray burst ash abundance distribution (though it did not contain nuclei with $Z < 8$) showed that as $\Gamma_{ij}$ is increased, the nuclei do indeed form crystalline planes, with a solid-liquid phase separation, and an accompanying chemical separation. It was observed that a solid lattice crystallizes above a liquid ocean. The liquid phase is greatly enriched with lighter $Z$ nuclei (particularly oxygen and although their simulation did not contain carbon, carbon could potentially become highly enriched in the liquid ocean), compared to the solid crust. Current thinking suggests that (at least for a pure plasma) a BCC lattice is the most likely, since this maximizes the distance between neighbors and so minimizes the electrostatic energy. Unless otherwise stated, a BCC lattice structure has been adopted throughout the heavy ion fusion calculations.

Another uncertainty is the the response of the lattice to the reaction taking place. Will the lattice remain statically ordered during the reaction or dynamically reorder during the tunneling event? These two possibilities impact the Coulomb barrier penetration, since the equilibrium distance between neighbors and reactants is different for these two scenarios.

An additional uncertainly in the lattice arises from imperfections and dislocations in the structure. This aspect could strongly affect the classical pycnonuclear
and thermally enhanced pycnonuclear domains, where the nuclei cannot move freely. Any dislocation is likely to change the number of nuclei packed into a region compared to what there would have been were the lattice to have remain perfectly periodical \[86\]. The net result would be a significant enhancement or suppression of the reaction rate.

It is difficult to put an estimate on the uncertainties arising from these considerations. Parameters which represent the limitations of our understanding can be built into an analytic expression for pycnonuclear reaction rates however. Varying the values of such parameters amounts to mapping the uncertainty in the fusion rates.

4.4 Formulation of Pycnonuclear Reactions

Historically authors have tackled the problem of deriving a pycnonuclear reaction rate by considering a one component plasma (OCP). This type of plasma is composed entirely of one nuclear species, \(i\), of charge \(Z_i\) and mass \(A_i\). This approach is suitable for a site such as the C-O core of a white dwarf, where, owing to the Coulomb barrier, the predominant reaction is C+C. A site such as a neutron star crust however is a multi component plasma (MCP), composed of many different species which are assumed to be isotropically mixed. Arguments developed for a OCP environment however can be extended to a multi component plasma (MCP), with some consideration for building in averaged quantities.

4.4.1 One Component Plasmas

The first authors to solve the problem of OCP pycnonuclear reactions in a robust manner were Salpeter and Van Horn in 1969 \[86\]. They derived the rate by firstly using the WKB approximation for the wave-functions of the reacting nuclei, and
then finding the transmission coefficient for barrier tunneling assuming two different approximations for the lattice potential. These two approximations correspond to a “static” or “relaxed” lattice. In the former all nuclei, as well as the center of mass of the reacting pairs, can be regarded as frozen in their respective lattice sites. In the latter the center of mass can be regarded as static, but surrounding nuclei can arrange themselves to minimize electron static energy after the reaction. The first approximation will underestimate the lattice potential and consequently the rate (since the average separation will larger than before the reaction), the second approximation will overestimate the rate (since the average separation will be less than before the reaction). Logically, the most likely lattice response is neither of these two options, but instead a dynamical motion to maintain equilibrium distances. These two approximations represent the maximum and minimum potentials, giving some estimate for the error of the lattice potential.

For a lattice composed entirely of species \( i \), constructed with a given packing structure, there are \( \nu_i \) closest neighbors. The pycnonuclear reaction rate between neighbors can be written as

\[
R_{\text{pyc}}^i = \frac{n_i}{2} < \nu_i p_i >_{av} \cdot cm^{-3} sec^{-1},
\]

where \( p_i \) is the reaction rate between a fixed pair of nuclei. The “av” subscript arises from performing the calculation over an ensemble of pairs. For a BCC lattice, \( \nu_i \) is eight, for an FCC lattice it is twelve.

Defining \( p_i \) as the product of the incoming flux, barrier transmission probability, and the probability that tunneling will lead to a given reaction (the \( S(E) \) factor), Salpeter and Van Horn wrote the \( T=0 \) OCP pycnonuclear rate as

\[
p_i = D_{\text{pyc}} \lambda_i^{3-C_{pl}} S(E^{pk}_i) \cdot \exp \left( \frac{-C_{exp}}{\lambda_i^{1/2}} \right) \cdot sec^{-1},
\]

73
where they assumed that $X_N = 1$. The quantity $D_{pyc}$ is a dimensionless parameter, representing the two extreme approximations for the lattice potential that was used in the WKB approximation.

The quantity $\lambda_i$ is the ratio of the Bohr radius to the lattice spacing. Physically, $\lambda_i$ introduces a density independence. The functional form of $\lambda_i$ is given by,

$$
\lambda_i = r_{Bi} \left( \frac{n_i}{2} \right)^{1/2} = \frac{1}{A_i Z_i^2} \left( \frac{1}{A_i} \frac{\rho X_N}{\gamma 6.7585 \times 10^{10} \text{gcm}^{-3}} \right)^{1/3},
$$

(4.38)

where $\gamma$ is the number of ions in a unit cell (this is 4 for a FCC lattice - an eighth of an ion from each corner, and half an ion from each face - and 2 for a BCC lattice - an eighth of an ion from each corner plus one whole ion in the center).

Substituting in the equation for the Bohr radius, eq. [4.35], and the reduced mass, eq. [4.5], and making a unit change to cm$^{-3}$ sec$^{-1}$, eq. [4.37] can be written numerically as

$$
R_{SVH}^i = C_{pyc} \times 10^{46} \rho X_i A_i Z_i^4 S(E_{pk}^i) \lambda_i^{7/4} \cdot \exp \left( \frac{C_{exp}}{\lambda_i^{1/2}} \right) \text{cm}^{-3} \text{sec}^{-1}.
$$

(4.39)

Uncertainty due to the lattice response to tunneling (static or relaxed) and lattice type, BCC or FCC, have been rolled into the dimensionless parameters $C_{pyc}$ and $C_{exp}$. The values of these parameters are given in table [4.1].

The typical reaction energy of the interaction nuclei is on the order of the plasma frequency multiplied by $\hbar$: $E_{pk}^i \approx \hbar \omega_i$.

4.4.2 Multi Component Plasma

After an X-ray burst has occurred, the results of Schatz et al [87] (plotted in fig. 1.3, and discussed in sec. 1.3.2) indicate that the ashes are composed of many different nuclei, such that reacting pairs must be described by $i$ and $j$. Consequently
the ingredients of the neutron star crust cannot be thought of as a OCP. In the context of realistic X-ray burst ashes, eq. 4.39 is clearly unsuitable. However eq. 4.39 can be generalized to an MCP plasma by performing modifications which rescale the inter-ion separations. In the discussion which follows, it has been assumed that the crust composition has a homogeneous distribution. It was touched on in sec. 4.3 that results from Horowitz [47] indicate that the ions may not distribute homogeneously however, instead it is possible that they form regions of enrichment and depletion. In this case the formalism presented here would have to be modified to reflect that the local lattice potentials cannot be described generally, and that averaged quantities, defined by eqs. 4.20 and 4.22 cannot be used.

Using the Bohr radius as defined by Eq. 4.35, dimensionless parameter $\lambda_i$ becomes $\lambda_i \rightarrow \lambda_{ij}$:

$$\lambda_{ij} = r_{B_{ij}} \left( \frac{n_{ij}}{2} \right)^{1/3} = \frac{A_i + A_j}{A_i A_j Z_i Z_j (Z_i^{1/3} + Z_j^{1/3})} \left( \frac{\rho X_N < Z >}{\gamma} \right) \left( \frac{6.785 \times 10^{10} \text{ g/cm}^3}{gcm^{-3}} \right)^{1/3}.$$  \hspace{1cm} (4.40)

The average ion charge and mass, $< Z >$ and $< A >$ are defined in eqs. 4.20 and 4.22.

From eq. 4.36, the pycnonuclear reaction rate for a MCP is

$$R_{ij}^{\text{pyc}} = \frac{n_i}{1 + \delta_{ij}} < \nu_{ij} p_{ij} >_{av} \text{ cm}^{-3} \text{ sec}^{-1},$$  \hspace{1cm} (4.41)

where $\nu_{ij}$ is the number of nearest nuclei $j$ around nucleus $i$. Following [74], for an isotopic distribution the number of ions $j$ around nuclei $i$ is given by the ratio of the number density of $j$ to the total number density, multiplied by the number of neighbors $i$ has,

$$< \nu_{ij} >_{av} = \frac{\binom{n}{2} n_j}{n}.$$  \hspace{1cm} (4.42)
The top number in the bracket refers to a uniformly mixed BCC lattice, the bottom to a uniformly mixed FCC lattice.

In eq. 4.41, \( p_{ij} \) gives the reaction rate per pair per second. Generalizing eq. 4.37, \( p_{ij} \) is given by,

\[
p_{ij} = D_{pyc} \frac{\lambda_{ij}^{3-C_{pl}} S(E_{pk}^{ij})}{hr_{Bij}^2} \exp \left( \frac{-C_{exp}}{\lambda_{ij}^{1/2}} \right) \text{sec}^{-1}. \tag{4.43}
\]

Substituting eq. 4.43 into eq. 4.41 yields

\[
R_{pyc}^{ij} = 4n_i n_j D_{pyc} \frac{LT < Z > S(E_{pk}^{ij}) r_{Bij}}{1 + \delta_{ij}} \frac{Z_i^{1/3} Z_j^{1/3}}{h} \frac{C_{pl}^{ij}}{\lambda_{ij}^{1/2}} \times \exp \left( \frac{-C_{exp}}{(\lambda_{ij})^{1/2}} \right) \text{cm}^{-3} \text{sec}^{-1}, \tag{4.44}
\]

where the quantity LT is again 8 for a BCC lattice, and 12 for an FCC lattice.

For numerical evaluations this can be written as,

\[
R_{pyc}^{ij} = 10^{46} C_{pyc} \frac{LT \rho X_N X_i X_j A_i A_j < A > Z_i^2 Z_j^2}{(1 + \delta_{ij})(A_i + A_j)^2} S(E_{pk}^{ij}) \lambda_{ij}^{3-C_{pl}} \times \exp \left( \frac{-C_{exp}}{\lambda_{ij}^{1/2}} \right) \text{cm}^{-3} \text{sec}^{-1}, \tag{4.45}
\]

where the \( \rho \) is expressed in g cm\(^{-3} \) and the astrophysical factor \( S(E_{pk}^{ij}) \) is in MeV b. The peak energy is \( E_{pk}^{ij} \simeq \hbar \omega_{ij} \). Eq. 4.45 recovers the OCP rate, eq. 4.39, in the event that \( i = j \). The main parameter that regulates the pycnonuclear reaction rate is \( \lambda_{ij} \), the dimensionless inverse length parameter measuring the ratio of the Bohr radius to the inter-ion spacing, since it is in the exponent argument. For sufficiently low mass densities \( \lambda_{ij} \) is very large, producing a tremendous suppression of the Coulomb barrier penetration and the pycnonuclear burning rate. With increasing \( \rho \) the barrier becomes more transparent and reaction rate increases, potentially
leading to efficient pycnonuclear burning at high densities.

Values of the dimensionless parameters used in eqs. 4.45, 4.44, and 4.39 are listed in table 4.1 for 11 different models (where s refers to static lattice, and r refers to relaxed lattice). The 11 different models correspond to 9 models from previous works, ([86], [88] and [74]) and a minimum and maximum rate proposed by [31].

The minimum and maximum rate of [31] are phenomenological models, obtained considering BCC lattice models, models 1-4 and model 9. The maximum rate is defined as a lattice which exhibits a relaxed response to a reaction, coupled with a large lattice screening potential. The values of $C_{exp}$ and $C_{pyc}$ (equal to 2.450 and 50 respectively) are set arbitrarily to include the numerical values of all other maximum BCC models from tab. 4.1 (i.e, models 2 and 3). The minimum rate of [31] on the other hand is a static response lattice, which has a low screening potential. The parameter values themselves ($C_{exp} = 2.65$, $C_{pyc} = 0.5$) were again selected with the requirement that they encompass existing models (i.e, models 1 and 4). The minimum and maximum rates represent the uncertainty in our state of the art understanding regarding lattice screening potentials and lattice reaction response.

Models 1-4 and model 9 are based in a BCC lattice; models 5-8 are for an FCC lattice. The minimum and maximum rates of [31] cover the limits of the BCC lattice. Though not used in the calculation of the rates in this thesis, the parameters $\alpha_{\omega_{ij}}$ and $\alpha_{dij}$ are listed in table 4.1 for completion. These parameters are fine-tune constants which reflect the fact that the rescaling in a MCP might not be as simple as approximating the equilibrium inter-ion spacing as the average of the two reactant ion spheres, as eq. 4.25 suggests. Instead the inter-ion sphere separation could deviate from this approximation. This could occur if the lattice is not periodic and
TABLE 4.1

COEFFICIENTS USED IN PYCNONUCLEAR REACTION RATE
FORMALISM

<table>
<thead>
<tr>
<th>No.</th>
<th>$C_{exp}$</th>
<th>$C_{pyc}$</th>
<th>$C_{pl}$</th>
<th>$C_T$</th>
<th>$\Lambda$</th>
<th>$\alpha_{\omega ij}$</th>
<th>$\alpha_{dij}$</th>
<th>Model</th>
<th>Refs.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.638</td>
<td>3.90</td>
<td>1.25</td>
<td>0.724</td>
<td>0.5</td>
<td>1</td>
<td>1</td>
<td>BCC; s</td>
<td>86, 88</td>
</tr>
<tr>
<td>2</td>
<td>2.516</td>
<td>4.76</td>
<td>1.25</td>
<td>0.834</td>
<td>0.5</td>
<td>1</td>
<td>1</td>
<td>BCC; r</td>
<td>86, 88</td>
</tr>
<tr>
<td>3</td>
<td>2.517</td>
<td>4.58</td>
<td>1.25</td>
<td>0.834</td>
<td>0.5</td>
<td>1</td>
<td>1</td>
<td>BCC; r</td>
<td>88</td>
</tr>
<tr>
<td>4</td>
<td>2.659</td>
<td>5.13</td>
<td>1.25</td>
<td>0.707</td>
<td>0.5</td>
<td>1</td>
<td>1</td>
<td>BCC</td>
<td>88</td>
</tr>
<tr>
<td>5</td>
<td>2.401</td>
<td>7.43</td>
<td>1.25</td>
<td>0.960</td>
<td>0.5</td>
<td>1</td>
<td>1</td>
<td>FCC; s</td>
<td>88</td>
</tr>
<tr>
<td>6</td>
<td>2.265</td>
<td>13.5</td>
<td>1.25</td>
<td>1.144</td>
<td>0.5</td>
<td>1</td>
<td>1</td>
<td>FCC; r</td>
<td>88</td>
</tr>
<tr>
<td>7</td>
<td>2.260</td>
<td>12.6</td>
<td>1.25</td>
<td>1.151</td>
<td>0.5</td>
<td>1</td>
<td>1</td>
<td>FCC</td>
<td>88</td>
</tr>
<tr>
<td>8</td>
<td>2.407</td>
<td>13.5</td>
<td>1.25</td>
<td>0.953</td>
<td>0.5</td>
<td>1</td>
<td>1</td>
<td>FCC</td>
<td>88</td>
</tr>
<tr>
<td>9</td>
<td>2.460</td>
<td>$1.8 \times 10^3$</td>
<td>1.809</td>
<td>0.893</td>
<td>0.5</td>
<td>1</td>
<td>1</td>
<td>BCC</td>
<td>74</td>
</tr>
<tr>
<td>10</td>
<td>2.450</td>
<td>50</td>
<td>1.25</td>
<td>0.840</td>
<td>0.35</td>
<td>1.05</td>
<td>0.95</td>
<td></td>
<td>31</td>
</tr>
<tr>
<td>11</td>
<td>2.650</td>
<td>0.5</td>
<td>1.25</td>
<td>0.738</td>
<td>0.65</td>
<td>0.95</td>
<td>1.05</td>
<td></td>
<td>31</td>
</tr>
</tbody>
</table>

regular, such that there is a fault which gives rise to either more or less ion packing in a given volume. The presence of more (or less) ions would locally distort the ion sphere radii, in which case the approximation of eq. 4.25 is too simple. Introducing a new parameter can give some estimate of how the rate changes in response to ion-sphere distortions. Though $\alpha_{\omega ij}$ and $\alpha_{dij}$ are accorded somewhat arbitrary minimum and maximum values here, they are throughout treated as unity. Changing them from unity is intended to provide some estimate of potential uncertainty in the inter-ion distances.
4.5 T=0 Pycnonuclear Rate Calculations

In order to understand the impact of the uncertainties surrounding temperature independent pycnonuclear rates, pycnonuclear reactions were calculated for three reactions. These reactions were \(^{12}\text{C}+^{12}\text{C}\), \(^{12}\text{C}+^{16}\text{O}\) and \(^{16}\text{O}+^{16}\text{O}\), calculated using eq. 4.45 and plotted in units of \(\text{cm}^{-3}\text{sec}^{-1}\). Astrophysical \(S(E)\) factors for the reactions were calculated following the prescription set out in section 3.1, where the fit parameters were taken from the tables II III and VI of ref.\[6\]. Mass fractions for \(^{12}\text{C}\) were taken to be \(X_C = 1\) for \(^{12}\text{C}+^{12}\text{C}\), \(X_C = 0.5\) for \(^{12}\text{C}+^{16}\text{O}\), and \(X_C = 0\) for the \(^{16}\text{O}+^{16}\text{O}\) calculation. In each case, \(X_N = 1\), even for mass densities greater than the neutron drip line.

Fig.4.4 shows the impact of the model uncertainties for these three reactions on a \(\log \rho \log R_{\text{pyc}}\) scale. For the two OCP plots (left and right panes), models for BCC lattices (models 1-4 and 9-11 of tab. 4.1) produce a 5 order of magnitude spread in the rate for \(^{12}\text{C}+^{12}\text{C}\), and an 8 order of magnitude spread for \(^{16}\text{O}+^{16}\text{O}\). Since the density dependence of the rates is extremely great however, with rates ranging over eighty orders of magnitude for an increase of between 2.5 and 3.5 orders of magnitude in the density, this error is not significant. Models 6 and 7 of tab. 4.1, for FCC lattices, show higher rates by \(\sim 2\) orders of magnitude for both OCP reactions. The higher rates associated with these models are a direct result of the smaller inter-ion separation for the FCC lattice compared to the BCC lattice.

There is a larger BCC model uncertainty impact for the binary ionic mixture (BIM), shown in the middle pane. Between the BCC models is a rate spread of \(\sim 14\) orders of magnitude. This arises largely from the rescaling of the inter-ion spacing. The FCC lattice shows an enhanced reaction rate, since the reaction rate, eq.4.45, depends on the exponent of the inter-ion separation through the parameter \(\lambda_{ij}\). This exponent is equal to \(\exp \left( \frac{-C_{\text{exp}}}{\lambda_{ij}^{1/2}} \right)\). As \(\lambda_{ij}\) scales as \(n_{ij}^{1/3}\) (eq.4.40), and \(n_{ij}\)
Figure 4.4. Calculation of the T=0 pycnonuclear reaction rate for three reactions, plotted on a log mass density - log reaction rate scale. The calculation was performed using eq. 4.45, where model parameters were taken from table 4.1. The $S(E)$ factors were determined from sec. 3.1.
is related the ion sphere radius by the negative cube power, (eq. 4.26), the exponent scales with the inter-ion spacing as $a_{ij}^{-1/2}$. Since FCC lattice have a smaller inter ion spacing than BCC lattices, rates are greater in FCC crystals.

The $\rho$ dependence of the T=0 pycnonuclear rates is illustrated in fig. 4.5. Pictured are fusion reaction rates, in units of cm$^{-3}$ sec$^{-1}$, for several heavy ion fusion systems, taken from table 2.1. The plotted rates range from stable systems to very neutron rich systems. Calculations for these rates were carried out using eq. 4.45, using model 1 of tab. 4.1. For each BIM the mass fractions were assumed to be $X_{\text{target}} = X_{\text{projectile}} = 0.5$, and $X_N$ was assumed to be 1 throughout.

Figure 4.5. Calculation of the T=0 pycnonuclear reaction rate for some C+C, C+O, O+O (left pane), Ne+Ne,Ne+Mg and Mg+Mg (right pane) fusion systems. Calculations were performed using model 1 of tab. 4.1 and eq. 4.45.
Figure 4.5 clearly demonstrates the mass density and charge dependence of the pycnonuclear rates. The strength of \( \rho \) dependence comes about since the exponent in eq. 4.45 scales not only with negative cube of the inter ion spacing, but also with \( \rho^{-1/6} \). Coulomb barrier repulsion is reflected in the figure; reaction rates between lower Z nuclei (for instance C+C, C+O and O+O) are higher than those between heavier Z nuclei (Ne+Ne, Ne+Mg, Mg+Mg). Reaction rates between nuclei with large \( A \) (e.g., \( ^{28}\text{O}+^{28}\text{O} \)) are also higher than reaction rates between lower \( A \) nuclei (e.g., \( ^{16}\text{O}+^{16}\text{O} \)). This effect is due to the mass dependence of \( \lambda_{ij} \) in the exponential, which scales with the compound nucleus mass as \( A_c^{-1/2} \).

Where the \( S(E) \) factor is very large, such as for \( ^{40}\text{Ne}+^{46}\text{Mg} \) where \( S(0) = 4.396 \times 10^{74} \text{ MeV b} \), the rate at sufficiently high density (in this case \( \sim 2 \times 10^{12} \text{ g cm}^{-3} \)) becomes greater than that involving lower Z nuclei. This highlights the importance of knowing the \( S(E) \) factor at extremely low energies, specifically the reality of hindrance and the behavior of the \( S(E) \) factor at very low energy.

4.6 Single Analytic Approximation

As the X-ray burst ashes descend through the neutron star crust, they are exposed to increasing density. From the surface of the star to the inner crust the processed ashes are expected to traverse all five burning regimes, depicted by the \( ^{12}\text{C} \) ignition curve in fig. 4.1. Since the ashes are exposed to a smoothly changing \( T-\rho \) plane, it is more useful to have a single analytic reaction rate expression which can reproduce the subtleties of individual domains and can be used in real time network solvers.

Since it is the Coulomb barrier tunneling parameter which is of the most importance in all regions, it is crucial to build an expression for this parameter which can yield the known forms in different \( \rho \) and \( T \) limits. Taking as a starting point the
classical thermonuclear regime, the Coulomb barrier parameter is given in eq. 4.34 by;

$$F_{th} = exp(-\tau_{ij}),$$  \hspace{1cm} (4.46)

which was defined previously as eq. 4.33.

With increasing \( \rho \), the shielding effects of plasma and electron screening become more significant, promoting the reaction rate by many orders of magnitude. The screening effect increases exponentially with temperature and density, modifying eq. 4.46

$$F_{th} = exp(-\tau_{ij}) \cdot exp(h_{ij}),$$ \hspace{1cm} (4.47)

where \( h_{ij} \) is the plasma screening for reaction between nuclei \( i \) and \( j \). It has been defined by ref. [104] as

$$h_{ij} = \frac{C_{ij}^{sc}\Gamma_{ij}^{3/2}}{\left(\left(C_{ij}^{sc}/\phi_{ij}\right)^4 + \Gamma_{ij}^2\right)^{1/4}},$$ \hspace{1cm} (4.48)

using unitless parameters \( C_{ij}^{sc} \) and \( \phi_{ij} \). These parameters in turn are dependent on the charges of the reactants and the compound nucleus, and the average charge of the plasma (assuming a uniform distribution) and are given by,

$$C_{ij}^{sc} = 0.9 \left(Z_c^{5/3} - Z_i^{5/3} - Z_j^{5/3}\right) \frac{Z_i^{1/3} + Z_j^{1/3}}{2Z_iZ_j},$$ \hspace{1cm} (4.49)

and

$$\phi_{ij} = \left(\frac{3 < Z^2 > (Z_i^{1/3} + Z_j^{1/3})^3}{8 < Z > Z_iZ_j}\right)^{1/2},$$ \hspace{1cm} (4.50)

respectively.
Turning next to the thermally enhanced pycnonuclear regime, the probability of a nuclei occupying quantum excited state is given by [86],

\[
\text{probability} = \exp\left(-\Lambda \frac{\hbar \omega_p}{k_B T}\right) = \exp\left(-\Lambda \frac{T_p}{T}\right) \quad (4.51)
\]

where the value of \( \Lambda \) is given in table 4.1 as 0.5 under most conditions, but as high as 0.65 to minimize the reaction rate, and as low as 0.35 to maximize the rate.

The thermal enhancement of the pycnonuclear rate (eq. 4.45) is defined by (ref.[104]) the exponent of the screening effect multiplied by the probability of being in an excited state, minus the ratio of the plasma temperature to the real temperature,

\[
F_{\text{enhance}} = \exp\left(-\Lambda \frac{T^p_{ij}}{T} + C_{sc} \Gamma_{ij} \phi e\left(-\Lambda \frac{T^p_{ij}}{T}\right)\right). \quad (4.52)
\]

Including the Coulomb tunneling term, and changing the temperature dependence of the parameters from the real temperature to a re-normalized temperature, eq.4.52 becomes,

\[
F = \exp\left(-\tilde{\tau}_{ij} + C_{sc} \tilde{\Gamma}_{ij} \phi e\left(-\Lambda \tilde{T}^p_{ij}/T\right) - \Lambda \frac{\tilde{T}^p_{ij}}{T}\right). \quad (4.53)
\]

The re-normalized temperature is introduced to connect the pycnonuclear regime to the classical thermonuclear region. In the former case, the energy of the ions is from zero point oscillations in the Coulomb lattice. In contrast, in the thermonuclear regime the ions posses thermal energy, equal to \( k_B T \) which comes from the thermal energy of the stellar gas. The definition of \( \tilde{T} \) is

\[
\tilde{T} = \sqrt{T^2 + C^2_{T} (T^p_{ij})^2} \quad (4.54)
\]
where \( C_T \) is a dimensionless parameter, listed in table 4.1.

Introducing \( \tilde{T} \) changes the definition of \( \Gamma_{ij} \) and \( \tau_{ij} \) accordingly:

\[
\tilde{\tau}_{ij} = \left( \frac{27\pi^2 \mu_{ij} Z_i^2 Z_j^2 e^4}{2k_B \tilde{T}^2 \hbar^2} \right)^{1/3}, \quad \tilde{\Gamma}_{ij} = \frac{Z_i Z_j e^2}{a_{ij} k_B \tilde{T}}. \quad (4.55)
\]

In the limit when \( T >> T_p \), \( \tilde{T} \rightarrow T \), \( \tilde{\Gamma}_{ij} \rightarrow \Gamma_{ij} \) and \( \tilde{\tau}_{ij} \rightarrow \tau_{ij} \).

Taking the limits of Eq. 4.53 to check that it reproduces the thermonuclear regime as well as the pycnonuclear region, when \( T >> T_p \), \( e^{-\Lambda T_{ip}} \rightarrow 1 \), \( \tilde{T} = \sqrt{T^2} \), and so \( F = \exp(-\tau_{ij}) \). This is the thermonuclear expression of Coulomb tunneling. When \( T \lesssim T_p \), the real temperature is replaced by the harmonic oscillator temperature in each of the three terms in eq. 4.53. This reproduces the thermally enhanced pycnonuclear region. Taking the limit when \( T \rightarrow 0 \), \( F = (-\tilde{\tau}_{ij}) \) and \( \tilde{T} = C_T T_{ip}^p \).

From eq. 4.45 the exponent for the classically pycnonuclear expression is \( F_{pyc} = \exp(-C_{exp}/\sqrt{\lambda_{ij}}) \). Substituting \( \tilde{T} \) in to \( \tilde{\tau}_{ij} \) of eq 4.55 and then replacing \( T_{ip}^p \) with eq. 4.29 and using the definition of \( \lambda_{ij} \), eq 4.40

\[
\tilde{\tau}_{ij} = 3 \left( \frac{\pi}{\lambda_{ij}} \right)^{1/2} \frac{1}{27/6 C_T^{1/3}}. \quad (4.56)
\]

Thus \( F_{pyc} = \exp(-C_{exp}/\sqrt{\lambda_{ij}}) \), where the constant \( C_{exp} \) is given by:

\[
C_{exp} = 3\sqrt{\pi}/(27/6 C_T)^{1/3}. \quad (4.57)
\]

Having checked for the correct behavior for the exponential function in all regions, a full phenomenological expression for the reaction rate in a uniformly mixed
MCP can then be written as, 

\[ R_{ij}(\rho, T) = R_{ij}^{pc} + \Delta R_{ij}(\rho, T), \quad \Delta R_{ij}(\rho, T) = \frac{n_i n_j S(E_{ij}) r_{Bij}}{1 + \delta_{ij}} P F \quad \text{cm}^{-3} \text{s}^{-1}, \]

\[(4.58)\]

where \( F \) is defined by eq. 4.53. The factor \( P \) comes from generalizing eq. 4.33 and is equal to

\[ P = \frac{8\pi^{1/3}}{3^{1/2}2^{1/3}} \left( \frac{E_G}{k_BT} \right)^\gamma; \]

\[(4.59)\]

where \( \gamma \) is a dimensionless parameter which connects the thermonuclear reaction rate pre-exponent constants to the pycnonuclear reaction rate pre-exponent constants. It can be found from the expression,

\[ \gamma = \frac{T^2 \gamma_1 + (T_{ij}^p)^2 \gamma_2}{T^2 + (T_{ij}^p)^2} \]

\[(4.60)\]

where \( \gamma_1 = 2/3, \gamma_2 = (2/3)(C_{pl} + 0.5) \).

For practical applications (such as network coding, required in eq. 5.8 of chapter 5) perhaps more useful than eq. 4.58, is the stellar reaction rate, which is in units of \( \text{cm}^{-3} \text{g}^{-1} \text{sec}^{-1} \). Expressing eq. 4.58 in terms of the stellar reaction rate,

\[ N_A < \sigma v > = \frac{R_{ij}(T, \rho) A_i A_j}{\rho^2 N_A X_i X_j} \quad \text{cm}^{-3} \text{g}^{-1} \text{sec}^{-1}. \]

\[(4.61)\]

The effective reaction energy at which \( S(E_{ij}^{pk}) \) is evaluated also has to be a composite of terms which collapse to give the correct expression in all regions. Specifically, in the thermonuclear regime, \( E_{ij}^{pk} \) is equal to

\[ E_{ij}^{pk} = \frac{T k_B \tau_{ij}}{3}, \]

\[(4.62)\]
and in classical pycnonuclear region the reaction energy must be given by the zero
point motion of the nuclei,

\[ E_{ij}^{pk} = \hbar \omega_{ij}^p. \] (4.63)

In the thermally enhanced regime the reaction energy must include a term which
rises with increasing temperature, and a term which reflects the excitation energy
of the nuclei as they start to become unbound,

\[ E_{ij}^{enh} = \hbar \omega_{ij}^p + \frac{Z_i Z_j e^2}{a_{ij}} \exp \left( -\Lambda \frac{T_{ij}^p}{T} \right). \] (4.64)

Combining eqs. 4.62, 4.63 and 4.64, the reaction energy is

\[ E_{ij}^{pk} = \hbar \omega_{ij}^p + \left( \frac{Z_i Z_j e^2}{a_{ij}} + \frac{k_B T \tau_{ij}}{3} \right) \exp \left( -\Lambda \frac{T_{ij}^p}{T} \right). \] (4.65)

4.7 T-\( \rho \) Nuclear Burning

Having established the framework for calculating rates as a function of mass
density and temperature for all burning regimes, it is now possible re-examine the
fusion reactions \( ^{12}\text{C}+^{12}\text{C} \), \( ^{12}\text{C}+^{16}\text{O} \), \( ^{16}\text{O}+^{16}\text{O} \) and extend the treatment of section
4.5 to include temperature effects.

Shown in fig. 4.6 is the temperature dependent reaction rate for these three
reactions, calculated with eq. 4.58. To see effect of the temperature, the density
was kept constant, at \( \rho = 5 \times 10^9 \text{ g cm}^{-3} \). The \( \text{S}(E) \) factors were obtained using the
formalism set out in sec. 3.1 where the reaction energy as a function of temperature
was obtained with eq. 4.65. Model parameters for eq. 4.58 were taken from table 4.1.

In all three panes of fig. 4.6 at temperatures lower than \( \sim 6.3 \times 10^7 \text{ K} \) the
fusion reaction demonstrates no temperature dependence, in direct contrast to the
thermonuclear domain. This is the region of the classical pycnonuclear temperature insensitivity. Since the Coulomb tunneling term is the most dominant element in any reaction rate, changing factors which determine it have a great impact on the rate. Once the temperature has been increased beyond \( \sim 6.3 \times 10^7 \text{ K} \), further increases in temperature result in an exponential increase in the calculated rate. This is true of all three rates - for \( ^{12}\text{C}+^{12}\text{C} \) the increase is \( \sim 35 \) orders of magnitude, for \( ^{12}\text{C}+^{16}\text{O} \) it is \( \sim 45 \), and for the reaction \( ^{16}\text{O}+^{16}\text{O} \) it is \( \sim 55 \) orders. It is the crucial sensitivity of the reaction rate to both temperature and density which gives rise to the wide range of burning times for \( ^{12}\text{C} \) shown in fig. 4.1.

Figure 4.6. Reaction cross section as a function of temperature for the reactions \( ^{12}\text{C}+^{12}\text{C}, ^{12}\text{C}+^{16}\text{O} \) and \( ^{16}\text{O}+^{16}\text{O} \), calculated using eq. 4.58 with model parameters from table 4.1.
It is also clear from fig. 4.6 that the pycnonuclear domain is plagued with far more uncertainties than the thermonuclear region. Models 1 - 11 of table 4.1 produce a spread in the reaction rate of between 10 (for $^{12}\text{C}+^{12}\text{C}$) and 18 (for $^{16}\text{O}+^{16}\text{O}$) orders of magnitude. In the thermonuclear regime models 1 - 11 yield virtually indistinguishably results. The reason for this disparity is largely due to the uncertainty shrouding the plasma potential in pycnonuclear region, and the uncertainties surrounding the lattice type. At higher temperatures these details are irrelevant, as the reaction rate contribution comes entirely from the unbound, thermal ions which characterize the thermonuclear domain.

Using model 1 of table 4.1 and eq. 4.58 it is possible to map the reaction rate for a given fusion reaction for a full range of temperature and density. Shown in fig. 4.7 is the reaction rate (in units of cm$^{-3}$ sec$^{-1}$) as a function of temperature and density for $^{12}\text{C}+^{12}\text{C}$, $^{12}\text{C}+^{16}\text{O}$ and $^{16}\text{O}+^{16}\text{O}$, for all five burning regions. All three rates show qualitatively the same features, namely a strong temperature dependence of the rate at high T (the thermonuclear regime), and a strong density dependence at high $\rho$, low T (the pycnonuclear regime).

Figure 4.8 demonstrates that the main features observed in reaction rates between stable nuclei are also seen in fusion reactions between nuclei far from the valley of stability, and so one can expect that all 946 reaction in table 2.1 will have the same form.

Note that the $\rho$ scale used in figs. 4.1, 4.4, 4.5, 4.6 and 4.7 is not truly accurate however, $^{12}\text{C}$ is unstable against EC at a mass density threshold of $3.9 \times 10^{10}$ g cm$^{-3}$, $^{16}\text{O}$ is EC unstable at a threshold of $2 \times 10^{10}$ g cm$^{-3}$. Neither isotope would really exist in stellar matter above these densities. The scale however does not affect the validity of the formalism and illustrates well the features of the reaction rates. Note also that a necessary change of units, to stellar reaction rate units of
Figure 4.7. Reaction rate as a function of temperature and density for the reactions $^{12}$C+$^{12}$C, $^{12}$C+$^{16}$O and $^{16}$O+$^{16}$O, calculated using model 1 of table 4.1 and eq 4.58.
Figure 4.8. Reaction rate as a function of temperature and density for the neutron rich reaction $^{40}\text{Ne} + ^{46}\text{Mg}$, calculated using model 1 of table 4.1 and eq. 4.58.

$\text{cm}^3 \text{g}^{-1} \text{sec}^{-1}$, will decrease the calculated rates by at least 23 orders of magnitude (i.e, Avogadro’s number).
CHAPTER 5

CRUST ISOTOPIC EVOLUTION

Evaluating the contribution played by density induced heavy ion fusion requires some understanding of the other burning modes occurring in the crust. Using the formalism presented in chapter 4, as well as a realistic EC formalism, it is possible to evolve the ashes of the X-ray burst and analyze the final abundance distribution. In order to perform this, one needs not only a realistic EC formalism, but also a mechanism for predicting masses (both stable and exceedingly neutron rich), and an estimate for \((n,\gamma)\) \((\gamma,n)\) reactions on these masses.

Once these formalisms have been established, a rapid network solver is required which can evolve the X-ray burst ash isotopic distribution through the types of reactions discussed here and in chapter 4. By these means it will be possible to arrive at a state of the art understanding of deep crust composition.

5.1 Crust Reaction Channels

After the burst has occurred, the ashes begin to experience EC reactions. The process transmutes the nuclei, producing lighter \(Z\) isotopes (the process is discussed more fully in secs.1.3.2 and 2.1). This step is necessary before heavy ion fusion reactions can occur, which would otherwise be suppressed do to repulsion. Other reaction channels can also occur before and during the heavy ion burning phase. Specifically, one must treat not only pycnonuclear fusion, but also the EC reactions
which drive the abundance distribution as a function of mass density, and neutron capture and inverse photo-dissociation. In conjunction with these, a reaction path must also be included for proton and $\alpha$ capture. The contribution of the proton capture channel will be very slight however, owing to the very high Q-value of proton capture on neutron rich nuclei and the fact that the rp process will have largely exhausted the proton abundance. The $\alpha$ abundance however is not insignificant. When the rp process terminates it does so in a cycle of Sn, Sb and Te isotopes:

$$^{105}\text{Sn} + p \rightarrow ^{106}\text{Sb} + p \rightarrow ^{107}\text{Te} \rightarrow ^{103}\text{Sn} + \alpha \ [87].$$

Photo-dissociation on proton rich Te isotopes lead to a build up of $\alpha$ particles in the X-ray burst ashes.

5.1.1 EC Calculations

Since the focus of this thesis is impact of heavy ion induced fusion reactions on the abundance distribution of the neutron star crust, the development and formalism of a realistic EC model has not been carried out here. Instead the EC model adopted is that of Gupta et al [35].

The a EC rate between a parent nucleus (in state $i$) and daughter nucleus (in state $j$) is given by

$$R = \frac{\ln(2) f_{ij}(T, \rho, E_f)}{(ft_{1/2})_{ij}}. \quad (5.1)$$

The parameter $f_{ij}$ in eq. [5.1] is the phase space factor. It represents the integral over electron energy and the allowed states which can be accessed by the transition. The comparative half life is given by $(ft_{1/2})_{ij}$. This parameter is related to the nuclear transition matrix elements for transition probability, $B_{ij}$, by

$$(ft_{1/2})_{ij} = \frac{D}{B_{ij}}; \quad D = \frac{2\pi^3 \hbar^7}{g^2 m_0^2 c^4}, \quad (5.2)$$
where $m_e$ is the mass of the electron, and $c$ is the speed of light, and $g$ is the $\beta$ decay strength constant.

Gupta et al have developed a realistic picture for electron capture reactions, which was obtained by solving for the nuclear transition matrix elements between parent and excited daughter states following the formalism set out in [70]. Once determined, the transition strengths were then tabulated as a function of daughter excitation energy. The phase space in eq. 5.1 was found using the fast analytic solver of [82]. Using this method means that electron captures can be solved in real time in a reaction network simulation of the neutron star crust.

Figure 5.1. Electron capture by nucleus (Z,N) happens when the electron Fermi energy is equal to the mass difference between parent and daughter. Odd-odd daughter nucleus (Z-1,N+1) will EC to a granddaughter state, which may have an excitation level beneath Fermi energy. Neutrons may be emitted too, if the separation energy is less than the excitation energy of the state.

To maintain a realistic EC transition picture, the model of [35] used Gamow
Teller (GT) transitions (in opposed to Fermi transitions) where the daughter states were multiplied by a phase space factor \( f_{ij} \) which corresponded to the Q-value for that decay. Consequently not all excited daughter states are accessible for a given EC reaction, only those which preserve the GT selection rules. Where the excitation energy of a daughter nucleus (or in the case of fig. 5.1 the granddaughter nucleus) is greater than the neutron separation energy for 1,2...6 neutrons, EC induced neutron emission (for up to six neutrons) is allowed.

Shown in fig 5.1 (taken from [35]) is the process which brings about even-even nuclei dominance in the crust discussed in sec. 2.1. A nucleus of \( Z,N \) undergoes an EC when the electron Fermi energy reaches the negative Q-value threshold for that reaction. The daughter product, characterized by \( Z-1,N+1 \) immediately EC to a granddaughter state \( Z-2,N+2 \), since the granddaughter nucleus has an excited state below the electron Fermi energy (i.e, the Q-value for the reaction is positive).

The formalism of [35] has however not been developed to cover all nuclei which can exist in a neutron star crust. Unfortunately there are no EC rates calculated for \( A < 20 \) or \( Z < 9 \), which means that there are no EC rates to bridge the gap from oxygen to carbon. Consequently where EC capture rates were needed for the reaction network crust simulation but not supplied by [35], they were calculated assuming that the transition was parent ground state to daughter ground state where the \( \log ft \) value for the reaction, defined by eq. 5.2, was set at a standard value of 6.

5.1.2 Neutron Capture

Required \((n,\gamma)\) rates (also \((p,\gamma)\) and \((\alpha,\gamma)\) where \(\gamma\) can be \(\gamma\), neutron, proton, \(\alpha\), deuteron or tritium) were obtained from a standard reaction rate library [81]. The rates in the library have been obtained by folding theoretical cross section calculates
with the Maxwell-Boltzmann velocity distribution shown in fig. 4.2. Theoretical cross sections were calculated in the context of the Hauser-Feshbach formalism for statistical reactions for compound nuclei.

Hauser-Feshbach formalism is framework for obtaining energy-averaged cross-sections for compound reactions [42]. It is a purely statistical model, based on the idea that when a projectile and target interact they produce a compound nucleus which has many closely spaced excitation levels. The spacing of the excitation levels is referred to as the level density. The assumption that compound nuclei have high level densities is valid if the target and projectile interact at high energy (forming a compound nucleus at high energy) or if the mass number of the compound nucleus is high (the number of resonances an isotope has scales with mass). For most of the neutron star crust density range considered here (see fig. 5.3) the neutrons behave as an ideal gas, moving in the lattice with a maxwell-Boltzmann distribution of energies (shown in fig. 4.2). Though (correlated with mass density) the target nuclei can be practically stationary, the neutron energy distribution is still sufficient for the reaction energy to populate excited states in the compound nucleus. Also the vast majority of nuclei for which neutron capture rates are required have a mass greater than $A=10$. These two factors justify using the Hauser-Feshbach theory for statistical reactions, so long as the neutrons maintain a Maxwell-Boltzmann distribution.

Cross sections in Hauser-Feshbach formalism can be obtained from the transmission functions for the formation ($T_{\text{form}}$) and dissociation ($T_{\text{dia}}$)of the compound nucleus, summed over the possible angular momentum ($J$) and parity ($\pi$) of the
compound resonance states,

\[
\sigma_{HF} = \frac{\pi \hbar^2}{2 \mu_{ij} E_{ij} (2J_i + 1)(2J_j + 1)} \sum_{J, \pi} (2J + 1) \frac{T_{form}(J, \pi) T_{dis}(J, \pi)}{T_{tot}(J, \pi)}. \tag{5.3}
\]

In eq. 5.3, \(J_i(J_j)\) represents the target (projectile) angular momentum, \(E_{ij}\) is the reaction center of mass energy and \(T_{tot}\) is the total transmission function for the residual nucleus, summed over all possible energetically assessable states in the entrance channel.

Reaction rates can now be found by folding the cross sections of eq. 5.3 with the reaction rate expression of eq. 4.9.

The usefulness of standard library rates becomes unsound when the assumption of a Maxwell-Boltzmann velocity distribution is not longer valid. In the case of neutrons, the gas adopts a Fermi distribution, indicative of degeneracy, when the thermal energy is less than the Fermi energy,

\[
\frac{3}{2} k_B T \ < \ \frac{\hbar^2}{2m} \left(3\pi^2 n\right)^{2/3} \tag{5.4}
\]

where \(m\) refers to the mass, and \(n\) to the number density of neutrons. The number density can be related to the mass density and the abundance of the neutrons by eq. 4.18. This allows eq. 5.4 to be recast as

\[
\frac{3}{2} \ < \ \frac{\hbar^2}{2m} \left(3\pi^2 \rho Y_n\right)^{2/3}. \tag{5.5}
\]

Re-arranging eq. 5.5, the neutron degeneracy becomes important when neutron abundance is greater than:

\[
\frac{T}{227 \rho^{2/3}} \ < \ Y_n^{2/3}, \tag{5.6}
\]

97
where $T$ is in Kelvin, and $\rho$ is in g cm$^{-3}$.

Using $T = 0.47$ GK and $\rho = 2 \times 10^{13}$ g cm$^{-3}$ (the simulation end point values, from fig. 5.3 in sec. 5.2) neutrons are degenerate when $Y_n$ is greater than to $1.49 \times 10^{-4}$.

It will be found in chapter 6 that $Y_n$ at $\rho = 2 \times 10^{13}$ g cm$^{-3}$ is much greater than this threshold value. This finding implies that it is not strictly appropriate to use standard library rates for $(n, \gamma)$ reactions at mass densities where the neutrons can no longer be treated as an ideal gas, since this last assumption is built into the theoretical calculations. Of particular concern is the treatment of neutron capture reactions which have negative Q-values. The negative Q-value energy for the reaction would be supplied by the Fermi surface of the degenerate neutron distribution, something which is clearly missed in ideal gas distribution. The blocking of inverse $(\gamma,n)$ reactions (due to filled neutron states) would also need to be considered. As yet however a formalism suitable for this has not been developed. As such, the Hauser-Feshbach formalism and the library rates have been used for neutron capture reactions even where it could be unphysical, with the caveat that a new set of $(n,\gamma)$ reactions need to be developed as a next step.

5.1.3 Nuclear Masses

A fundamental ingredient in nuclear reaction rate calculations are the nuclear masses of the reactants involved. In terms of EC reactions, the difference between the parent and the daughter mass dictates the Q-value threshold required before the reaction can be activated. This makes EC reactions highly sensitive to nuclear mass input, since a change in mass model could result in a change in parent-daughter mass difference. This would affect the density at which a particular EC reaction is activated, and could affect the evolution of the crust abundance distribution. In
general, mass models affect the amount of energy it requires to separate a proton or neutron from a nucleus, impacting which nuclei are bound and which are unbound in the crust. This is of particular relevance for very neutron rich nuclei (it is also of importance for very proton rich nuclei, but those are not a concern in the neutron star crust environment).

Though an understanding of the impact of the mass model on crust isotopic evolution is clearly of critical importance, it is beyond the immediate scope of this thesis. Instead, the aim was to maintain a consistent mass set as input into the reaction network code. To this aim, nuclear masses were obtained theoretically, even when experimental data did exist (except for proton and neutron masses which were experimental).

In this thesis nuclear masses and ground state deformation parameters are from one of two sources, shown in fig. 5.2. Where they have been calculated, nuclear masses and deformations were provided by the finite range droplet model (FRDM) [71]. This mass calculation compilation covers a range from A = 20, Z=8 up to A = 339, Z= 136 (not all of this range was taken, only nuclei up to tin were included in the network calculations). Adoption of the FRDM mass model is in keeping with the treatment of [35], who used this mass model to develop the formalism for EC reactions described in sec. 5.1.1.

Where the masses outside of the FRDM mass model were required (for instance, $^{92}\text{Cr}$ from the pycnonuclear fusion of $^{46}\text{Mg}+^{46}\text{Mg}$ or $A < 20 \ Z < 9$) they were supplied by the analytic Hilf mass formalism [43]. These nuclei are shown in blue on fig. 5.2.
5.2 Equation of State

In order to study the heavy ion abundance distribution as a function of increasing mass density in the crust, some assumptions were made about the neutron star. Simulations were performed assuming a fixed radius (R) and mass (M) of the neutron star equal to 10 Km, and $M = 1.4 \ M_\odot$ respectively. Accretion was assumed to be spherically even over the star, with an accretion rate of $\dot{M} = 3.0 \times 10^{17} \ g \ s^{-1}$ (4 \times 10^{-9} \ M_\odot \ \text{year}^{-1})$. Local accretion was given by $\dot{m} = 2.6 \times 10^4 \ g \ s^{-1} \ cm^{-2}$. This work does not attempt to embark upon a global study of the impact of heavy ion fusion as a function of $(M, \dot{M}, R)$.

Shown in Fig.5.3 is the temperature and density profiles used for the neutron star. It was obtained from [35], where the required density profile as a function of...
radial coordinate, $r$, was obtained from the expression:

$$\rho = \rho_0 \left(1 - \left(\frac{r}{R}\right)^2\right)$$

$$\rho_0 = \frac{15}{(8\pi) R^3}$$

(5.7)

Figure 5.3. Temperature and mass density profile used to model star. This was not obtained self consistently, but from [35].

Because the radial coordinate vector points towards the surface, $\rho_0$ is defined as the density at the core of the star. It should be noted here that the thermal profile was optimized for [35] by a process of iterating over the local heat deposited in the crust due to reactions, and then reconstructing the thermal profile as a function of time from this. Strictly speaking the same process should be carried out to construct a self-consistent thermal profile in this case also. It is possible that a self consistent thermal profile would lead to a better estimate for the thermally
enhanced pycnonuclear reactions, but given the existent uncertainties in the regime (particularly due to the plasma screening) it is unlikely to improve the uncertainties significantly. Also, since Gupta et al. found that heating from the EC was fairly insensitive to the temperature, and the classical pycnonuclear reactions have no thermal sensitivity whatsoever, this profile can be adopted here.

5.3 The Reaction Network Code

The initial abundance vector was evolved a function of time \( t \), temperature and mass density using a generalized reaction network solver provided by Hix and Thielemann [45]. Since the code followed the thermal and density trajectory described in 5.2 rather than determining a dynamic profile in response to the nuclear reaction path, it is termed a post-processing solver. Though a post-processing code is simpler than the alternative, a hydrodynamic solver which determines \( T \) and \( \rho \) based on reactions which are occurring, it has some advantages. For instance, post-processing codes are typically faster than hydrodynamic codes. A second advantage is that as the uncertainty in the nuclear reaction input grows (because the abundance distribution is far from stability where the necessary data is entirely from theory) thermal trajectories could become highly unstable, causing the code to fail. Predetermined trajectories remove the likelihood of the code stalling and speed up calculations.

Abundances are evolved by the solver according to the equation,

\[
\frac{dY_i}{dt} = \sum_j N^i_j \lambda_j Y_j + \sum_{j,k} N^i_{j,k} \rho N_A <\sigma v>_{ij} Y_j Y_k + \sum_{j,k,l} N^i_{j,k,l} \rho^2 <\sigma v>_{j,k,l} Y_j Y_k Y_l,
\]

(5.8)

where the nuclear abundances of isotopes \( j, k \) and \( l \) are given by \( Y_j, Y_k \) and \( Y_l \). The
first term refers to one body reactions (i.e., EC reactions), where \( \lambda_j \) is the inverse of the mean life time of \( j \), the second term refers to two body reactions, and the third term to three body reactions. Parameters \( N_{ij}^j \), \( N_{jk}^i \), and \( N_{jkl}^i \) can be positive or negative, and indicate how many particles of species \( i \) were created or destroyed at a given time step. The heavy ion fusion reaction rate formalism developed in chapter 4 is a two body reaction. In order to use the formalism with eq. 5.8, eq. 4.61 was used as the two body reaction rate.

Time stepping in the routine was determined by an implicit solver. Practically this meant that at a given time, \( t \), the new time step, \( dt \), was found by evolving the abundances to \( t+dt \) and then testing for convergence. If convergence was not found, then the \( dt \) was halved, and the abundances were determined at \( t+dt/2 \). The abundances were then retested for convergence. If they passed, the time step was accepted, else the time step was rejected, the abundances were reset, and the process begun again. Though this method can be computationally slow, it is advantageous because in general, it allows the code to take long time steps when the reaction rates are slow. This spares the CPU from calculating the abundance unnecessarily for many times when there are no significant abundance changes.

An additional test involved checking each time step against all EC reactions occurring at that point. This was necessary because there are sharp thresholds at which EC reactions are triggered. A long time step could easily step over the fine threshold of an EC reaction, leading to either a lack of abundance flow resolution for these reactions, or worse, causing the routine to fail altogether as it fruitlessly halved the time step looking for a convergence point.

Convergence itself was defined as occurring when the sum of the abundance changes (\( \Delta Y \)) divided by the sum of the abundances at that point was less than \( 1 \times 10^{-4} \). That the sum of the mass fractions equaled 1 (with an error threshold
of $1 \times 10^{-6}$) was also checked for each time step. To solve for convergence, the Newton-Raphson method was used to find $\Delta Y$.

In order to minimize noise effects in the network, the lowest abundance which was tracked in the convergence calculation was set to a threshold of $1 \times 10^{-30}$, abundances less than this were set to zero. In order to prevent the time step from being too small however, only nuclei with abundances greater than $1 \times 10^{-8}$ were used in the time step calculation. Realistically however, abundances of less than $1 \times 10^{-14}$ should be treated with caution, because of internal precision of the computing processor.
CHAPTER 6

RESULTS OF NETWORK CALCULATIONS

Before tackling realistic X-ray burst ashes it is informative to follow in the footsteps of another author [38] and investigate the isotopic composition evolution if the crust is assumed to be composed entirely of $^{56}\text{Fe}$. This is an easier situation to investigate since it involves less isotopes and fewer reaction paths.

6.1 Pure $^{56}\text{Fe}$ Matter

Starting with $X_{^{56}\text{Fe}}=1$, a neutron star crust simulation was performed assuming a starting temperature and mass density of 0.34 GK and $2.3 \times 10^7$ g cm$^{-3}$ respectively (equivalent to a Fermi energy of $\sim 0.73$ MeV). The simulation was performed until the Fermi energy reached $\sim 36.3$ MeV (and the mass density was $2.6 \times 10^{13}$ g cm$^{-3}$, which is the end of the density profile, shown in fig. 5.3). Figure 6.1 shows a pictorial representation of the initial (top) and final (bottom) abundance distribution.

6.1.1 Analysis of Reaction Flows

Shown in fig. 6.2 is the abundance distribution as a function of time for the A=56 chain. Using FRDM masses, the initial $^{56}\text{Fe}$ is stable against EC up to a Fermi energy of 6.67 MeV. When an EC does occur, it is a GT transition from the ground state ($0^+$) of Fe to a 1+ excited state in $^{56}\text{Mn}$ at an excitation energy
Figure 6.1. Initial (top) and final (bottom) abundance distributions for a pure $^{56}$Fe simulation. At the end of the simulation the initial $^{56}$Fe composition has been evolved to a mixture of predominantly free neutrons ($Y_n = 0.934$) and $^{40}$Mg ($Y_{40Mg} = 1.156 \times 10^{-3}$), with a trace amount of $^{46}$Si ($Y_{46Si} = 8.514 \times 10^{-11}$).
of 2.52 MeV. The $^{56}\text{Mn} \rightarrow ^{56}\text{Cr}$ has a ground state - ground state EC threshold of 0.77 MeV, but since the $J^\pi$ of the $^{56}\text{Mn}$ and $^{56}\text{Cr}$ ground states are $3^+$ and $0^+$ respectively, the EC cannot proceed from the ground state of $^{56}\text{Mn}$ to the ground state of $^{56}\text{Cr}$. Instead the transition is from the Mn ground state to an excited state in $^{56}\text{Cr}$, and proceeds at a Fermi energy of 3.95 MeV. Since this is below the $^{56}\text{Fe}$ EC threshold however, this second EC proceeds as soon as the first occurs. $^{56}\text{Cr}$ is stable against further EC until the electrons have a Fermi energy of 10.09 MeV, equal to the negative Q-value needed for $^{56}\text{Cr} \rightarrow ^{56}\text{V} + \nu_e$. This transition is actually to a very low lying excited state in $^{56}\text{V}$. Since $^{56}\text{V}$ is an odd nucleus however, the EC threshold for $^{56}\text{V} \rightarrow ^{56}\text{Ti}$ is at the lower value of 6.18 MeV, resulting in yet another two-step EC process. The flow of this reaction path is shown in the top pane of fig. 6.3. The neutron number (N) for the element is given along the bottom, the proton number up the side. Red lines are defined as flows from lower N to higher N, green lines define flows from higher N to lower N. The style of the lines (whether they are solid or dashed) indicates the magnitude of the flow. Solid lines are fluxes up to $1 \times 10^{-5}$, dashes lines are fluxes between $1 \times 10^{-5}$ and $1 \times 10^{-6}$. Dark gray squares represent the valley of stability. An amount of $\beta^-$ decay can be seen competing with the EC between the isotopes $^{56}\text{V} \rightarrow ^{56}\text{Cr}$ and $^{56}\text{Sc} \rightarrow ^{56}\text{Ti}$, however the main path pushes material down the A=56 chain.

A branching point is reached at nucleus $^{56}\text{Ca}$ (middle pane of fig. 6.3). This nucleus requires a Fermi energy of 22.8 MeV before EC to an accessible state in $^{56}\text{K}$. Once $^{56}\text{K}$ has been made however, it is unstable against EC at a threshold of 20.89 MeV. This is greater than the Q-value for EC (to $^{56}\text{Ar}$) and 2 neutron emission to $^{54}\text{Ar}$ however, which is 20.08 MeV. Consequently $^{56}\text{K} \rightarrow ^{54}\text{Ar} + 2\text{n} + \nu_e$. The thermonuclear neutron capture rate of $^{56}\text{Ca}$ is about $N_A < \sigma v > = 6.32 \times 10^2 \text{ cm}^3 \text{ gs}^{-1}$, and so the remaining $^{56}\text{Ca}$ (which have not yet captured electrons; there is
Figure 6.2. Plot of the abundance as a function of time for the A=56 chain. The simulation was performed assuming an initial composition of $X_{\text{56Fe}} = 1$, $Y_{\text{56Fe}} = 0.0179$

A width to the EC reactions given by $k_B T$ which enables capture to start roughly 0.5 MeV before the threshold is met) capture neutrons to produce $^{57}\text{Ca}$. The EC threshold for $^{57}\text{Ca}$ is lower than that for $^{56}\text{Ca}$, it is only 19.96 MeV, and so $^{57}\text{Ca}$ immediately undergoes EC capture to produce $^{57}\text{K}$. Since $^{57}\text{K}$ requires a Fermi energy of 21.57 MeV in order to EC, it too immediately captures an electron. However the Q-value for EC plus 1 neutron emission is only 18.94 MeV, and so $^{57}\text{K} \rightarrow ^{56}\text{Ar} + \text{n} + \nu_e$, adding to the neutron abundance. The presence of the free neutrons, coupled with isotopes with positive (n,γ) Q-values, leads to the production of $^{58,59,60,61}\text{Ca}$, $^{58,59,60}\text{K}$ and $^{54,55}\text{Ar}$.

A distribution of isotopes is slightly dissimilar to the result of [38], who found that EC reactions lead directly to $^{56}\text{Ar}$. The discrepancy is directly due to the mass model used, [38] used the compressible liquid drop model, here masses are either from FRDM or the Hilf model (see fig. 5.2). However it should also be noted
that the authors of [38] tracked the evolution of just one Wigner-Seitz cell. This implicitly assumed that the total crust mass fraction at any given depth was totally represented by that test cell. As such, no more than once species of isotope could exist at any one time.

6.1.2 Production of $^{40}$Mg

By tracking the composition, the effects of pycnonuclear reactions can be observed. One key pycnonuclear isotope is $^{40}$Mg. This particular isotope can be formed from the following reaction chain:

$^{54}$Ar (EC = 27.31 MeV) $\rightarrow$ $^{53}$Cl + n (EC = 25.22 MeV) $\rightarrow$ $^{48}$S + 5n (EC = 27.49 MeV) $\rightarrow$ $^{45}$P + 3n, $^{45}$P + n $\rightarrow$ $^{46}$P + n $\rightarrow$ $^{47}$P (EC = 28.45 MeV) $\rightarrow$ $^{42}$Si + 5n (EC = 30.39 MeV) $\rightarrow$ $^{41}$Al + n (EC = 29.72 MeV) $\rightarrow$ $^{36}$Mg + 5n, $^{36}$Mg+ n $\rightarrow$ $^{37}$Mg + n $\rightarrow$ $^{38}$Mg + n $\rightarrow$ $^{39}$Mg + n $\rightarrow$ $^{40}$Mg.

The reaction chain is plotted in the lower pane of fig. 6.3.

The $^{36}$Mg is formed at a density of $\sim 6.5 \times 10^{11}$ g cm$^{-3}$, but is stable against EC only up to a density of $4.67 \times 10^{11}$ g cm$^{-3}$. The EC rates are on the same order ($\sim 10$ cm$^3$ g$^{-1}$ sec$^{-1}$) as the competing thermonuclear neutron capture rates, which leads to a branching point with the formation of $^{37,38,39,40}$Mg on one hand, and the formation of $^{35}$Na on the other (the phase space does not allow a $^{36}$Mg $\rightarrow$ $^{36}$Na transition). However a natural question here is why does the lower pane of fig. 6.3 not show $^{36}$Mg undergoing pycnonuclear fusion? Fig. 6.5 shows a plot of the (thermonuclear) $^{36}$Mg(n,$\gamma$), $^{38}$Mg(n,$\gamma$) and $^{40}$Mg(n,$\gamma$) rates against the $^{36}$Mg+$^{36}$Mg, $^{36}$Mg+$^{38}$Mg, $^{38}$Mg+$^{38}$Mg, $^{40}$Mg+$^{40}$Mg and $^{20}$C+$^{40}$Mg heavy ion fusion rates as a function of mass density, in units of cm$^3$ g$^{-1}$ sec$^{-1}$. Since the thermonuclear neutron capture rate for $^{36}$Mg at $\rho = 6.5 \times 10^{11}$ g cm$^{-3}$ is greater than the pycnonuclear rate, $^{36}$Mg captures a neutron to form $^{37}$Mg. The criteria is true of other Mg isotopes also and so the neutron capture chain continues to produce $^{40}$Mg. This isotope has
Figure 6.3. Plot of the fluxes for a simulation assuming an initial composition of $X_{Fe} = 1$ at three different times. Neutron number is given along the bottom, proton number up the side. Grey squares mark the valley of stability. Red lines represent flows from lower N to higher N, green from higher N to lower N. Dashed lines represent flows between $1 \times 10^{-5}$ and $1 \times 10^{-6}$. 
an extremely low \((n,\gamma)\) reaction rate, and so does not neutron capture.

Following again the EC chain, \(^{35}\text{Na}\) (EC = 25.27 MeV) \(\rightarrow\) \(^{31}\text{Ne} + 4\text{n}\), \(^{31}\text{Ne} + \text{n} \rightarrow \(^{32}\text{Ne}\) (EC = 30.25 MeV) \(\rightarrow\) \(^{31}\text{F} + \text{n}\) (EC = 29.02 MeV) \(\rightarrow\) \(^{25}\text{O} \rightarrow \(^{24}\text{O} + \text{n} \rightarrow \(^{23}\text{N} + \text{n}\) (EC = 24.4 MeV) \(\rightarrow\) \(^{18}\text{C} \text{ and } ^{20}\text{C}\). The first \(^{18,20}\text{C}\) produced fuses with \(^{40}\text{Mg}\) forming \(^{58,60}\text{Ar}\), and is quickly exhausted. A second formation of \(^{18,20}\text{C}\) is at a density and temperature of \(6.6 \times 10^{11}\) g cm\(^{-3}\) and \(\sim 0.50\) GK respectively. Fig. 6.4 plots the reaction curve for \(^{18,20}\text{C} + ^{18,20}\text{C}\) under these conditions, which correspond to thermally enhanced pycnonuclear burning. The reaction curve for all three C+C reactions increases with mass density, reaching a maximum at \(\sim 1 \times 10^{12}\) g cm\(^{-3}\), when the rate begins to decline as \(X_N\) becomes less than 1. At mass densities less than this, the reaction rate curves show structure which reflects the change in \(<Z>\). At greater mass densities, the rates reflect the change in electron and number density.

Fusion between \(^{18,20}\text{C}\) and \(^{18,20}\text{C}\) results in the formation of \(^{36,40}\text{Mg}\), which can be seen in the top pane of fig. 6.6. Effectively, the EC on \(^{36}\text{Mg}\) populates a reaction path which ultimately produces the isotopes \(^{18,20}\text{C}\), which, through heavy ion fusion, repopulate \(^{36}\text{Mg}\) and \(^{40}\text{Mg}\). Neutron capture on \(^{36}\text{Mg}\) also in turn leads to a build up of \(^{40}\text{Mg}\).

6.1.3 Flows at Higher Densities

Both neutron capture on \(^{31}\text{Ne}\) and EC on \(^{36}\text{Mg}\) lead to the production of \(^{32}\text{Ne}\), at a density of \(\sim 6.5 \times 10^{11}\) g cm\(^{-3}\). Fusion between \(^{18,20}\text{C}\) and \(^{32}\text{Ne}\) result in the production of \(^{50,52}\text{S}\), whereas fusion between \(^{18}\text{C}\) and \(^{40}\text{Mg}\) manufactures \(^{58}\text{Ar}\) at the slightly higher mass density of \(7.1 \times 10^{11}\) g cm\(^{-3}\) (top pane in fig. 6.6).

Neutron capture on to Ar isotopes, produced by both EC and pycnonuclear reaction mechanisms, lead to a string of neutron rich isotopes up to \(^{62}\text{Ar}\) (middle
Figure 6.4. Density induced fusion rates as a function of mass density for the reactions $^{18,20}$C+$^{18,20}$C and $^{18,20}$C+$^{32}$Ne.

pane fig. 6.6). This particular isotope can EC at a threshold of 32.6 MeV, producing $^{57}$Cl + 5n and $^{56}$Cl + 6n. Since neutron capture rates for these isotopes are greater than EC rates, both of these daughter isotopes capture up to $^{61}$Cl, which transitions to $^{55}$S + 6n. The stellar rate for the thermonuclear photo-dissociation of $^{55}$S is $2.25 \times 10^7$ cm$^{-3}$ g$^{-1}$ sec$^{-1}$, resulting in $^{54}$S. Since the Fermi energy is 32.6 MeV when $^{54}$S is formed, but the EC threshold for this nucleus is 30.94 MeV, it captures an electron and produces $^{49}$P. This in turn transitions via EC to $^{44}$Si which undergoes 2 neutron capture to form $^{46}$Si.

Plotted in fig. 6.7 is the abundance as a function of time for the isotopes $^{18,20}$C, $^{36,40,44}$Mg (upper pane) and $^{58,60,62}$Ar, $^{44,46}$Si (lower pane). At a time of $\sim 9 \times 10^{10}$ sec (corresponding to $\rho=2.9 \times 10^{11}$ g cm$^{-3}$ and Fermi energy $\sim 22.5$ MeV), $^{18}$C starts to fuse with itself, producing $^{36}$Mg. There is also a small decrease in $^{20}$C at
Figure 6.5. Thermonuclear neutron capture rates and heavy ion fusion rates (calculated using model 1 of table 4.1 and eq. 4.58) for the isotopes $^{36}\text{Mg}$, $^{38}\text{Mg}$ and $^{40}\text{Mg}$. Fluctuations in the heavy ion rates at high densities reflect dynamic changes in electron abundance and number density in the network simulation. At low densities structure reflects changes in $<Z>$. 
Figure 6.6. Plot of the fluxes for a simulation assuming an initial composition of $X_{56Fe} = 1$ at three different times. Neutron number is given along the bottom, proton number up the side. Grey squares mark the valley of stability. Red lines represent flows from lower N to higher N, green from higher N to lower N. Dashed lines represent flows between $1 \times 10^{-5}$ and $1 \times 10^{-6}$. 
this time, corresponding to an increase in $^{40}$Mg. An increase in $^{58}$Ar at $t = 1.9 \times 10^{11}$ sec marks the formation of this isotope through EC and neutron capture. At a Fermi energy of $30.32$ MeV ($\rho = 6.9 \times 10^{11}$ g cm$^{-1}$) $^{58}$Ar start to decay through EC. This steep decay edge is arrested by the fusion of $^{18}$C + $^{40}$Mg occurring at a time of $3.3 \times 10^{11}$ sec ($\rho = 7.5 \times 10^{11}$ g cm$^{-3}$). Heavy ion fusion of $^{20}$C + $^{40}$Mg to produce $^{60}$Ar starts to occur at $t = 4.47 \times 10^{11}$ sec ($\rho = 1.2 \times 10^{12}$ g cm$^{-3}$, Fermi energy equals 33.6 MeV). The Fermi energy threshold for $^{60}$Ar is 30.32 MeV. At the density at which $^{20}$C + $^{40}$Mg fusion starts to produce $^{60}$Ar, it is able to capture an electron. The thresholds for $^{60}$Ar EC and 5 and 6 neutron emission are 30.10 MeV and 31.50 MeV respectively, both beneath the Fermi energy. The daughter nuclei, $^{55}$Cl and $^{54}$Cl are both unstable against EC, and transition to Sulfur isotopes. The chain of EC and neutron emission continues, producing $^{46}$Si.

The abundance of $^{46}$Si as a function of time is shows a number of peaks and troughs reflecting the play off between the reactions which yield $^{46}$Si populating that isotope and the competing EC decay of $^{46}$Si which destroys it.

The bottom pane of fig. 6.6 shows the flows at the end of the simulation. The fusion reaction $^{40}$Mg + $^{40}$Mg $\rightarrow ^{80}$Cr can be seen occurring, but as demonstrated in fig. 6.5 the rate for this fusion is very small (on the order of $\sim 10^{-24}$ cm$^3$ g$^{-1}$ sec$^{-1}$)). This is different to the findings of [38], who predicted that $^{36}$Ne, formed from EC on $^{40}$Mg (which has a EC threshold of 37.03 MeV in the FRDM framework), would be the first isotope to undergo pycnonuclear fusion. The discrepancy is due to the fact that the simulation used in this thesis follows many nuclei, not just one cell. Removing this restriction opens up new reaction paths that populate a distribution of reacting isotopes. As such reactions can be observed which were prohibited in the work of [38]. This leads to a different reaction path than those authors observed.

The final abundance distribution is shown in the lower pane of fig. 6.1. At the
Figure 6.7. Abundance as a function of time for $^{20,22}$C, $^{40,44}$Mg, $^{60,62,64}$Ar and $^{46}$Si. The $^{40}$Mg is formed initially through neutron capture on $^{36}$Mg, then at later times by the heavy ion fusion of $^{20}$C. The formation of $^{62}$Ar follows neutron capture on $^{60}$Ar, formed by $^{20}$C+$^{40}$Mg. After the initial formation of $^{46}$Si via EC on $^{62}$Ar, a cycle of $^{46}$Si production is set up, where pycnonuclear reactions between C and Mg isotopes lead to isotopes of Ar, which in turn EC to $^{46}$Si, which EC back to lighter elements, releasing energy.
end of the simulation there is a build up of free neutrons ($Y_n = 0.953$), $^{40}\text{Mg}$ ($Y_{^{40}\text{Mg}} = 1.156 \times 10^{-3}$) and a small amount of $^{46}\text{Si}$ ($Y_{^{46}\text{Si}} = 8.514 \times 10^{-11}$). It has been predicted by authors such as Haensel and Zdunik ([38], [39], [40]), Schramm and Koonin ([88]) that an isotope such as $^{40}\text{Mg}$ will fuse through pycnonuclear reactions, rather than build up. In the pycnonuclear formalism established here however, the rates depend exponentially on $<A>$, $<Z>$ and $X_N$, through the parameter $\lambda_{ij}$. Shown in fig. 6.8 are these three quantities as a function of mass density for this simulation. At $\rho \sim 9 \times 10^{11}$ g cm$^{-3}$ $X_N < 1$. This occurs because neutrons start to drip out of the nucleus. Since $\lambda_{ij}$ (eq. 4.40) scales proportionally with $X_N$, the exponent in eq. 4.45 scales with $X_N$. As such, as $X_N \rightarrow 0$, so $\exp(-C_{exp}/\lambda_{ij}) \rightarrow 0$, meaning that the heavy ion fusion rates decrease exponentially after the neutron drip density. As shown in the lower pane of fig. 6.6 pycnonuclear fusion of $^{40}\text{Mg}$ does occur, but it is inhibited at $\rho \sim 9 \times 10^{11}$ g cm$^{-3}$.

### 6.1.4 Integrated Energy Generation

The integrated energy deposited into the crust as a function of mass density is plotted in fig. 6.9 where the red line represents the simulation without the inclusion of the pycnonuclear channel and the green line with the pycnonuclear channel. The amount of energy deposited at each time step for an abundance distribution composed of $k$ isotopes can be calculated from the change in the nuclear mass excess, the change in the electron Fermi energy, and the amount of heat deposited by neutrino loss (due to EC) via,

$$\frac{dQ}{dt} = \left( \sum_k d\Delta_k dY_k \right) + E_f dY_e - \sum_k \frac{dY_k}{4}(E_f - E_{k,\text{thr,gs-gs}}).$$

where $E_f$ is the Fermi energy, in MeV, $\Delta_k$ the mass excess of isotope $k$, $Y_k$ the mass fraction of isotope $k$, and $E_{k,\text{thr,gs-gs}}$ is the energy of the excited state of the
Figure 6.8. Average mass, proton number, and the mass fraction contained in the nucleus as a function of mass density, for a $X_{56Fe} = 1$ simulation. At $\sim 9 \times 10^{11}$ g cm$^{-3}$ $X_N < 1$. This marks the neutron drip point.
At mass densities less than $\sim 8 \times 10^{11}$ g cm$^{-3}$, the deposited energy comes entirely from EC reactions. The step-like features in the plot come from individual EC reactions switching on as a function of density. The dip in the energy generation rate at $1.5 \times 10^{12}$ g cm$^{-3}$ occurs when the mass model used to calculate mass excess switches from FRDM to Hilf formalism, i.e. when electron captures occur between nuclei with $Z < 8$. In this respect it is an artifact, rather than real physical process.
Expanding the FRDM mass model calculations to cover all of the nuclei included in the network code would eliminate the dip feature, though such an expansion is beyond the immediate scope of this thesis.

When \( \rho \) is greater than \( \sim 1.8 \times 10^{12} \text{ g cm}^{-3} \) (corresponding to a Fermi energy of \( \sim 33.4 \text{ MeV} \)), including pycnonuclear reactions increases the energy deposition by a factor of \( \sim 4.6 \). It is interesting to note that this is approximately the same finding as [41], even though they observed a slightly different isotopic evolution (due to a different mass model).

The main reason for the energy enhancement is that several pycnonuclear channels feed the production of \(^{46}\text{Si} \left( ^{18,20}\text{C} + ^{36,40}\text{Mg} \right) \) reactions produce \(^{58,60}\text{Ar} \), which then decay through a chain of EC reactions and neutron emissions to \(^{46}\text{Si} \), plotted in fig. 6.7. These processes all occur at a Fermi energy above that required to activate EC on \(^{46}\text{Si} \). Therefore heavy ion production of \(^{46}\text{Si} \) is accompanied by EC capture which in turn produces first \(^{41}\text{Al} \), then \(^{36}\text{Mg} \) through a two-step EC process. Sequential neutron captures on \(^{36}\text{Mg} \) results in \(^{40}\text{Mg} \), which can fuse with remaining carbon isotopes to begin the cycle again. However it must be stressed that the neutron capture rates used throughout the simulation are thermonuclear rates. According to eq. 5.6 neutrons are degenerate when the neutron abundance is greater than,

\[
Y_n > \left( \frac{T}{227} \right)^{3/2} \frac{1}{\rho}. \tag{6.2}
\]

Since the simulation end point conditions (\( T = 0.47 \text{ GK} \) and \( \rho = 2 \times 10^{13} \text{ g cm}^{-3} \)) indicate that the neutrons are degenerate when \( Y_n > 1.49 \times 10^{-4} \), and fig. 6.1 shows that the final neutron abundance is 0.934, the \((n,\gamma)\) rates cannot be treated as thermonuclear. Thermonuclear formalism does not account for the energy of the neutrons owing to filled neutron states. Much like the EC situation, this neutron energy sea could activate negative Q-value \((n,\gamma)\) reactions, and block
some \((\gamma, \text{n})\) reactions from occurring (since low energy neutron states are filled). As such, thermonuclear neutron capture rates could significantly underestimate the realistic \((\text{n}, \gamma)\) reaction rate for a given isotope. It is possible that changing the neutron capture formalism at high mass densities could result in a build up of different, more exotic neutron rich isotopes that are far beyond the neutron drip line. These nuclei would be stable against neutron emission (owing to filled states in the neutron Fermi sea), could be stable against EC and \(\beta^-\) decay (because of filled electron Fermi states) and maybe stable against heavy ion fusion, depending on the Coulomb barrier.

6.1.5 Error in the Pycnonuclear Rate

In order to gage the effects of the uncertainty in the pycnonuclear model on the integrated energy generation curve, the pure \(^{56}\text{Fe}\) simulation was repeated for 7 different parameter sets from table 4.1. The parameters selected are all for BCC lattice types.

Shown in the top half of fig. 6.10 are the pycnonuclear rates calculated for the reaction \(^{40}\text{Mg}^+ + ^{40}\text{Mg}\). The different pycnonuclear models do not have a significant effect on the stellar reaction rate at lower mass densities, where the reaction rates are extremely small, on the order of \(10^{-60}\) cm\(^3\) g\(^{-1}\) sec\(^{-1}\). By the end of the simulation however, the difference between model 10 and 11 (by definition the models which produce the minimum and maximum rates) is 10 orders of magnitude in the reaction rate. An uncertainty of this magnitude agrees approximately with the findings of sec. 4.5 and represents the current limitation of understanding.

The lower half of fig. 6.10 illustrates the impact of the rate uncertainty on the integrated energy generation curve. It is an interesting feature of this plot that there is not an even spread of integrated energies, rather there are models which
Figure 6.10. Impact of the uncertainty in the pycnonuclear reaction rate formalism on the stellar reaction rate (top) and integrated energy generation curve (bottom) for the reaction $^{40}\text{Mg} + ^{40}\text{Mg}$. The 7 models plotted represent BCC lattice types, and are taken from table 4.1.
yield $\sim 2.4$ MeV/u, and models which yield $\sim 1.8$ MeV/u. The stratification is caused by the lattice response to a tunneling event - either static or relaxed. The static lattice model underestimates the rate yielding a lower energy generation. The relaxed lattice model overestimates the reaction rate, resulting in a larger energy generation.

6.2 Other Pure Stable Nuclei Compositions

To investigate the dependence of the final composition abundance distribution on the initial seed abundance distribution in the X-ray burst ashes, an array of other initial stable nuclei were selected, and the simulation repeated. As for the case of $X_{56Fe}=1$, each simulation was assumed to be initially composed of a single isotope. Simulations were begun with a starting temperature, density and Fermi energy of $0.34$ GK, $2.3 \times 10^7$ g cm$^{-3}$ and $0.73$ MeV respectively, and performed until the mass density reached $2.6 \times 10^{13}$ g cm$^{-3}$.

Fig. 6.11 shows the evolution of $<A>$, $<Z>$ and $<N>$ as a function of mass density for the initial nuclei $^{104}$Pd, $^{102}$Ru, $^{98}$Mo, $^{88}$Sr, $^{84}$Kr, $^{68}$Zn, $^{74}$Ge, $^{38}$Ar, $^{36}$S, $^{30}$Si and $^{56}$Fe (for comparison).

For each simulation the composition remains unchanged until the mass density reaches a threshold at which EC reactions set in. The threshold is coupled to the initial nucleus composition, but can be estimated from the middle pane of fig. 6.11. Broadly speaking, heavier isotopes begin to EC at shallower depths than lighter isotopes. For instance, $^{106}$Pd starts to EC at $\rho = 5 \times 10^8$ g cm$^{-3}$, whereas $^{36}$S undergoes EC at a threshold of $\rho = 1 \times 10^{10}$ g cm$^{-3}$. When EC reactions are triggered for each composition, initially there is no accompanying neutron emission. This can be inferred from the plot of average mass number, which remains the same as the initial composition mass number until a mass density of $\sim 9 \times 10^{12}$ g cm$^{-3}$. 

123
Figure 6.11. Average mass number (top), proton number (middle) and neutron number (bottom) for 11 different starting compositions, as a function of mass density.
The lower pane of fig. 6.11 illustrates average neutron number increasing as average proton number decreases also until a threshold of $\sim 9 \times 10^{11} \text{ g cm}^{-3}$, when there is a sudden decrease in $<N>$. This threshold is virtually independent of initial nucleus composition, and marks the point at with the neutron drip line is reached.

The effects of pycnonuclear reactions are clearly visible in simulations where the initial composition was light, such as $^{38}\text{Ar}$, $^{36}\text{S}$ and $^{30}\text{Si}$. Since these compositions start out light (low $<Z>$ and $<A>$), EC reactions for these simulations produce low proton number isotopes ($Z = 6 - 12$) in the density range $10^{11} - 10^{12} \text{ g cm}^{-3}$. These nuclei can undergo heavy ion fusion. This is borne out by a rise in $<N>$ at $8 \times 10^{11} \text{ g cm}^{-3}$, indicating fusion reactions. Heavier initial compositions yield a range of $Z = 25 - 35$ over the same density interval, which preclude the composition from pycnonuclear reactions.

Where pycnonuclear reactions are taking place, such as the pycnonuclear fusion of $^{30}\text{Ne}$ (initial composition $^{36}\text{Si}$), the resulting nucleus undergoes EC induced neutron emission to produce an average composition of $Z=12$, $A=40$. This is true of heavier initial compositions also, indicating that no matter what the one-nucleus initial composition is, at the end of the simulation the ashes are dominated by free neutrons and $^{40}\text{Mg}$. Though the pycnonuclear fusion reaction rate of $^{40}\text{Mg} + ^{40}\text{Mg}$ is non zero, as fig. 6.12 shows, the reaction rate (in stellar reaction rate units of $\text{cm}^3 \text{ g}^{-1} \text{ sec}^{-1}$) is not significant when $X_N$ is less than 1.

At very high mass density the low $^{40}\text{Mg}+^{40}\text{Mg}$ rate indicates that $X_N < 1$. The rigid Coulomb lattice is dissolving into effectively a soup of free neutrons, some electrons (most have been lost through EC), and some stable ions. The formalism for heavy ion reactions developed here is not suitable for this physical situation. Since the majority of the pressure now must come from neutron degeneracy (rather than electron degeneracy), nor is the equation of state or even the thermonuclear
Figure 6.12. Stellar reaction rate as a function of mass density for 5 different values of $X_N$. At mass densities greater than the neutron drip, $X_N < 1$. Since the pycnonuclear reaction rate depends exponentially on $X_N$, reduction in $X_N$ translates into a many order of magnitude decrease in the reaction rate.
6.3 Realistic X-Ray Burst Ash Composition

Having examined the compositional end point for different single species nuclei, a simulation was performed using the realistic X-ray burst ashes of Schatz et al [87], shown in fig. 1.3. The simulation was performed for 2329 nuclei, assuming a starting temperature and mass density of 0.25 GK and $4.6 \times 10^6$ g cm$^{-3}$ respectively (equivalent to a Fermi energy of $\sim 0.33$ MeV). The abundance distribution was evolved until the Fermi energy reached $\sim 36.2$ MeV, and the mass density was $2.6 \times 10^{13}$ g cm$^{-3}$. The initial and final abundance distributions are shown in fig. 6.13. The final abundance distribution is dominated by free neutrons, with smaller amounts of $^{40}$Mg and $^{46}$Si.

Fig. 6.14 shows a plot of the reaction flows for this simulation where again, red lines represent flows from lighter A to greater A, and green lines show the reverse direction. There are a lot of flows for a simulation involving so many isotopes and so to keep the figure reasonably readable, not all fluxes are plotted. Red and green lines represent fluxes of up to $1 \times 10^{-4}$, gray dashed lines represent fluxes between $1 \times 10^{-4}$ and $1 \times 10^{-5}$).

A strong feature of fig. 6.14 is that the EC reactions map out a path of constant mass for a given reaction chain up to a limit close to the neutron drip line, where $(n,\gamma)$ ($\gamma,n$) reactions and multi neutron emission EC reaction dominate. This drives the paths away from the initial mass chain. The EC reactions are the dominant form of nuclear reaction, right out to the neutron drip line.

As the composition becomes more neutron rich, $(n,\gamma)$ reactions start to occur. This effect charts the region where Q-value EC thresholds are great enough to prevent EC reactions from taking place (without a rise in Fermi energy), but the Q-
Figure 6.13. Initial (top) and final (bottom) abundance distributions for a network simulation involving realistic x-ray burst ashes. Similar to the previous examples studied, the final abundance distribution is composed of free neutrons ($Y_n = 0.9483$), $^{40}$Mg ($Y_{^{40}Mg} = 1.292 \times 10^{-3}$), and a smaller amount of $^{46}$Si ($Y_{^{46}Si} = 3.21 \times 10^{-7}$).
values for neutron capture and emission are positive, and so equilibrium can develop. Once the threshold for EC has been reached for a neutron rich isotope however, it often decays to a state in the daughter nucleus with an excitation energy greater than the neutron separation energy for multiple (up to 6) neutrons. The daughter nucleus can then EC to a granddaughter excited state, which is also at an energy above multiple neutron separation. Since the Q-value thresholds for EC reactions are similar for nuclei at the drip line, the granddaughter nucleus transitions via EC to a great granddaughter excited state which can also result in multiple neutron emission. The process (called an Electron Capture Cascade by ref. [36]) continues, efficiently and rapidly processing the material from heavier A,Z to lighter A,Z with a large accompaniment of neutron emission. Without this process, density induced fusion could not occur at all.

In the initial ashes there is a small amount of $^{12}$C ($Y_{12C}=5.64\times10^{-4}$). It is the burning of this initial distribution which is thought to perhaps power super-bursts. Fig 6.15 plots the abundance evolution of the initial $^{12}$C as a function of time.

The $^{12}$C begins to burn in the thermonuclear with strong screening domain, to form $^{24}$Mg on a timescale of hundreds of years. This happens at a Fermi energy of 4.7 MeV, corresponding to mass density of $\sim 2.1 \times 10^9$ g cm$^{-3}$ (T=0.5 GK). The $^{24}$Mg requires a Fermi energy of 6.81 MeV before it can EC to a 0.16 MeV excited daughter state in $^{24}$Na. As an odd A odd Z nucleus, $^{24}$Na requires a threshold of just 1.45 MeV to EC to the ground state of $^{24}$Ne. At a Fermi energy of 15.61 MeV, $^{24}$Ne captures an electron to form $^{24}$F, which undergoes 2-neutron emission induced EC to produce $^{22}$O. Through a two-step process of EC and 1 neutron emission, $^{22}$O is processed in to $^{20}$C, which undergoes pycnonuclear fusion resulting in an initial build up of $^{40}$Mg. As discussed in sec. 6.1 this nucleus is not only stable against EC until a threshold of 37.03 MeV, it also has a low $(n,\gamma)$ reaction rate. The other
Figure 6.14. Plot of the fluxes for a simulation assuming a composition of realistic X-ray burst ashes. Neutron number is given along the bottom, proton number up the side. Grey squares mark the valley of stability. Red lines represent flows from lower N to higher N, green from higher N to lower N. Dashed lines represent flows less than $1 \times 10^{-5}$ of the maximum flow.
Figure 6.15. The abundance evolution of the initial $^{12}\text{C}$ as a function of time. At a Fermi energy of 4.7 MeV, the Carbon begins to fuse forming $^{24}\text{Mg}$. This nucleus is unstable against EC at 6.81 MeV, and so $^{24}\text{Ne}$ is rapidly formed at greater crust depths.
production mechanism for $^{40}$Mg, is neutron capture on lighter Mg isotopes that either comprised the original composition, or else were produced though electron capture on other ($Z > 12$) isotopes. It is interesting to note that the production mechanisms of $^{40}$Mg for a realistic isotopic distribution is very similar to that of pure $^{56}$Fe. There are no EC reactions which directly feed into $^{40}$Mg, and similarly the threshold for EC is sufficiently high that the only other reaction channel left is heavy ion fusion. A flux from $^{40}$Mg to $^{80}$Cr can be seen in fig. 6.16 (the same as fig. 6.14 but plotted over a smaller isotope range for clarity). This path starts to open up at a mass density of $\sim 3.2 \times 10^{12}$ g cm$^{-3}$ (a Fermi energy of 36.3 MeV), which corresponds to classical $T=0$ pycnonuclear burning. However, as demonstrated in secs. 6.1 and 6.2, this path is suppressed initially by low density and then by $X_N < 1$ at mass densities greater than the neutron drip density.

Shown in fig. 6.17 are $< A >$, $< Z >$ and $< N >$ as a function of mass density. Initially, the ashes have an average composition of $^{88}$Zr (due to combination of $^{104,105}$Cd with $^{72}$Se, $^{68}$Mo, $^{64}$Zn). Electron capture reactions drive $< Z >$ down, while increasing $< N >$. Maximum $< N >$ occurs at $\rho \sim 9 \times 10^{11}$ g cm$^{-3}$, and corresponds to the neutron drip point.

Intriguingly, final $< A >$, $< N >$ and $< Z >$ are 40, 28, and 12 respectively. This is the same result as was obtained using pure compositions in sec. 6.2. This result indicates that as the Coulomb lattice begins to dissolve at $\rho > 2 \times 10^{12}$ g cm$^{-3}$, the ashes are processed into free neutrons, and the same stable nuclei, regardless of the initial abundance composition.

The integrated energy deposited into the crust as a function of mass density is plotted in fig. 6.18. Owing to the small Q-values required to trigger EC on heavy isotopes (i.e., $^{104}$Cd, which has a threshold of 0.93 MeV), energy generation starts at a shallower depths in the crust for realistic X-ray burst ashes than compared
Figure 6.16. Zoomed section of fig. 6.14 showing nuclei of relevance to pycnonuclear reactions.
Figure 6.17. Average mass number, proton number and neutron number, as a function of density, for an abundance vector composed of x-ray burst ashes.
Figure 6.18. Integrated energy deposited in the crust as a function of mass density. The feature at $\sim 3.9 \times 10^{11} \text{ g cm}^{-3}$ is a model artifact, and corresponds to the switch between FRDM masses and Hilf masses.

to an ash composed entirely of $^{56}\text{Fe}$ (fig 6.9). As such, a small amount of energy generation is observed in fig. 6.18 up to a density of about $\sim 2.5 \times 10^{9} \text{ g cm}^{-3}$ (a Fermi energy of $\sim 4.7 \text{ MeV}$). At densities higher than this, other EC reactions switch on, transitioning the material towards lighter products. At a mass density of $\sim 3.9 \times 10^{11} \text{ g cm}^{-3}$ (a Fermi energy of 25 MeV) there is a drop in the energy generation curve. This is a model artifact, highlighting the switchover between different mass model formalisms, discussed in sec. 6.1.4.

The effects of pycnonuclear reactions can be seen particularly at densities greater than $1 \times 10^{12} \text{ g cm}^{-3}$. This is approximately the same density region as was the case for pure $^{56}\text{Fe}$ composition, fig 6.9. The inclusion of ion fusion reactions in the simulation above this density (and using model 1 of table 4.1) results in an energy generation of approximately 1.8 MeV/u, which is almost identical to the findings
of sec. 6.1. The results from sec. 6.1.5 can be used to estimate the uncertainty in this value attributable to heavy ion fusion; the energy generation is between 1.8 MeV/u and 2.4 MeV/u, depending on the model of Coulomb barrier penetration, and lattice response used.

As was the case for the pure $^{56}$Fe composition, the heating at higher densities is not so much from the pycnonuclear reactions themselves as it is from the EC by the products of the fusion reactions.

Since the results for compositionally pure $^{56}$Fe verses realistic X-ray burst ashes are so similar (in terms of integrated energy generation and averaged plasma quantities; $< A >$, $< Z >$ and $< N >$), once passed a mass density region of $\sim 2 \times 10^{12}$ g cm$^{-3}$ the abundance distribution comprising the deep crust is practically independent of the initial composition.

In itself this is perhaps a good result, since it means that one does not need to know the reaction flows in detail to obtain the essential physics of the neutron star crust. On the other hand this is also a difficult result, since it means that observing the light curve in quiescence may tell us nothing more about what neutron star crust processes can occur, and for which nuclei.
DISCUSSION AND CONCLUSIONS

The purpose of this thesis has been to explore the effects of density induced reactions, coupled with realistic EC reactions, on the abundance distribution of realistic X-ray burst ashes. This has been achieved by firstly developing a formalism for calculating $S(E)$ factors for heavy ion fusion reactions of interest, and then developing a framework for calculating the reactions in real time so that they could be included into a network code along with other types of nuclear reactions (e.g., EC, $(n,\gamma)$, $(p,\gamma)$ etc). For the first time, the effects of heavy ion fusion reactions involving nuclei of different species in an MCP have been included in a network code, to provide a state-of-the-art understanding of crust composition evolution which models from post x-ray burst surface ashes to the inner crust.

It had been thought that the heating effects of pycnonuclear reactions could be particularly significant as an internal heat source. This work has shown that pycnonuclear reactions can indeed occur, though perhaps not with the magnitude that has been previously estimated. The main reason for this is that the rates are suppressed after the neutron drip density (as the electrostatic lattice begins to dissolve, so the distance between neighboring ion pairs is no longer periodic). Those ions which do end up next to each other can still fuse, whilst others do not have neighbors close enough to fuse with.

One of the main results to come out of this thesis is that the final abundance distribution is to large effect independent of the initial composition. This is counter
intuitive. The reason for it is that the EC reactions sequentially process material down a given Z chain. At the the neutron drip, EC reactions result in multiple neutron emission, breaking the nuclei up. At greater densities, pycnonuclear reactions fuse light nuclei (isotopes of C, O, Ne and Mg) to form heavier nuclei which are almost always able to immediately EC. What results at the end of the simulation are nuclei ($^{40}$Mg and $^{46}$Si) that are either stable against EC at that density, or a product of EC by pycnonuclear fusion products, which are in the process of decaying via electron capture. Under the reaction rate assumptions used in the crust simulation (assumptions such as a Maxwell-Boltzmann neutron distribution, that closed shells are not affected by high neutron excess, and that FRDM and Hilf masses can be used safely) there is a build up of $^{40}$Mg. There a few reasons for this build up. Firstly the closed N=28 neutron shell results in a negative Q-value for the reaction $^{40}$Mg, suppressing neutron capture. Secondly the high Coulomb barrier, coupled with $X_N < 1$ means that heavy ion fusion rate $^{40}$Mg + $^{40}$Mg is hindered. Thirdly, the electron Fermi energy is not great enough to switch on EC for $^{40}$Mg, but is sufficiently high to block $\beta^-$ decay.

It would be interesting to re-evaluate the initial assumptions which lead to the selection of pycnonuclear isotopes, and allow pycnonuclear fusion channels for other nuclei (i.e., odd A and/or odd Z). This may change the reaction flows, for instance producing $^{61}$Ar via pycnonuclear fusion of $^{19}$C + $^{40}$Mg. However because of the pairing effects discussed in sec. 2.1 odd nuclei (like $^{19}$C) would not be stable and so would not survive EC in the crust to undergo heavy ion fusion. Inclusion of odd pycnonuclear nuclei is therefore unlikely to change the final nuclei or the energy generation curve.

Another interesting avenue to explore is the fate of the compound pycnonuclear nucleus. In the current framework once a pycnonuclear reaction has occurred, the
compound nucleus can only de-excite by $\gamma$ emission: the p, n, and $\alpha$ channels are all blocked. Consequently the pycnonuclear fusion of $^{12}\text{C} + ^{12}\text{C}$ seen in fig. 6.16 results in $^{24}\text{Mg}$, the reaction channels $^{12}\text{C}(^{12}\text{C},\alpha)^{20}\text{Ne}$, $^{12}\text{C}(^{12}\text{C},p)^{23}\text{Na}$ and $^{12}\text{C}(^{12}\text{C},n)^{23}\text{Mg}$ are all suppressed (though the neutron exit channel may be suppressed in any case due to a high neutron Fermi energy). Incorporating a framework for particle emission in the compound nucleus exit channel could have a significant impact on the final abundance distribution. Allowing particle decay channels would increase the abundance of lighter nuclei (ie, $^{56}\text{S} + \alpha$, and $^{59}\text{Cl} + p$ instead of $^{60}\text{Ar}$ from the reaction $^{20}\text{C}+^{40}\text{Mg}$). Any protons or $\alpha$s released would be rapidly captured, adding perhaps significantly, to the energy generation curve.

Though it is beyond the scope of this work, it would be highly beneficial to either develop a new theoretical mass formalism which can cover the entire mass range of interest, or else to expand the FRDM mass range to include both lighter, and neutron unbound nuclei. This would remove the artifact seen in the energy generation curves, and would potentially increase the integrated energy. In turn, this would provide a cutting edge estimate for energy generation. Another important issue to be addressed is the use of thermonuclear $(n,\gamma)$ Hauser-Feshbach rates at densities where the neutrons do not constitute a Maxwell-Boltzmann distribution. The use of these library rates is fundamentally flawed at high densities, since they do not include effects of neutron emission blocking (due to filled neutron states) or the negative Q-value neutron capture reactions that could still proceed. However, it has been seen that by far the greatest uncertainty in the energy generation curve comes from the uncertainties surrounding the plasma aspects of the neutron star crust. Somewhat dishearteningly, one author at least has speculated that the reduction of these theoretical errors could be hard to achieve.

On this note, it is important to stress the number of uncertainties in the model
which has been presented in this dissertation. In terms of the pycnonuclear rates, there are uncertainties arising not only from the reaction $S(E)$ factors, but also the model dependencies which factor into the rate calculations. Broadly speaking, these uncertainties fall into two categories, those relating to nuclear physics, and those relating to astrophysics. In terms of the nuclear physics, the main uncertainties arise from a general lack of understanding of neutron rich, exotic nuclei, both from a mass/structure point of view (i.e., shell closure locations, masses, neutron separation energies) and a fusion point of view (effects of hindrance, effects of thick neutron halos). In the context of astrophysics, uncertainties arise from our lack of knowledge concerning the neutron star lattice plasma potential and crust structure (BCC or FCC, lattice imperfections, and distribution of nuclei, isotropic or otherwise). These errors represent the limit in our state-of-the-art understanding of neutron star crust physics and are hard to quantify. The pycnonuclear rates themselves can have up to a 14 order of magnitude spread, depending on which model from table 4.1 is adopted. Consistently, model 1 of table 4.1 has been used throughout the calculations performed here. The uncertainties surrounding the pycnonuclear rates however just underline how little is known for certain about neutron star physics, and how much work is left.

7.0.1 How Could We Detect Pycnonuclear Reactions?

One way could be to study observable properties of known neutron stars, such as initial cooling curves. After the star has had a spell (on order years) of accreting matter, the accretion can shut off. When it does, the thermal energy in the crust, which is the result of extended accreting and accreting induced reactions, dissipates over the whole star. The dissipation rate depends on crust properties such as the crust thickness, thermal conductivity, neutrino cooling, and reaction heat sources
(such as pycnonuclear reactions). Measuring the cooling curve will allow some constraints to be placed on models, especially those relating to deep crust heating sources.

Another way could be to measure the energy emitted from a neutron star surface when the star is in a period of quiescence. X-ray burst light curves are associated with accretion driven spells of activity on the neutron star surface. Quiescence on the other hand are associated with spells of inactivity, when accretion from a companion object (see sections 1.3 and 1.3.1) is switched off or suppressed.

When the X-ray burst occurs, the energy from the thermonuclear reactions involved in the runaway, as well as the energy released as the ashes begin to sink, is lost via photon emission and does not penetrate the crust of the neutron star. Pycnonuclear reactions however occur at deep depths, occurring at densities of between $\rho = 2.1 \times 10^9 \text{ g cm}^{-3}$ for $^{12}\text{C} + ^{12}\text{C}$ and $\rho = 3.2 \times 10^{12} \text{ g cm}^{-3}$ for $^{40}\text{Mg} + ^{40}\text{Mg}$. These densities corresponds to a between a few hundred metres, and a kilometre into the neutron star crust. At these depths the energy released from nuclear processes, $\sim 1.8 \text{ MeV/u}$ or $\sim 2.4 \text{ MeV/u}$, goes into crust heating. The temperature profile of the crust is a reflection of how the released energy is transported through the crust. Though it is beyond the scope of this work, comparing measured quiescence curves of neutron stars crusts during thermal relaxation to the energy generation estimates such as presented here, could be one way of validating deep crustal heating from pycnonuclear reactions and EC on pycnonuclear products.

The signature of pycnonuclear reactions (specifically the $^{46}\text{Si}$ production and burning cycle that they lead to, described in sec. 6.1.3), should show up in deep crustal heating of neutron stars. Though it is beyond our present technological capabilities, improved sensitivity in a new generation of X-ray observatories may eventually be able to pick out subtle changes in neutron star luminosity. Such lu-
minosity variations could be signatures of deep crustal heating in accreting neutron stars.


