

Simulating Enhanced C12+C12 Reaction Rates for Carbon Shell Burning in Massive Stars

Matt Bundas

Advised by Jennifer Ranta, Dr. Sean Couch

Abstract

A major factor in the dynamics of stars as they pass through burning stages is how easily a given fusion reaction takes place, which is directly tied to the reaction rate. Reaction rates directly affect the composition and structure of a star which in turn affects other processes in the star. Reaction rates and in particular the Carbon-12 + Carbon-12 (C12-C12) rate are not easily measured in a laboratory setting, leading to dispute in their values. A recent paper from A. Tumino et. al experimentally found using the Trojan Horse Method (THM), underlying resonances in the C12-C12 to Mg 24 reaction rate, leading to a much enhanced rate compared to the standard Caughlan-Fowler 88 (CF88) rate. To test the potential effects of the newly found THM rate we ran two 20,000s 2-D simulations of a 25 solar mass star undergoing carbon shell burning using the hydrodynamical astrophysical code FLASH, one implementing the CF88 C12-C12 rate and one implementing the THM rate. I examine the increase in nuclear energy production, increase in strength of convection, and change in element abundance within the star.

1. Introduction

Throughout a star's lifetime it will pass through many burning stages, progressing from fusing light elements like Hydrogen and Helium to, if massive enough ($M_{\text{sun}} > 8$), heavier elements such as Carbon. Such a star will spend roughly 7,000,000 years burning Hydrogen, 700,000 years burning Helium, just 600 years burning Carbon, and a year burning heavier elements up to Silicon. Carbon burning encompasses just a fraction of a star's lifetime and is the subject of this paper.

C12-C12 fusion has multiple channels which are discussed in section 5. Like any fusion reaction the frequency at which these reactions takes place depends on a mathematical quantity called the reaction rate. A reaction rate is essentially how many fusion reactions will take place at a given temperature and density and has the units $\text{cm}^3/\text{s}/\text{mol}$. The exact value of fusion reaction rates are difficult to measure, as direct measurement requires stellar environment conditions which are not easily induced in a laboratory setting, leading to dispute in values. Many new studies regularly are released finding reaction rates which are much slower (4) and much enhanced compared to the long standard Caughlan-Fowler 88 rates (2). In this work we simulate one particular fusion reaction rate found by A. Tumino et al. which found using the Trojan Horse Method, underlying resonances in the C12-C12 fusion rate (3) leading to a

much enhanced rate compared to CF88. In the remainder of this paper the Caughlan-Fowler rates will be referred to as the CF88 rates and Trojan Horse Method rates will be referred to as the THM rates. At relevant stellar burning temperatures the THM reaction rate is between 2 and 20 times enhanced, meaning given the same conditions the THM rates will induce between 2 and 20 times as many C12 fusion reactions. The Trojan Horse method allowed for measuring of the rates at lower energies than typical, around the Gamow peaks and at these energies were where the resonances were found.

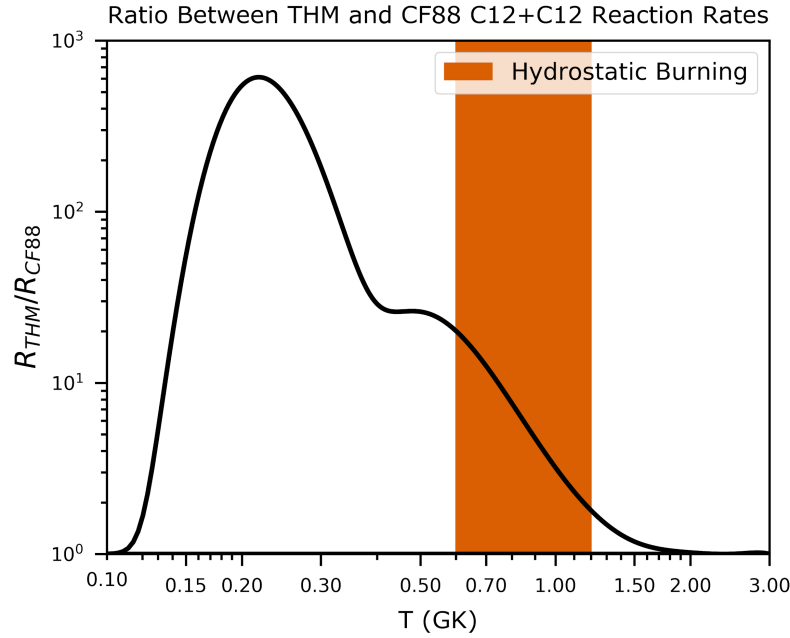


Figure 1. | The ratio between the Trojan Horse Method C12-C12 rates (THM) and the Caughlan-Fowler 1988 rates (CF88) for different temperatures.

Many papers have been written exploring the effects of different C12-C12 fusion reaction rates, exploring the effects on the s-process and p-process (5), Type Ia Supernova (6), stellar evolution (7) but not much work has been done in 2-D. In this study we expand on previous work performed in 1D and extend it to 2D using the magnetohydrodynamic code FLASH (8). 2-D simulations allow for physics that does not exist in 1-D simulations, allowing for deeper and more meaningful analysis of the problem.

In this paper, section 2 explains the methods used to perform the study including the code utilized, details of the progenitor, and the reaction rates tested. Section 3 explores the increase in nuclear energy production as a result of the THM rates. Section 4 explores the effects of the THM rates on convection. Section 5 examines the change in isotope abundance. Section 6 and 7 include conclusions and discussion of future work.

2. Methods

As mentioned before we make use of the magnetohydrodynamic multidimensional code FLASH from the University of Chicago's Flash Center for computational science. FLASH, written in Fortran-90 is capable of running many different astrophysical scenarios in 1-D, 2-D and 3-D including Type Ia supernova, core-collapse supernova, cosmology, general fluid dynamics, and in our case, stellar evolution. It is publically available and highly modular allowing for the customization of the code to suit specific needs or introduce additional mechanics into simulations.

In this study we examine a 25 solar mass star which is already well into the carbon shell burning stage. This type of star was chosen to ensure the study of the THM rates was meaningful as this star well beyond the mass range required to burn Carbon and is already doing so when our simulations begin. To obtain this star, Modules for Experiments in Stellar Astrophysics (MESA) (9) was used to simulate the life of a 25 solar mass star in 1-D from birth to death and a snapshot of the star during carbon shell burning was extracted as essentially a line of data and then mapped into 2-D into a form which FLASH could understand. Our progenitor was chosen much based on a Kippenhahn diagram shown in Figure 2. In this figure the x axis is the model number which is essentially a proxy for time scaled logarithmically where at small model numbers large periods of time are represented and at bigger model numbers smaller time periods are represented. This figure shows the shells of different isotopes where a vertical slice represents the abundance of material growing radially. The model number we selected is represented by a dashed line and in this slice we see the carbon shell region between the yellow and blue lines and that convection is occurring (mixing) in this region, indicating carbon shell burning is taking place. Because this model has a convective carbon shell we selected it to be mapped into FLASH and serve as our progenitor.

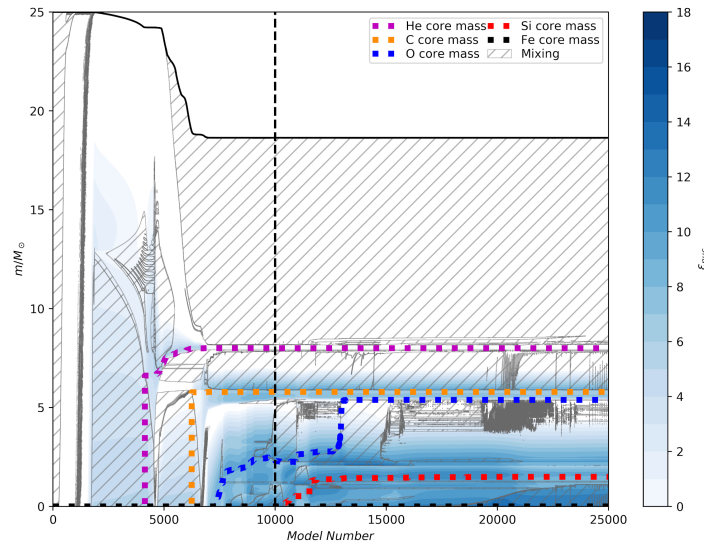


Figure 2. | A Kippenhahn diagram of our MESA run which produced the progenitor used in the main simulations. Model number is a proxy for time scaling logarithmically, the model used in our main simulations is marked by the vertical dashed line.

In part because the progenitor comes from a separate simulation, our FLASH simulations essentially start as a hunk of isotopes at specified conditions (density, temperature etc.), where no processes such as fusion are taking place. This allows the simulation to develop and evolve entirely in its FLASH setting moving forward, but also has the effect of creating initial transients where the star behaves out of the ordinary physically. There is a period of time called the turnover time where the effects of these transients no longer affect the star going forward and is about 2,000s in this case. Our simulations are roughly 20,000s, allowing for several turnover times to pass by ensuring the results we find are not a result of initial transients or other factors but are as a result of the physics FLASH simulates.

Two simulations were run as part of this study. One was run using entirely the standard CF88 rates and the other implemented the CF88 rates except for the enhanced C12-C12 THM fusion rate. FLASH uses a fusion reaction network which is made up of 21 isotopes from Hydrogen to Nickel-56 called Aprox21 where each reaction in the network has a subroutine which calculates the reaction rate on any given timestep. To implement the THM rates a new subroutine was created which calculated the THM fusion rate using the formula shown in Figure 3. The formula used in the standard CF88 subroutine is shown in Figure 4. The simulation using only the CF88 rates called the standard C12-C12 subroutine in the network while the THM simulation called the newly created THM rate subroutine.

$$N_A \langle \sigma v \rangle = \sum_{i=1}^3 f_i = \sum_{i=1}^3 \exp[a_{i1} + a_{i2}T^{-1} + a_{i3}T^{-1/3} + a_{i4}T^{1/3} + a_{i5}T + a_{i6}T^{5/3} + a_{i7}\ln(T)]$$

a_i	f_1	f_2	f_3	f_{16}	f_{20}	f_{30}	f_{11}	f_{21}	f_{31}
a_{11}	1.22657×10^2	9.03221×10^1	2.28039×10^2	1.22687×10^2	9.03982×10^1	2.28056×10^2	3.21570×10^2	6.08741×10^2	3.14593×10^3
a_{12}	0.557112	-8.35888	-1.16039×10^1	0.557664	-8.35720	-1.15681×10^1	-0.815182	-1.42976×10^1	-2.26169×10^1
a_{13}	-9.05657×10^1	-6.17552×10^1	-2.40364×10^2	-9.05616×10^1	-6.17282×10^1	-2.40343×10^2	3.17671×10^1	3.43845×10^2	1.36110×10^3
a_{14}	-6.83561×10^1	-1.07514×10^2	-9.21375×10^1	-6.83178×10^1	-1.07358×10^2	-9.21156×10^1	-4.22173×10^2	-1.11874×10^3	-5.16494×10^3
a_{15}	1.42906×10^1	7.20344×10^1	1.25411×10^2	1.42891×10^1	7.20835×10^1	1.25484×10^2	5.23691×10^1	1.73098×10^2	7.85965×10^2
a_{16}	-2.43583	-1.37501×10^1	-3.25984×10^1	-2.46506	-1.38060×10^1	-3.24417×10^1	-6.35869	-2.33743×10^1	-1.29447×10^2
a_{17}	9.32623	-1.91793×10^1	-1.10903×10^2	9.35304	-1.91920×10^1	-1.10961×10^2	1.34509×10^2	3.60334×10^2	1.60224×10^3

Figure 3. | Above is the formula and coefficients used to calculate the THM C12-C12 rate in the simulation implementing these rates given by Tumino et al. (3). T represents temperature in GK.

$$\text{C12+C12 (MG24)} \quad Q = 13.933 \quad 4.27\text{E+26} * \text{T9A56} / \text{T932} * \text{EXP}(-84.165 / \text{T9A13} - 2.12\text{E-03} * \text{T9A} = \text{T9} / (1. + 0.0396 * \text{T9})$$

Figure 4. | The formula used to calculate the CF88 C12-C12 rate in the simulation implementing the CF88 rates (2). T9 represents temperature in GK, and the coefficients after T9 or T9A represent the power the value is raised to. Ex. T9A56 is T9A raised to the 56 power.

The simulations themselves were run on Michigan State University's High Performance Computing Center in 2-D, making use of several hundred thousand core hours, taking about a month constantly running to eclipse 20,000s simulation time. FLASH produced data in two forms, a data file and plot files. Plot files contain an enormous amount of information about each block in the grid which makes up the simulation such as the temperature, velocity, density, isotope abundances etc. and were produced once every second simulation time. The data file is written to every time step and contains information about the entire star such as the total mass of various isotopes, the total nuclear energy, kinetic energy and momentum. As a result we obtained a lot of data which we could dig into and explore. This data was analyzed in python, making use of the data visualization package yt (10) and was the focus of the study. We aimed to analyze the data from the simulation to examine how the THM rates might affect the dynamics of the star by looking at quantities from the plot and data files which could teach us about the nuclear energy production, strength of convection and change in element abundance.

3. Nuclear Energy Production

Perhaps the most obvious, but also a very important, quantity to examine when studying different reaction rates is the energy produced from fusion, and the difference in production as a result of the modified rates. In our THM simulation we are increasing the fusion reaction rate so naturally we would expect more nuclear energy production, more fusion means more energy released. During a fusion reaction the products of the reaction are less massive than the reactants, but mass must always be conserved so this discrepancy is solved in the release of energy, powering the star.

From the CF88 simulation to the THM simulation we are only changing one reaction rate, the C12-C12 rate, but see a very noticeable increase in nuclear energy production in the carbon shell burning region as essentially all of the fusion in this location is C12-C12 fusion. We see this increase in nuclear energy production throughout our simulation from beginning to end, shown in Figure 5. Essentially all of the carbon fusion is occurring on the inner surface of the carbon burning shell, so our plots are centered around this region. Throughout the simulation there is roughly 1.5x the nuclear energy production in this region when comparing the THM and CF88 simulations. Because the only modification between the two simulations is the enhanced C12-C12 rate it can be assumed that this difference in nuclear energy production is due to the enhanced rate.

We notice that the nuclear energy production is decreasing throughout the simulation, likely because at the beginning of our simulations there is a higher abundance of C12 in the region where burning occurs and as the simulation evolves there is less and less fuel to be burned. It is worth noting that although the total nuclear energy production is decreasing with time in our simulations, the factor of nuclear energy production in the THM simulation versus the CF88 remains at a steady 1.5. This factor of increase in nuclear energy production from the two simulations is in line with what is expected. Analytically at the temperature around the surface of the carbon shell burning region, 1.26 GK, the ratio between the THM rate and the CF88 rate is 1.6. This can be seen as a direct test that the rates we are implementing are behaving as expected. Carbon is shown burning early in our simulation because our progenitor was taken

from a model where the star was already undergoing carbon shell burning, so from the start the star has the necessary conditions to begin burning.

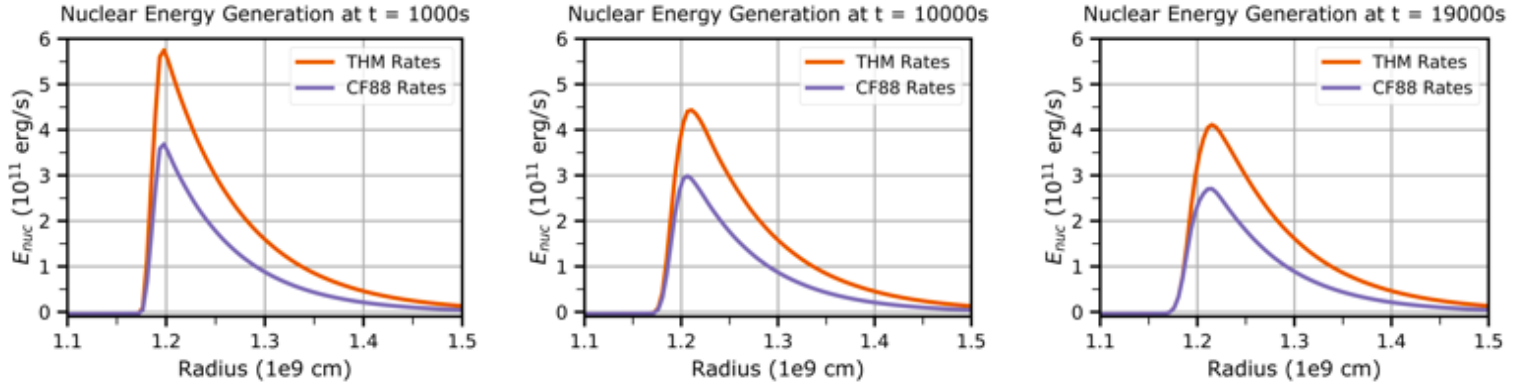


Figure 5. | Nuclear Energy Production radial profiles at roughly the beginning, middle and end of our simulation. Plots are centered around the inner surface of the Carbon burning shell.

Nuclear energy production serves as the energy source for the star, so it of course plays a large role in a star's life. The increase in nuclear energy production by itself is not all that interesting, but any energy produced in the star must go somewhere and affects other processes in the star, in particular convection.

4. Convection

The enhanced THM C12-C12 fusion rates has many impacts on the star's dynamics and processes but perhaps none more important than the process of convection. Convection is an important process for any star and occurs when there is a steep enough temperature or pressure gradient such that a parcel of material rises because of its discrepancy in pressure or temperature in relation to its neighbors. When material is heated, in our case at the inner carbon shell surface, it becomes hotter than the material in its surroundings and if hot enough the material will rise (11). This creates a mechanism for energy transport and also serves the purpose of mixing the material within the star, allowing for material to be transported to a region which it otherwise would not have. The transport of material from one region to another can serve to increase the efficiency of fusion by pulling matter which otherwise would not be in the burning region down to the burning region where it can be fused (12), and also can allow isotopes to mix together which otherwise would not.

Because convection is driven by energy generation associated with fusion, when we modify the rate at which fusion reactions take place we would expect to see a change in the convection. In this study's case we are enhancing the carbon fusion rates, resulting in more C12-C12 fusion, more energy production and as a result see an increase in the strength of convection. Convection already occurs in the carbon shell burning region with the standard

CF88 rates, but in the simulation implementing the THM rates we see a significant increase in the strength of convection throughout the simulation.

To study the change in convection we compared two quantities between the simulations, the non-radial energy generation and the velocity of material. The visualization of the velocity of material in the carbon shell region is perhaps the most telling and is shown in Figure 6. In these velocity magnitude plots we are only showing about the inner third of the star with respect to radius, which encompasses the carbon burning shell, and have adjusted the color bar to reflect the velocity in the carbon shell burning region. We ran two separate simulations but in these figures we are portraying them side by side for visualization purposes. These plots show a few things. Most apparently is that the THM simulation shows that the material in this convective carbon shell is moving much quicker than in the CF88 simulation throughout the spanned time. Also in the THM simulation we see there are many more and stronger convective nodes where the material swirls around in a circular pattern. It is also worth noting that at the 1000s timestep we have indication that carbon is igniting sooner in the THM simulation as a result of requiring a lower temperature for ignition due to the enhanced rates.

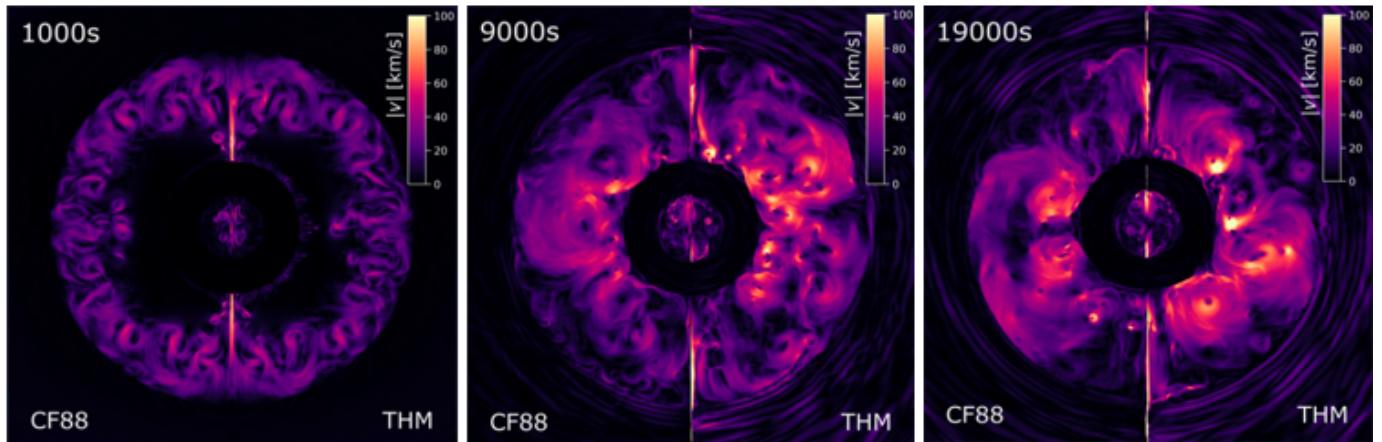


Figure 6. | Slice plots at 1000s, 9000s and 19000s showing the magnitude of velocity of material within the inner $r=4e9$ cm of the star. On the left of each panel is the CF88 simulation and on the right of each panel is the THM simulation.

A more quantitative measurement of the strength of convection is the non-radial energy production, shown in Figure 7. Radial energy can be thought of as the energy of the material traveling in the radial direction while the non-radial energy is the energy of material traveling in the direction perpendicular to the radial component. This quantity is stored in our data file and thus is the non-radial energy in the entirety of the star, not just the carbon shell burning region, shown in Figure 6. The non-radial energy generation is essentially a direct way to measure the

strength of convection as it tells us with what amount of energy the material is moving with in the star.

In Figure 7 we see that throughout the simulations, the THM simulation has a larger non-radial energy production and thus stronger convection. The THM simulation shows much higher non-radial energy especially towards the beginning of the simulations before about 10000s or so at which point the CF88 simulation somewhat catches up. This is likely because at the beginning of the simulation the two simulations start with the same amount of fuel to burn but because the THM rates are much enhanced it is able to burn through that fuel much quicker right away until it reaches a relative equilibrium point. Both simulations seem to reach a relative equilibrium where the non-radial energy fluctuates less but the THM simulation remains having a higher non-radial energy throughout. It is worth noting that the period from 0s to roughly 2000s is under the influence of an initial transient which is a feature of our simulations beginning and does not physically represent the situation well. After this initial transient and after a turnover time period has passed the features of the simulations are entirely due to the physics FLASH imposes.

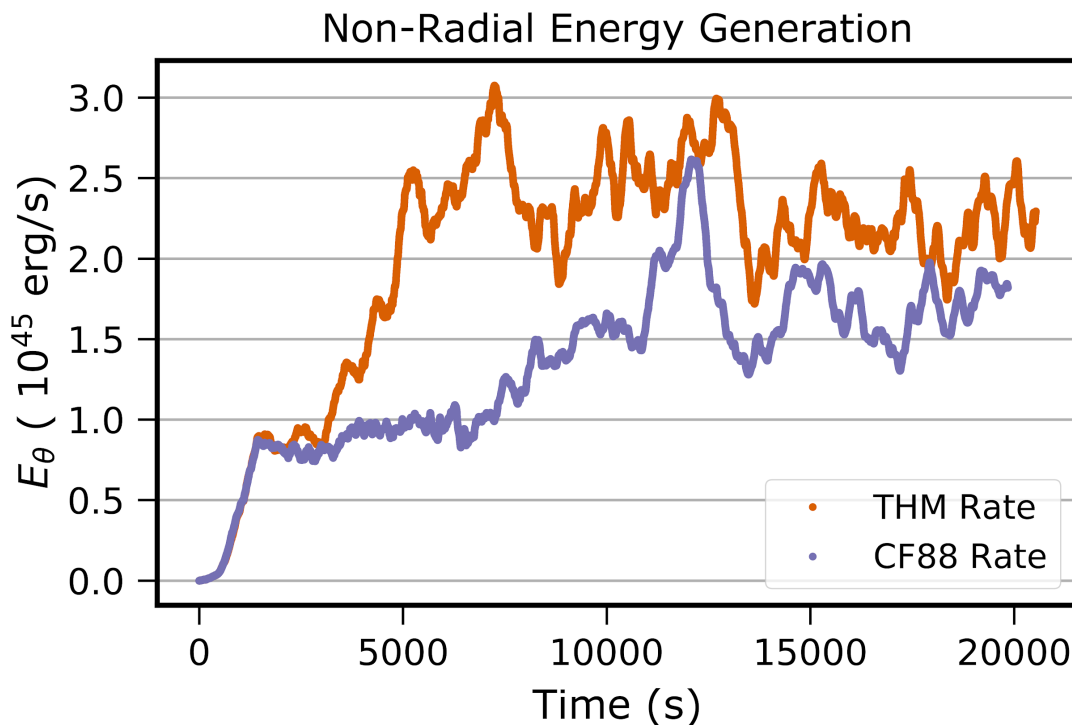


Figure 7. | Non-Radial Energy generation in both simulations with time, quantity reflects the star's full domain.

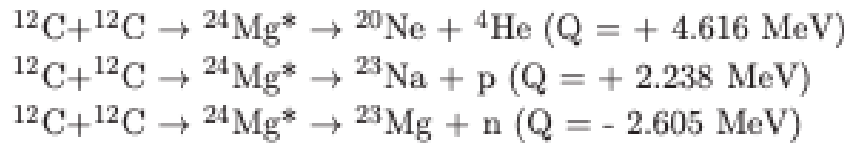
We have shown that when enhancing the C12-C12 fusion rate in a star undergoing carbon shell burning there is much stronger, more energetic convection in this burning region. This will serve the purpose of better mixing the material within the star leading to more efficient

burning and other possible side effects which would need to be studied more in the future such as how the increase in convection affects the structure of the star.

5. Element Abundance

Another consequence of changing the C12-C12 fusion reaction rate is a change in element abundance. During the process of fusion isotopes of one type react and produce isotopes of another form so it is not surprising that by changing the rate at which these fusion reactions take place would affect the abundance of elements.

C12-C12 burning takes place through three main channels:



These channels are all possible, but have different probabilities for multiple reasons, primarily because some are more energy favorable than others. The first two channels dominate C12-C12 burning and have roughly the same probability of occurring (5) so they were the main focus of our study. It is worth noting that the reaction rates discussed in this paper is the rate which encapsulates all 3 of these channels. In FLASH all of these fusion reactions occur but they depend on one common rate.

To study the effects of the THM rates on isotope abundance we compared the levels of the key isotopes in these different channels at the very end of our simulations, shown in Figure 8 which is centered around the inner surface of the carbon shell burning region. In this way we are seeing how the rates affected the levels of elements throughout the simulation, as both simulations start with the same progenitor and thus the same abundance of isotopes. In Figure 8 we see examine the three isotopes associated with the first fusion channel; C12, Mg24 and Ne20. In this reaction C12 and C12 fuses to form Mg24 which alpha decays into Ne20 and He4. Because we are increasing the rate at which C12 fuses in the THM simulation we see, when comparing the THM and CF88 simulations, a decrease in C12 abundance in the THM simulation and increases in Mg24 and Ne20 because they are products of the first C12-C12 fusion channel. This change in element abundance at present only occurs where carbon is being fused, directly on the inner surface of the carbon shell. Magnesium builds up on this surface and shows a large enough deposition such that it is pushed slightly inward and slightly outwards from the surface as well.

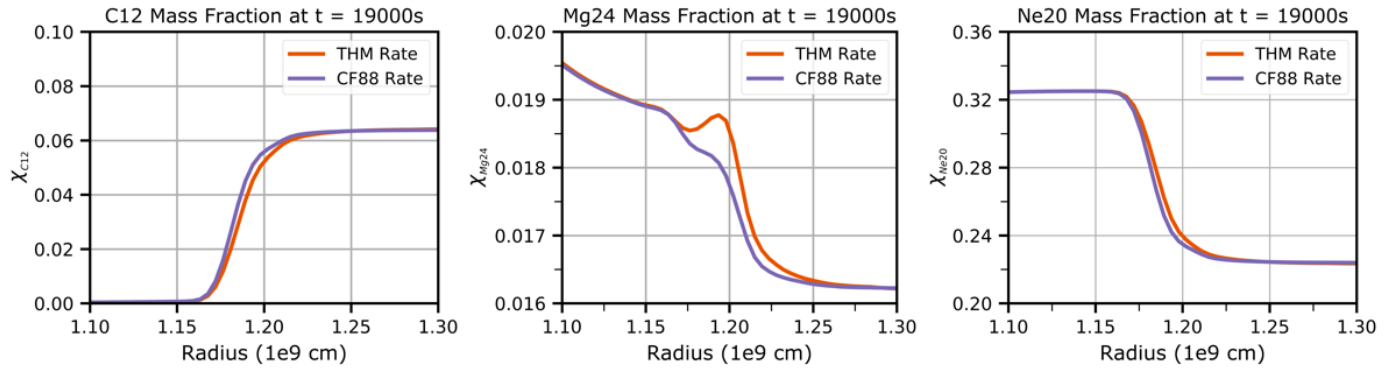


Figure 8. | Radial profiles of the mass fraction of the isotopes involved in the first C12-C12 fusion channel at the end of our simulations. Radius axis is centered around the inner surface of the carbon shell burning region, where the fusion is taking place.

Also in our analysis we notice a small increase in the products associated with the first two channels, He4 and p (H1). These changes in isotope abundance as a result of the THM rates can have a large impact on the star's future, mostly in the extra proton and alpha particle production. Alpha particles and protons can be used in proton and alpha particle captures such as $\text{Ne22} + \alpha \rightarrow \text{Mg25} + n$, which is the primary source for neutrons in the s-process of massive stars (5). These enhanced rates could also affect the isotope abundances in other stages of a star's not studied here, but has been studied in other papers such as Bennet et al 2012, and Pignatari et al. 2012, which have a very distinct impact on future fusion processes.

In this work we have shown that the enhanced THM C12-C12 rates undoubtedly have an impact on the star's chemical makeup as a direct result of enhancing the C12-C12 rate. Our simulations ran for only 20,000s which although is lengthy for a FLASH simulation, does not encapsulate a very significant part of a star's lifetime. It is perhaps reasonable to say that showing there is a change in isotope abundance on this time scale is significant because this affect will not go away as the star continues its evolution. It is also reasonable to say that these changes in isotope abundance may have an impact on other fusion reactions whose efficiency depends on the abundance of reactants.

6. Conclusion

In this work we studied the potential effects of enhancing the C12-C12 fusion reaction rate and studied in particular the effects of the rates A Tumino et al 2018 found using the Trojan Horse Method, which are much enhanced compared to the standard Caughlan-Fowler rates. We ran two identical simulations of a 25 solar mass star undergoing carbon shell burning, except one implemented the CF88 C12-C12 rate and one implemented the THM rate. We compared these two simulations to determine the impact of these enhanced rates and examined three main quantities, the nuclear energy production, strength of convection and isotope abundance. We found a 1.5x increase in nuclear energy production, a significant increase in strength of convection, and noticeable changes in isotope abundance in the THM

simulation. Our simulations ran for 20,000s simulation time, encompassing just a small portion of the star's lifetime but is relatively significant in terms of burning stages and covered several stellar turnover times. These affects could perhaps grow as the star experiences enhanced rates for a larger portion of its lifetime.

7. Looking Forward

To continue exploring the effects of enhanced C12-C12 fusion rates or the THM in particular, it will likely be useful to study a larger piece of the star's lifetime which is difficult to do in FLASH and in 2-D. The simulations performed in this work took hundreds of thousands of core hours so it would be more reasonable to use another code such as MESA which can simulate a much larger portion of a star's history in a more reasonable amount of time. This would also allow us to study the effects of enhanced rates on not just carbon shell burning but carbon core burning as well, and examine how a star will look different when it spends its entire lifetime with enhanced rates instead of just a snapshot of its life. We also can continue to explore the copious amounts of data produced by our FLASH simulations and continue to look for differences in the simulations by examining other parameters not studied in this paper.

References

- 1) <http://astrosun2.astro.cornell.edu/academics/courses/astro201/highmass.htm>
- 2) Caughlan, Fowler, 1988, "Thermonuclear reaction rates V"
- 3) A. Tumino et al., 2018, "An increase in the $^{12}\text{C} + ^{12}\text{C}$ fusion rate from resonances at astrophysical energies"
- 4) Jiang C. L. et al., 2018, "Reaction rate for carbon burning in massive stars"
- 5) M. Pignatari et al., 2012, "The $^{12}\text{C} + ^{12}\text{C}$ reaction and the impact on nucleosynthesis in massive stars."
- 6) K. Mori et al., 2018, "Impacts of the New Carbon Fusion Cross Sections on Type Ia Supernovae"
- 7) Halabi, El Eid, 2014, "Effect of $^{12}\text{C}+^{12}\text{C}$ Reaction & Convective Mixing on the Progenitor Mass of ONe White Dwarfs"
- 8) FLASH code, <http://flash.uchicago.edu/site/flashcode/>
- 9) Paxton et al., 2018, "Modules for Experiments in Stellar Astrophysics (MESA): Convective Boundaries, Element Diffusion, and Massive Star Explosions"
- 10) <https://yt-project.org/>
- 11) E. A. Spiegel, 1972, "Convection in Stars"
- 12) Chiosi, 2007, "Convection and mixing in stars: theory versus observations"
- 13) Bennett et al., 2012, "The effect of $^{12}\text{C} + ^{12}\text{C}$ rate uncertainties on the evolution and nucleosynthesis of massive stars"