Nova Nucleosynthesis Calculations: Robust Uncertainties, Sensitivities, and Radioactive Ion Beam Measurements

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Abstract.
We examine the quantitative impact of nuclear physics uncertainties on predictions of nova models via Monte Carlo simulations wherein, for the first time, the uncertainties of all relevant nuclear reactions are considered simultaneously. We determine uncertainties in predictions of isotope synthesis - including radioisotopes which may be observable tracers of novae - resulting from uncertainties in the input nuclear physics. We also detail the reaction rate sensitivity of radioisotope production, and discuss reactions which need further study. Finally, we examine the influence on nova nucleosynthesis of two new reaction rates - ^{17}F(p,γ)^{18}Ne and ^{14}O(α,2p)^{16}O - that were studied in recent ORNL measurements with radioactive ion beams.

MOTIVATION

The very high temperatures and densities of nova outbursts - greater than 10^8 K and 10^4 g/cm^3, respectively - enable unstable nuclei produced by capture [e.g., (p,γ)] reactions to undergo further reactions before they decay. The resulting sequences of reactions (the hot CNO cycles and rapid proton capture process) differ substantially from reaction sequences in non-explosive stellar environments [1], with energy generation rate up to 100 times greater. Furthermore, the resultant pattern of synthesized abundances are also different from solar, with overabundances of ^{13}C, ^{15}N, and ^{17}O, as well as Ne, Na, and heavier elements in some explosions. Long-lived radioactive nuclei such as ^{18}F and ^{22}Na are also synthesized and ejected, and their observation may provide stringent constraints on nova models [2, 3].

Progress in probing the nova phenomena can be made with improved determinations of the rates of the important reactions as a function of temperature. The sensitivity of nova model predictions of energy generation and element synthesis to selected reaction rates has been demonstrated in numerous studies (e.g., [4, 5]). Especially important are reactions involving proton-rich radioactive nuclei with relatively short ($\lesssim$ 1 minute) lifetimes [6, 7]. Experimental determinations of some of these reaction rates are now becoming possible with the availability of beams of radioactive nuclei at a number of facilities worldwide [7]. Since these beams are difficult to produce, it is crucial to guide experimental programs by determining which nuclear reactions have the largest impact on predictions of nova outburst simulations. Ideally, the correlation between all relevant reaction rates and all synthesized isotopes should be determined. Furthermore, it is desirable to determine to what accuracy any given rate should be measured, especially in light of the uncertainty of all the other reaction rates. We have addressed these issues with our Monte Carlo studies of nova nucleosynthesis, where - for the first time - we simultaneously consider the uncertainty of *all* input nuclear reaction rates to determine *all* correlations between rates and abundance synthesis predictions. It is also important to determine the impact of new determinations of reaction rates, and we have addressed this by varying individual rates and examining the changes in model predictions. Finally, our study is the first to quantitatively determine the uncertainties on abundance predictions in novae considering the uncertainties of all nuclear reaction rates. This enables statistically robust comparisons of nova model predictions to observations.

NOVA NUCLEOSYNTHESIS CALCULATIONS

The temporal evolution of the isotopic composition in novae was followed using a nuclear reaction network [8] containing 169 isotopes, from hydrogen to ^{54}Cr with nuclear reaction rates drawn from REACLIB [9]. We have examined the nucleosynthesis in 3 nova models: on a 1.00 $M_\odot$ CO White Dwarf (WD), and on 1.25 $M_\odot$ and 1.35 $M_\odot$ ONeMg WDs. The first two are representative of the most prevalent classes nova, while the third represents a more energetic outburst. The calculations for the 1.25 $M_\odot$ and 1.35 $M_\odot$ ONeMg WDs begin with a set of initial abundances for 169 nuclides, adopted from Politano et al. [10]. They assumed a solar composition mixed with 50% by mass oxygen, neon and magnesium. The initial abundances for the 1.00 $M_\odot$ CO WD nova was 50% solar and 50% products of He burning (an equal mix of ^{12}C and ^{16}O with a trace of ^{22}Ne). The enhancement in each case was representative of the envelope material mixing with the matter from the underlying white dwarf [11].

We utilized a post-processing approach where the nucleosynthesis is decoupled from the hydrodynamics of the burst. Since our reaction variations did not appreciably change the nuclear energy generation nor, therefore, the temperature and density history of the explosion, this approach was deemed valid. We simulated the explosion by extracting hydrodynamic trajectories – time histories of the temperature and density – from one-dimensional hydrodynamic calculations with a limited reaction rate network for outbursts on 1.0, 1.25, and 1.35 $M_\odot$ WDs similar to Ref. [4]. Different mass elements ("zones") of the envelope at different radii generate unique trajectories. In our simulations, the ejecta of each of the nova models consists of between 26-31 zones. For our studies of the sensitivity of individual reactions, separate nuclear reaction network calculations with the full complement of nuclei and nuclear reactions were carried out to study the nucleosynthesis details within each zone; no mixing of the zones was included. To calculate the final total predicted abundances in the ejecta of each explosion, a sum was made of abundances over the zones, weighted by the ratio of the zone mass to the total envelope mass. These calculations are more realistic than previous post-processing nucleosynthesis calculations which used constant temperatures and densities and those which considered only the hottest zones of the explosion (e.g., [5]).

MONTE CARLO SIMULATIONS

To investigate the extent to which nuclear reaction uncertainties translate into abundance variations, we use a Monte Carlo technique which assigns a different, uncorrelated, random enhancement factor to *each* reaction rate in the simulation. The nucleosynthesis is calculated with these modified reaction rates, the results stored, and the process repeated with different enhancement factors. After 10000 iterations, the mean values and 90% confidence limits are determined from the distribution of abundance predictions. In this paper, we present results from the innermost zone of a 1.25 $M_\odot$ WD nova model, though the method can examine the impact on entire outburst models. A representative example for the radionuclide ^{22}Na is shown in Figure 1.A., where the upper and lower 90 % confidence limits differ by a factor of 3.6. Monte Carlo methods have been employed with great success in the analysis of Big Bang nucleosynthesis [12], but have not previously been applied to other thermonuclear burning scenarios. These confidence limits are the first statistically robust uncertainties determined for nova nucleosynthesis. They have important implications for determining the sensitivity of orbital observatories (e.g., INTEGRAL) for detection of gamma rays from novae.

The reaction rate enhancement factors are distributed according to the log-normal distribution, which is the correct uncertainty distribution for quantities like reaction rates which are manifestly positive [13],

$$p_{log-normal}(x) = \frac{1}{\sqrt{2}\pi\beta x} \exp\left(-\frac{(\ln x - \alpha)^2}{2\beta^2}\right) \ , \tag{1}$$

where α and β are the (logarithmic) mean and standard deviation, respectively, and $p(x)dx$ is the probability of finding p in the range x to $x+dx$. Our use of the log-normal distribution for the reaction rates represents a significant improvement over previous Monte Carlo calculations. For small uncertainties ($< 20\%$), the difference between the log-normal distribution and the normal (gaussian) distribution is small. However, for uncertainties of larger sizes like those encountered in this problem, the difference is important. Figure 1 shows the difference between normal and log-normal distributions for the abundance prediction of one isotope, ^{22}Na. We have assigned uncertainties of $\sim 50\%$ $[\beta = \ln(1.5)]$ to rates whose measurement would require radioactive ion beams, and uncertainties of a factor of 2 for rates calculated by Hauser-Feshbach methods. Beta decay rates are given their tabulated values [14]. For all other rates we assign $\beta = \ln(1.2)$. We have deliberately used uncertainties that are somewhat underestimated to ensure that our resulting Monte Carlo uncertainties are not unduly inflated. Even so, many of the abundant metals have 90% confidence limits with a width of a factor of 2 or larger, such as ^{16}O (2.7), ^{17}O (2.7), ^{18}O(3.3), and ^{30}Si (5.6). The predicted abundances of radionuclides also have large uncertainties: for ^{18}F, the 90% confidence level spans a factor of 3.3, and for ^{26}Al, it spans a factor of 3.6.

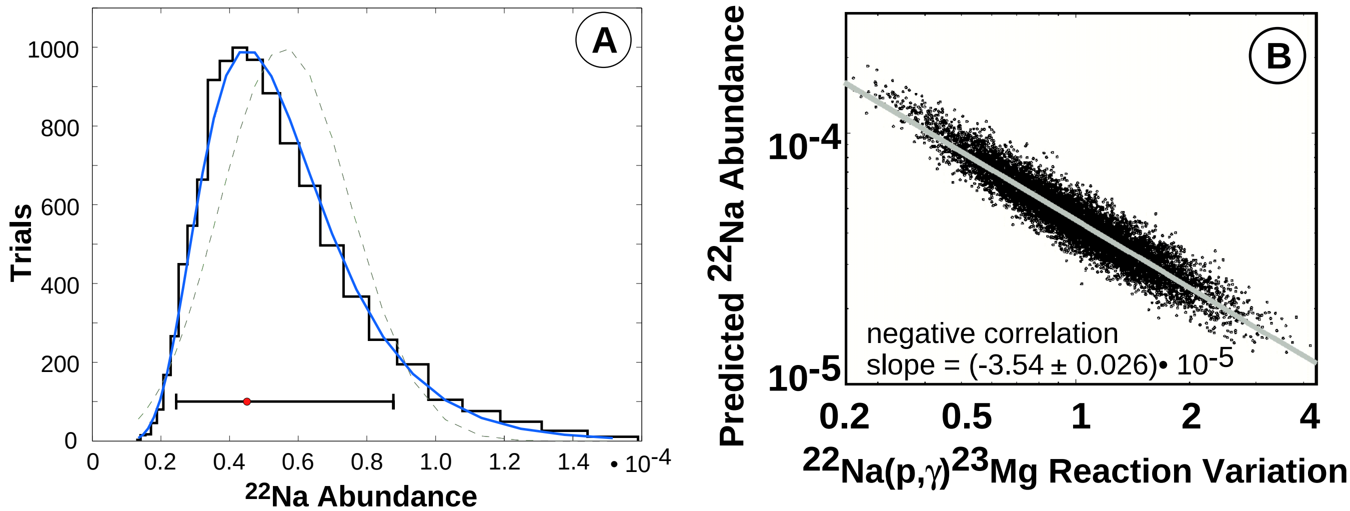

FIGURE 1. A. Histogram of the deviations of the predicted ^{22}Na abundance from the mean in the Monte Carlo simulation. The solid (dashed) curve is the log-normal (normal) distribution with logarithmic (arithmetic) mean and standard deviation from the Monte Carlo. The mean abundance and 90 % confidence levels are shown by the horizontal bar. B. Distribution of the predicted ^{22}Na abundance with the variation in the ^{22}Na(p,γ)^{23}Mg reaction rate. A linear fit and the slope are also indicated.

We also determine the correlation between small variations of *all* relevant reaction rates and *all* synthesized isotopes in the outburst. Figure 1.B. shows a representative result - the distribution of the predicted ^{22}Na abundance with the variation in the ^{22}Na(p,γ)^{23}Mg reaction rate. A linear fit determines that, in this case, there is a negative correlation – as the capture rate increases, the resulting ^{22}Na abundance decreases – and that the correlation is statistically significant – the slope is more than a few standard deviations different from zero. We have used our analysis, for example, to determine a prioritized list of reactions that most influence the production of radioisotopes that may be observable tracers of novae. For ^{18}F, the critical reactions are (in order of importance) ^{17}O(p,γ)^{18}F, ^{17}F(p,γ)^{18}Ne, ^{16}O(p,γ)^{17}F, ^{18}F(p,α)^{15}O, and ^{17}O(p,α)^{14}N. For ^{22}Na, the most important reactions are: ^{22}Na(p,γ)^{23}Mg, ^{20}Ne(p,γ)^{21}Na, ^{23}Na(p,α)^{20}Ne, ^{23}Na(p,γ)^{24}Mg, and ^{21}Na(p,γ)^{22}Mg. For ^{26}Al, the most important reactions are ^{23}Mg(p,γ)^{24}Al, ^{26}Al(p,γ)^{27}Si, ^{23}Na(p,γ)^{24}Mg, ^{23}Na(p,α)^{20}Ne, ^{20}Ne(p,γ)^{21}Na, ^{25}Mg(p,γ)^{26}Al, and ^{25}Al(p,γ)^{26}Si. Radioactive beams are required to study a number of these reactions, and our calculations can be used to set priorities for reaction measurements.

REACTION RATE SENSITIVITY STUDIES

A recent measurement of the excitation function for the ^{1}H(^{17}F,p)^{17}F reaction at ORNL's Holifield Radioactive Ion Beam Facility was used to obtain the first unambiguous evidence for the $J^{\pi} = 3^{+}$ state in ^{18}Ne and precisely determine its energy and total width [15]. This was in turn used to determine a new ^{17}F(p,γ)^{18}Ne reaction rate [16], which

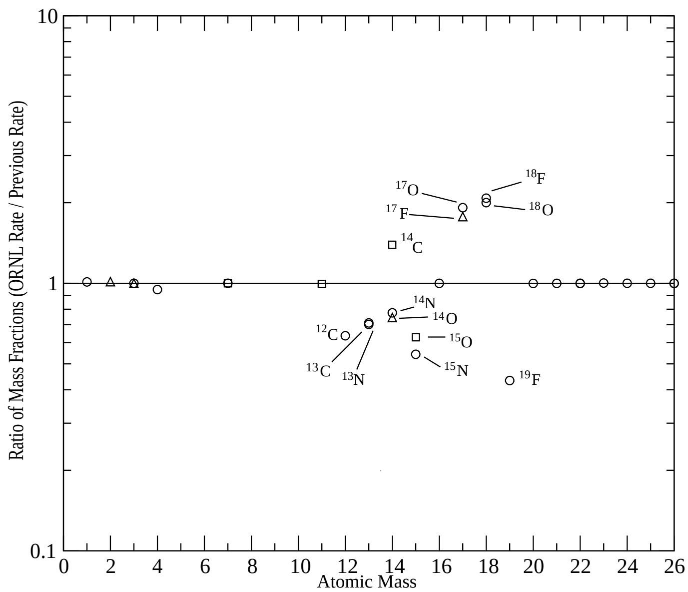

FIGURE 2. The ratio of mass fractions using the ORNL to that from one previous rate estimate [17] plotted against nuclide mass for the entire envelope of a 1.25 $M_\odot$ white dwarf nova. The ORNL rate changes the mass fractions of some nuclei by up to a factor of 2. Changes in the hottest zones are up to a factor of 600. The circle symbols mark species with mass fractions greater than 10^{-8}, the square symbols mass fractions between 10^{-8} and 10^{-16}, and the triangle symbols mass fractions less than 10^{-24}.

was up to a factor of 30 slower than the widely-used rate [17] found in REACLIB. We analyzed these rates in our post-processing nucleosynthesis code to determine the impact of the new HRIBF measurement [18]. The ratios of abundances produced using the two rates is shown in Figure 2. We find that in the 1.25 $M_\odot$ WD nova, for example, the new rate changes the abundances of ^{18}F, ^{18}O, ^{17}F and ^{17}O synthesized in the hottest zones up to a factor of 600 compared to some previous estimates, and produced significant changes in the abundances of ^{18}F, ^{18}O, ^{17}F, ^{17}O, ^{19}F, ^{15}N, ^{15}O, ^{12}C , ^{13}C, ^{13}N, ^{14}N and ^{14}O by up to a factor of 2.1 when averaged over the entire exploding envelope. The changes are even larger (to a factor of 14,000 in the hot zone and 3.7 overall) for the 1.35 $M_\odot$WD nova, but almost negligible for the cooler 1.0 $M_\odot$WD nova.

The production of the important, long-lived radionuclide ^{18}F is increased in the hottest zones of the nova by the network using the slower ORNL ^{17}F(p,γ)^{18}Ne rate. This is because a faster ^{17}F(p,γ)^{18}Ne rate creates ^{18}F sooner after the peak of the outburst (from decay of ^{18}Ne) and therefore at higher temperatures – where it is more likely to be destroyed by ^{18}F(p,α)^{15}O. The network with slower ^{17}F(p,γ)^{18}Ne rate delays the production of ^{18}F and therefore creates more of it at a lower temperature – where it is more likely to remain as a mass 18 isotope. This effect does not, however, carry over to the outer zones of the explosion, because the overall lower temperatures of these zones limits the post-peak destruction of freshly-synthesized ^{18}F. If only the hottest zones were considered, an incorrect conclusion would have been drawn regarding the change in the synthesis of ^{18}F – showing the importance of considering the nucleosynthesis throughout the nova model. Mixing of the zones, which was not included in our calculations, could also significantly affect the final calculated abundances.

Another sensitivity study was motivated by an ORNL measurement that found a possible simultaneous two-proton decay out of a resonance in ^{18}Ne via a measurement of the ^{17}F(p,2p)^{16}O reaction using a radioactive ^{17}F beam [19]. This suggests that there is a reaction link ^{14}O(α,2p)^{16}O, proceeding through this resonance in ^{18}Ne, which is not currently included in the nucleosynthesis network. To determine the possible impact on nova nucleosynthesis that this reaction could have, we varied the rate of this reaction (as multiples of the rate of the competing ^{14}O(α,p)^{17}F reaction) and inserted this into our reaction network. The results showed that there is no change in nova nucleosynthesis for strengths of this reaction equal to or weaker than the ^{14}O(α,p)^{17}F reaction. Our analysis shows that the sum of the mass flow of nuclei via ^{14}O(α,p)^{17}F and via ^{14}O(α,2p)^{16}O(p,γ)^{17}F is roughly constant. We also carried out detailed sensitivity studies for the ^{14}O(α,p)^{17}F reaction and determined that this reaction has little influence on element synthesis in novae [20].

ACKNOWLEDGMENTS

ORNL is managed by UT-Battelle, LLC, for the U.S. Department of Energy under contract DE-AC05-00OR22725. W.R.H. is supported by NASA under contract NAG5-8405, NSF under contract AST-9877130, and by funds from the Joint Institute for Heavy Ion Research.

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