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Message from the Assistant Deputy Administrator for Stockpile Stewardship, Chris Deeney

A number of years ago, Dr. Richard Carlson penned the runaway best seller "Don't Sweat the Small Stuff…And It's All Small Stuff." This may be good advice for achieving serenity in our lives, but the articles in this issue of the Stockpile Stewardship Quarterly demonstrate that, in pursuit of stewardship, the small stuff really does matter. Whether it be the change in distribution of energetic ions at a boundary layer in a fusion plasma, through twining in solids to diffusion in mix, the details matter. This is one of the reasons that I find the stewardship program so exciting by being both intellectually challenging and impactful. The stewardship community must perform rigorous science at all scales leading to managing the lifecycle of the nuclear deterrent, thus enabling national policy. This is a great motivation for many in our program.

The human element remains key to stewarding the deterrent and we sadly (for us) have to acknowledge the retirement of three members of our team at NNSA Headquarters: Dr. Jeff Quintenz, Dr. Tom Finn and Mr. David Dixon. At the same time, we celebrate the awards received by Professor Jolie Cizewski, the American Physical Society's Woman Physicist of the Month award, and Dr. Mark Herrmann, Fusion Power Associate's 2012 Excellence in Engineering Award. Those who are starting their careers, and thus becoming part of our human element, should take note of DOE's prestigious Computational Science and Stewardship Science Graduate Fellowship programs. Please encourage talented graduates to apply. The competition is fierce, but the opportunities are immense! An example of the scientific opportunity is the article by Robert Hoffman et al. When we achieve ignition, the resultant neutron fluence will enable new experimental opportunities to study nuclear science relevant for radiochemistry and nuclear synthesis studies.

Finally, to revisit my opening comments on serenity, let me acknowledge the great uncertainties I know many of you have as those of us inside the beltway work through an apparently never ending series of budget crises and issues. We all understand the worries, but NNSA management at all levels believes in the strength, quality and importance of our program. With your superior work to underpin our claims, we are well positioned for the decisions to come. Keep up the excellence, and we will work through the budget crises. Unfortunately, our ability to predict hydrodynamic turbulence use exceeds our predictive abilities on budget and politics inside Washington, DC at the moment, so we can offer no timescales yet for stability. However, be comforted that our program is broadly supported.

Retirement Roll Call

The Office of Stockpile Stewardship bid farewell to Dr. Jeff Quintenz, Director, Office of Intertial Confinement Fusion in November 2012. We also said goodbye to Dr. Tom Finn, Physical Scientist and Program Manager in January 2013 and Mr. Dave Dixon, a Project Manager and Procurement Officer based out of the Albuquerque Service Center. Their numerous contributions, level of excellence, and fine service to the nation will long be remembered. We wish them a very happy retirement. They will be missed!

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Comments
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Accounting for Energy Changes in Hydrodynamic Mixing: The Role of Enthalpy Diffusion

by Andrew W. Cook and Jeffrey A. Greenough (Lawrence Livermore National Laboratory)

Turbulent mixing of dissimilar materials, subject to strong driving forces, is a ubiquitous phenomenon in supernovae events, inertial confinement fusion (ICF) experiments and other applications. In ICF, for example, the interface between the plastic shell and the nuclear fuel becomes unstable during the implosion, leading to interpenetration and mixing of the two fluid species. The first step in any numerical simulation of such phenomena is to determine a complete set of equations governing the system, including all of the physically relevant terms. In setting forth the governing equations to be solved, informed choices must be made as to which terms to include and which terms to neglect. A complete description of diffusion physics would involve a rather large set of equations; however, in many cases, the system can be simplified by neglecting various effects. Of course, the danger in neglecting certain effects is that some important physics might inadvertently be left out.

One effect in particular, which has often been neglected in simulations of turbulent mixing, is *enthalpy diffusion*. Enthalpy is the amount of energy in a system available for doing mechanical work. It includes molecular energy as well as the work required to create space for the system by displacing its environment. The role of enthalpy diffusion can be understood by considering two ideal gases, say helium and xenon, sitting next to each other in thermodynamic equilibrium. As the gases diffuse across their common interface, helium molecules exchange places with xenon molecules on a one-to-one basis. Since xenon molecules are heavier than helium molecules, the mass on the helium side of the interface increases, while the mass on the xenon side decreases. Molecular diffusion thus generates a net mass flux through the interface. Furthermore, since diffusion neither adds heat nor does work on the system, the enthalpy per unit volume must remain the same on both sides of the interface. This means that the enthalpy per unit mass must change in accordance with the mass flux. The enthalpy diffusion term in the energy equation accounts for this change in enthalpy per unit mass resulting from species diffusion.[1]

The role of enthalpy diffusion can be understood by considering how changes in density come about when two initially quiescent ideal gases diffuse into each other. Density itself does not diffuse; i.e., there is no diffusion term in the mass-conservation equation. Changes in density can only occur if the velocity field is perturbed. According to the conservation-of-momentum equation, a nonzero velocity can only be generated if there is a pressure gradient. If the gases start out in thermodynamic equilibrium, then the only term in the energy equation capable of perturbing the pressure field is the enthalpy diffusion term. If this term is neglected, then species concentrations become decoupled from the other flow variables; i.e., although species concentrations may temporally evolve due to diffusion, other flow variables will remain fixed. This has the unphysical side effect of generating anomalous temperature spikes, since mixture specific heats depend on (changing) concentrations and (fixed) energy. By including the enthalpy diffusion effect, species concentrations become properly coupled to the other flow variables and mixing/diffusion is more physically captured.

Enthalpy diffusion has recently been incorporated into Ares, an Advanced Simulation and Computing (ASC) code for ICF and astrophysics. The code incorporates a Fickian diffusion flux, which drives species from high to low concentration. Simulations with and without enthalpy diffusion have been performed for the simple case of diffusion between helium and xenon, with both gases initially at standard temperature and pressure. Results of Ares' simulations are shown in Figure 1.

In the absence of enthalpy diffusion, the density field does not change from its initial configuration. By incorporating the additional physics, the density gradient properly relaxes, as seen by the solid black curve in the left plot.

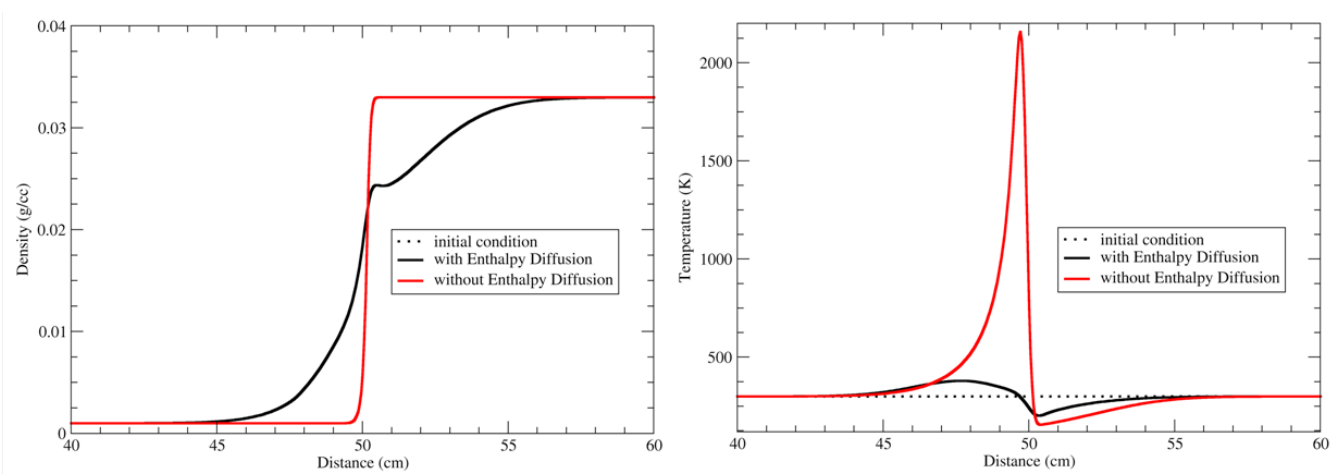

Figure 1. Density (left) and temperature (right) for diffusion between helium and xenon using a constant diffusivity of 1000 cm^2/s. The solid black curves are with enthalpy diffusion and the red curves are without enthalpy diffusion at the final time of 2 milliseconds. The dotted curves are the initial conditions.

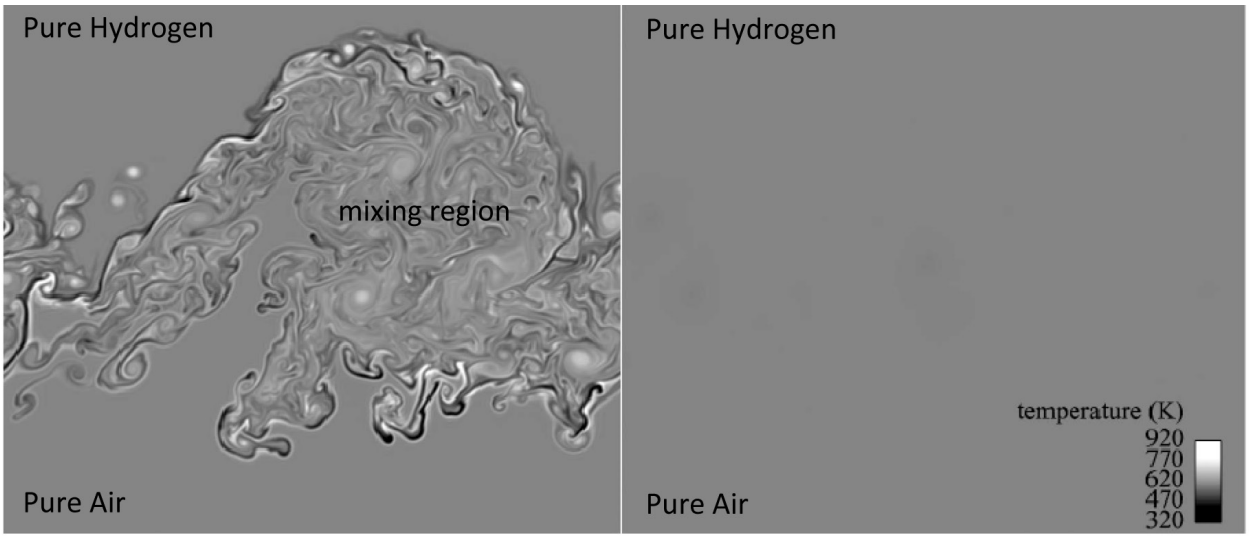

Figure 2. Temperature in a fully developed shear flow between pure hydrogen and pure air excluding (left) and including (right) enthalpy diffusion.

The temperature field exhibits striking differences with and without enthalpy diffusion. With the term excluded, the maximum temperature rises by nearly 700% above ambient conditions; however, by including the term, the peak temperature rises by only 20%. Anomalous temperature spikes, as seen here, can have dire consequences in flows with temperature-threshold effects, such as ignition of fuel-oxidizer mixtures.

Beyond this simple example, omission of enthalpy diffusion leads to anomalous temperatures in turbulent flows as well. Figure 2 shows the temperature field for a turbulent hydrogen-air shear layer, with and without enthalpy diffusion, as calculated by the Miranda code.[2] This flow is formed by a high speed stream of hydrogen gas encountering a low speed stream of air. The unstable interface between the gases develops into a turbulent flow. In the simulation with enthalpy diffusion (right frame), the temperature field appears nearly uniform. Without enthalpy diffusion, hot and cold regions spontaneously develop in the mixing region. In the left image, white regions exceed the ignition temperature of the mixture.

In simulating interfacial instabilities and turbulent mixing, ignoring enthalpy diffusion can lead to unphysical behavior of flow variables. In particular, the temperature of mixed zones depends sensitively on a correct accounting of energy changes resulting from changes in composition. Now that enthalpy diffusion has been implemented in Ares, simulations employing mixing models produce more physically correct results. Evaluations of the effects of enthalpy diffusion on problems of programmatic interest are currently underway. The Miranda research code is currently being used to ascertain whether additional physics (e.g., pressure and temperature-driven diffusion) is necessary to properly account for species mixing in ICF and other applications. Miranda's results will be used to guide the implementation of additional physics terms in Ares and serve to validate the new results.

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Fracture Model for Beryllium and Other Materials by Alek Zubelewicz and Abigail Hunter (Los Alamos National Laboratory)

The commonly used phenomenological constitutive models rely on a long-term, trial and error approach, which led to the development of physically and numerically robust material descriptions. The phenomenology means that the models are "good" in the domain already verified by experiment. Quite often though, extrapolation of the models into the regimes not tested can be troublesome. For instance, these models don't generally account for specific mechanisms of irreversible deformation such as the dislocation glide plasticity and partly (often fully) recoverable twinning; the latter is linked to crystallographic reorientations. Beryllium seems to provide an example for such difficulties. In beryllium, we observe brittle-ductile transitions associated with complex fracture processes and the deformation mechanisms include plasticity and twinning. We break the phenomenology and, instead, construct a mechanisms-based model that includes the two deformation mechanisms, while capturing brittle and ductile fracture.

Over several decades, Los Alamos National Laboratory (LANL) developed a set of excellent strength and fracture models for metals. While learning from the successes, the work has not stopped there because we believe that alternative modeling approaches should be pursued and validated, giving the chance for broadening the menu

of LANL's modeling capabilities. In here, we introduce the mechanisms-based visco-plasticity model capable of replicating brittle and ductile fracture processes. The model is tested for beryllium showing excellent agreement with experimental data.

Mechanisms-Based Approach

We adapted our earlier results[1] and constructed the mechanisms-based visco-plasticity model with built-in fracture in the framework of a tensor representation theory.[2] First, physics-based insight dictates the selection of relevant mechanisms of inelastic deformation models due to plasticity and twinning. Next, the magnitudes of the plastic flow and twinning are determined in terms of appropriate invariant strain rates. In our description, we enforce the principle of objectivity and, from there we derive equivalent (invariant) stresses compatible with plastic deformation and twinning. It is emphasized that the invariant measures are derived and not assumed. In this model, the equivalent stresses are coupled with the equivalent strain rates. Also, we include the contribution of the dynamic overstress, which plays a role when the rate of the energy redistribution and dissipation is slower from the rate the energy that is pumped into the material. Again, the formula for the overstress is derived and is based on thermodynamics considerations.[3] Thus, the flow rules (mechanisms for plasticity and twinning) along with the rate dependent constitutive relations and, lastly, the dynamic overstress, complete the description of the inelastic behavior of beryllium. The visco-plasticity model has unique features, among which is the ability to capture the ductile-brittle transition, strain rate effects from quasi-static up to extreme conditions, shear localization at elevated temperature and cleavage at high strain rates and/or low temperatures.

Brittle Fracture

A frequent assumption is that brittle fracture arises from a set of non-interacting penny-shaped micro-cracks randomly distributed in an otherwise homogeneous material.[4] Since the crack opening strain is collected from the individual micro-cracks, these descriptions are suitable for predicting the material's responses at early stages of the damage process. The cracks are characterized in terms of the crack surface area, while their orientations are defined in terms of stresses. One open issue in brittle materials is that these models predict an unlimited strength under bi-axial compression. This prediction seems unrealistic and, in fact, experimental observations gathered for various brittle materials provide arguments to the contrary.[5,6] The penny-shape crack approach has been further extended in Reference 7, but the previously mentioned concern of the non-interacting micro-cracks remains unsolved. In these constitutive models, fracture processes are built into the

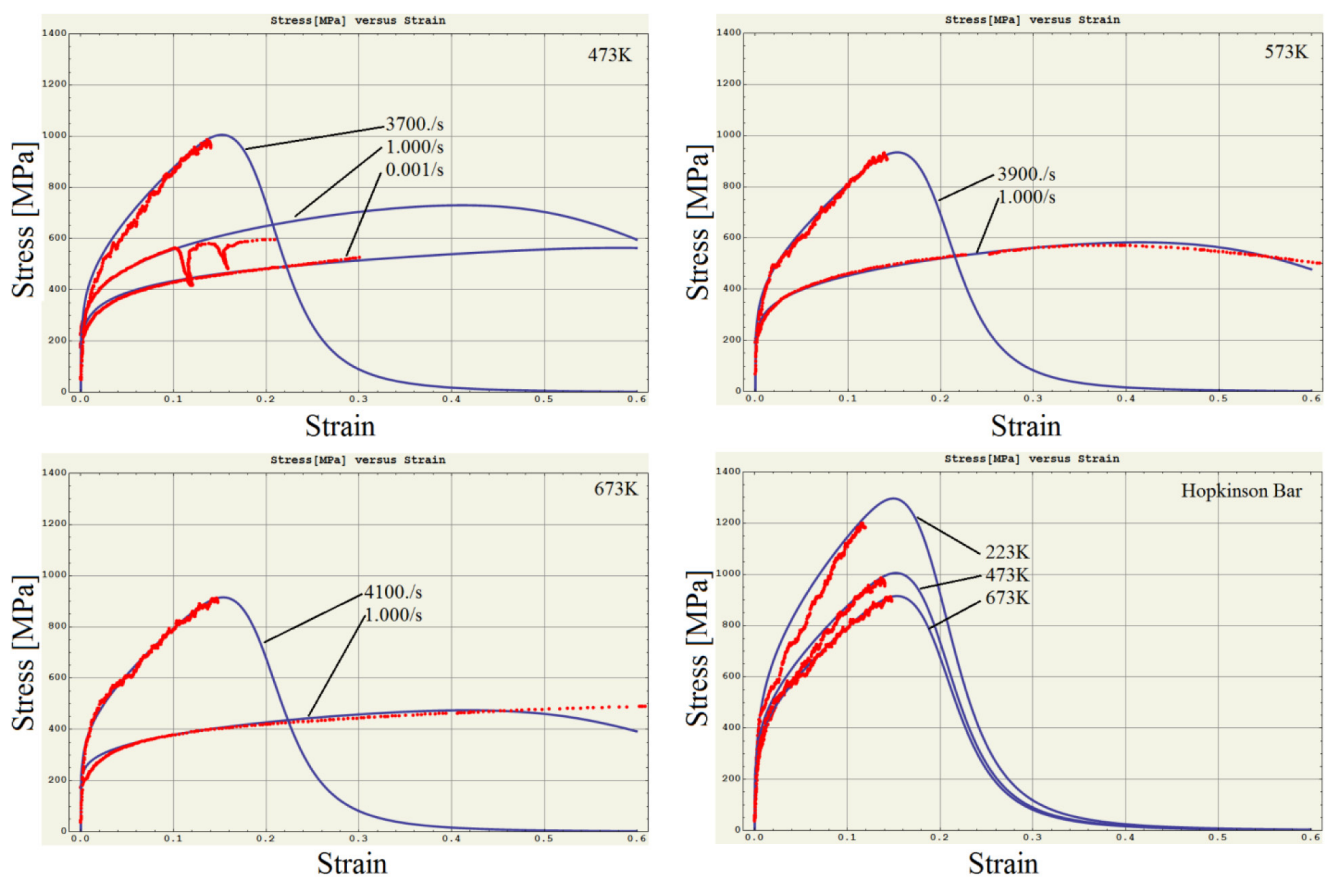

Figure 1. Uniaxial stress-strain responses in beryllium at various temperatures and strain rates. The red lines depict the LANL experimental data, while the blue lines represent to the model predictions.

constitutive description by degrading either the material's strength or elastic constants such as shear modulus.

Introduction of the micro-plane model[8] marks significant progress in the understanding of the behavior of brittle/frictional materials. The model predicts the damage initiation and progressive growth and it captures fracture mechanisms occurring within a representative volume element (RVE).[9] However, the introduction of RVE is a troublesome assumption, especially when considering an advanced stage of the post-critical behavior. The RVE homogenization technique fails at conditions where the cracks break up the volume. Also, the micro-plane model is quite complex and may present a challenge when applied to a large-scale numerical analysis. A relatively simpler model based on an analogous idea is proposed in Reference 1. In this description, the fracture processes are monitored in terms of stress tractions along the dominant load directions, while the stresses are acting on the crack opening displacements. As in many other cases, the fracture planes are co-rotational with principal stresses; therefore, this model produces fracture that is stress-co-rotational, thus isotropic. Despite this deficiency, the model is strong in its simplicity and surprisingly good predictability.

In metals, damage processes are often assumed to follow the Gurson's ductile mechanism.[10] This mechanism accounts for the progression of a distributed damage due to the growth of voids in an already plastically deformed material. However, it has been long known that other ductile and brittle fracture mechanisms are present in various metals and, among them, in beryllium. The mechanisms can be sorted into two groups:

- Ductile/brittle process zone due to either void growth and coalescence (ductile) or growth and coalescence of micro-cracks (brittle). Both processes follow the direction of the maximum tensile stress.
- Shear localized zones caused by a shear dominant loading. As before, we may have a brittle fracture (cleavage) and there is temperature assisted shear localization.

The brittle and ductile fracture processes are included in elastic energy, which is a potential expressed in terms of elastic strains and elastic constants. The elastic properties undergo a directional degradation, thus making the material anisotropic. Following experimental observations, brittle fracture in beryllium includes mode I cracking (triggered by maximum tensile stress) and cleavage (mode II fracture) in compression. Also, we account for the brittle-ductile fracture transition in tension and shear. The transitions are observed in the range of 200 °C and at high strain rates.

Model Calibration for Beryllium

The proposed fracture model is calibrated using the existing experimental data at LANL. The model reproduces the material behavior (see Figure 1) quite well. Yet, in our assessment, the calibration cannot be considered complete. For instance, there is a coupling of the inelastic deformation due to twinning and plasticity but the interactions are not well understood. In here, we assume that some twins cannot be recovered in the presence of plastic deformation but we do not know the exact fraction of stored twins at various temperatures and strain rates. Also, the ductile-brittle transition appears to be not only temperature but also rate sensitive.

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Nuclear Plasma Interactions on the National Ignition Facility

by Robert D. Hoffman, George Zimmerman, Mau Chen, and Charles Cerjan (Lawrence Livermore National Laboratory)

With the advent of the National Ignition Facility (NIF), increasing interest has focused on plasma physics processes that might be observed for the first time, in particular those mediated by electrons that could alter the populations of low-lying nuclear excited states. Inclusion of such processes into our simulation codes could also impact our interpretation of radiochemical ratios measured during the underground test program if the nuclear cross sections proceeding on a ground state versus a low lying nuclear excited state differ. (For example: the radiochemical ratio ^{170}Tm/^{168}Tm is formed when (n,2n) and (n,γ) reactions that proceed on ^{169}Tm produce the radioactive species ^{168}Tm and ^{170}Tm. Such radiochemical ratios are used to infer the overall neutron fluence in a plasma environment that has experienced nuclear interactions). ^{169}Tm is an important nucleus for stockpile stewardship radiochemistry as well as being an *s*-process branch point in stellar nucleosynthesis theory.

There are several nuclear decay and excitation processes mediated by electromagnetic coupling with atomic electrons. In cold, neutral atoms, since there are no valence electrons and no inner shell vacancies, the only process

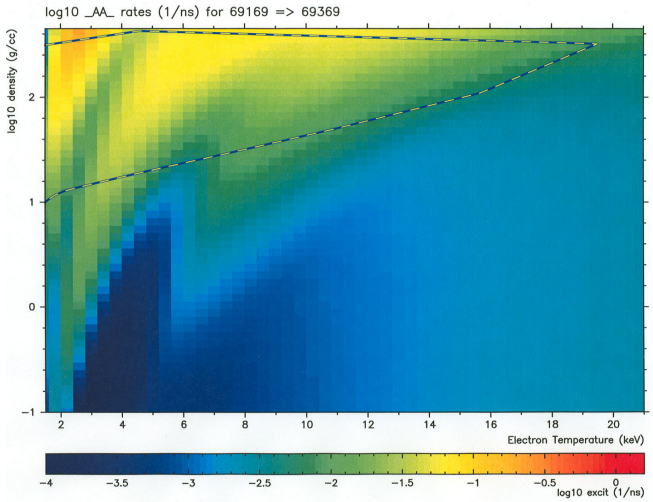

Figure 1. Electron-induced nuclear excitation rate as a function of electron temperature and density for the 8 keV ground to first excited state transition in ^{169}Tm.

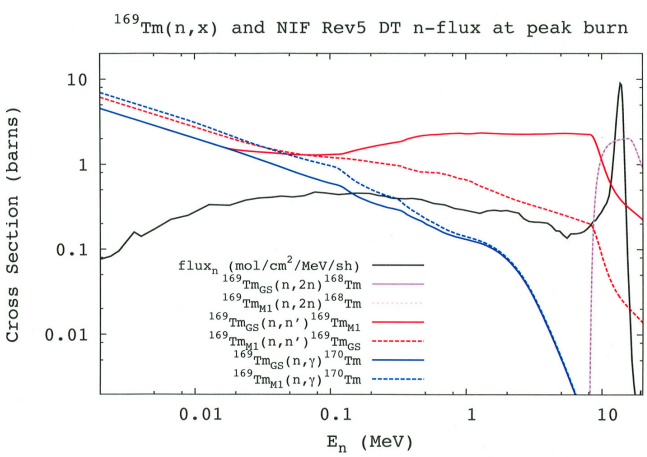

Figure 2. Neutron-induced cross sections on ground and first excited state targets of ^{169}Tm and the neutron flux at peak burn in the NIF Rev5 ignition capsule.

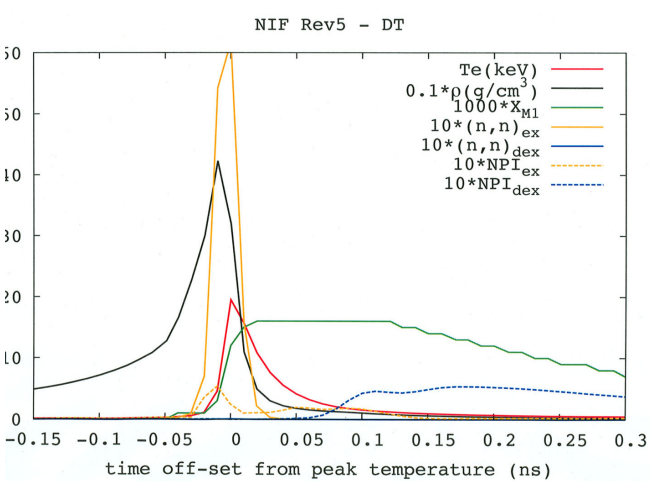

Figure 3. Quantities affecting the population of the 8 keV first excited state in ^{169}Tm.

that can occur is for the nuclear gamma decay energy to be transferred to a bound electron and typically ejected into the continuum, i.e., internal conversion (IC). This process is well understood theoretically and experimentally. However, in a high temperature plasma environment, there are both free electrons and many inner-shell and outer-shell vacancies that make other nuclear processes possible. For example, nuclear decay can excite a bound electron to an unoccupied bound state i.e., bound internal conversion (BIC). Conversely, the inverse of each process can also occur in a plasma environment. The inverse of IC occurs when a free electron is captured into the atomic bound state and transfers the released energy to an excited state in the nucleus, i.e., nuclear excitation by electron capture (NEEC).[1] The inverse of BIC occurs when the electron goes from a higher level to a lower level and resonantly transfers the decay energy to excite the nucleus, known as nuclear excitation via electron transition (NEET).[2]

We recently explored for the first time inclusion of these electron-induced nuclear excited state population effects in a simulation of the NIF Rev5 ignition capsule[3] that incorporates ^{169}Tm as a radiochemical tracer. In our simulation, we loaded 7.4x10^{14} atoms of ^{169}Tm into the innermost 5 mm ablator layer. With a 50-50 DT fuel mix, the Rev5 capsule provides a yield of 15.7 MJ of energy and a neutron yield of 5x10^{18} neutrons.

Electron & Neutron Preliminaries

Figure 1 shows the electron-induced nuclear excitation rates (NEET + NEEC + γ-absorption) for the 8 keV ground to first excited state transition in ^{169}Tm tabulated over a range of electron temperatures ($2 < T_e < 20$ keV) and densities ($0.1 < \rho < 490$ g cm^{-3}). A similar plot showing electron-induced de-excitation rates (IC + BIC + γ-decay) is given in Reference 4. Overlaid on the rates is the thermodynamic evolution of the DT burn region in our Rev5 capsule simulation. At peak burn (T_e=19.5 keV, ρ=319 g cm^{-3}), the excitation rate is 7.7x10^{-3} ns^{-1}, while the de-excitation rate is 6.0x10^{-3} ns^{-1}.

Figure 2 shows the most important neutron-induced cross sections in this work as well as the instantaneous neutron flux sampled in the DT burn region at peak burn. These are but a small fraction of the full reaction network used for this survey,[4] but they illustrate the main points. For each channel, we show the cross section proceeding on the ground state (GS: solid line) and on the 8 keV first excited state (M1: dashed line) of ^{169}Tm. Note that the neutron scattering cross section proceeding on the (loaded) ground state will preferentially populate the excited state for neutron energies > 0.1 MeV. Population by either the electrons or neutrons would lead to an enhancement of ^{170}Tm due to the 30% larger (n,γ) cross section that proceeds on the ^{169}Tm first excited state, thus providing a potential radiochemical signal. By contrast, the same amount of ^{168}Tm would be made no matter what distribution of ^{169}Tm ground or first excited state population prevails due to the identical (n,2n) cross sections. We will explore the difference in resulting radiochemical ratios with the electron excitation rates turned on and turned off.

Results

Figure 3 shows the temporal evolution of the DT burn region in our Rev5 capsule simulation (offset at peak burn time = 0 ns) for the scaled quantities: electron temperature (T_e, red), density (ρ, black), and the population of the 8 keV first excited state of ^{169}Tm (X_{M1}, in green). We have normalized the initial population of the ground state by the loaded amount to make X_{GS} = 1, and present all populations in terms of mass fraction. At peak burn X_{M1} = 0.017, or 1.7%. Also shown are three *nuclear flows* (the product of a target state population and a "reaction rate") which we use to gauge how fast X_{M1} is populated due to the neutrons and electrons.

The solid gold curve is the neutron excitation flow $(n,n)_{ex}$ (X_{GS} times the integral over all neutron energies of the product of the flux and the (n,n') cross section in Figure 2). The dashed gold curve shows the electron-induced excitation flow NPI_{ex} (X_{GS} times the excitation rate in Figure 1). Over the duration of the burn, the neutrons clearly dominate the contribution to X_{M1}. The dashed blue curve is the electron de-excitation flow NPI_{dex} that de-populates X_{M1} after the capsule comes apart. The de-excitaion flow for the neutrons is not visible (due to a small X_{M1}).

The populations of ^{170}Tm and ^{168}Tm at the end of our NIF Rev5 DT simulation with the electron rates turned on were 2.4×10^{-4} and 3.64×10^{-2}, respectively, making for a radiochemical ratio of ^{170}Tm/^{168}Tm = 6.6×10^{-3}. *These quantities were the same (to within 4 significant figures) with the electron-induced rates turned off.* The reason was not because the capsule didn't get hot (at ~20 keV, it did), or that the neutron flux was small (it wasn't), but rather there was no time for either excitation flow to populate X_{M1} enough to allow for substantial neutron capture to take place on the excited state (T_e was above 1 keV for only 0.14 ns). However, if one could maintain peak conditions long enough for the electron excitation and de-excitation rates to come into equilibrium (73 ns) X_{M1} would reach 36%, more than enough to distinguish a difference in the radiochemical ratio due to enhanced neutron capture when including the electron rates (vs. not).

In conclusion, the Rev5 capsule design on NIF, with its short DT burn timescale, is not a viable platform to observe NEEC or NEET using the ^{169}Tm first excited state transition.

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Knudsen Layer Reduction of Fusion Reactivity

by Kim Molvig and Nelson M. Hoffman (Los Alamos National Laboratory)

The work is a collaboration with Eric M. Nelson, Brian J. Albright, and Evan Dodd (LANL) and George Zimmerman and Ed Williams (LLNL). The idea of Knudsen losses of fuel ions was first suggested by Robert B. Webster (LANL).

Introduction

Over-prediction of fusion energy yield has been a persistent enigma in inertial fusion systems for over 50 years. Presented is a new piece of physics to help to resolve this puzzle. Our best (clean) theory and code predictions have systematically calculated higher energy yield from fusion than observed in experiments by factors of two and more. This yield over-prediction has traditionally been attributed to the "mix" of impurities into the fuel. Many models of such mix have been developed, refined and applied over the years. Nonetheless, current mix models fall short of being fully satisfactory. This work is motivated by the belief that it is missing physics beyond "mix" that is needed to account for yield over-prediction (although we certainly expect mix to play a role and have combined it with the new physics in simulating experiment). The Knudsen layer effect we describe briefly here (and published in Physical Review Letters[1]) is such a piece of physics that fundamentally reduces the fusion reactivity by depleting the high energy tail population of fuel ions that are primarily responsible for the yield.

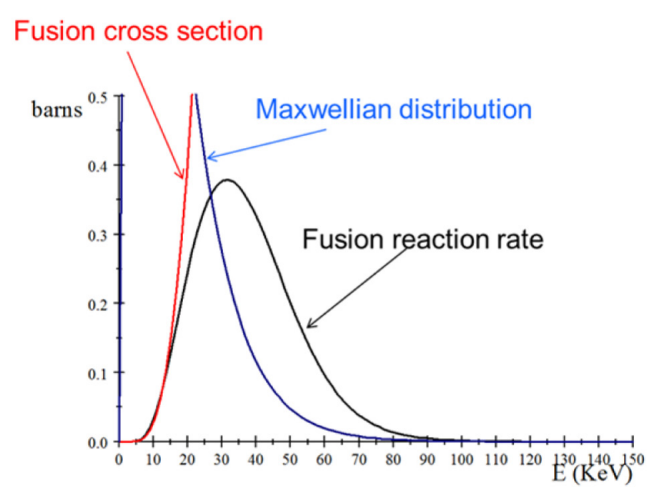

Figure 1. Competing energy dependences of Maxwellian ion distribution and fusion cross section determine Gamow peak in the fusion reactivity.

Basic Theory of Fusion Reactivity and the Knudsen Layer

Nuclear fusion reactions at energies below several hundred keV involve quantum tunneling through the repulsive Coulomb barrier that keeps nuclei from interacting. The probability of successful quantum tunneling rises rapidly as the energy of nuclei increase, which makes the fusion cross section (i.e., the probability of fusion) a rapidly rising function of energy as well (red curve in Figure 1). In the calculation for fusion reactivity, the rapid increase of cross section competes with the rapid decrease of the number of ions present at a given energy (the ion distribution function, called a *Maxwellian distribution* in thermal equilibrium; blue curve in Figure 1). This competition results in the *Gamow peak* in fusion reactivity (black curve in Figure 1), which shows where most of the fusion reactions occur. The Gamow peak energy is well above the average energy of the thermal ions.

Inertially confined fusion systems typically have plasma fuel enveloped by a cold non-reacting region or *wall*. Typically, thermal ions have mean free paths for Coulomb scattering that are short compared to the distance to this wall. But owing to the rapid decrease of collision probability as ion energy increases, the mean free path for the fusing ions at the Gamow peak can be 10 to 50 times longer. These ions can reach the wall before undergoing a thermalizing collision and therefore be lost to the system, resulting in a depletion of the high energy tail ions that account for most of the fusion reactivity. In practical terms, the way this works is shown in Figure 2, where the boundary of a spherical fuel volume is shown as a blue circle. A reference display point at 80% of the fuel radius is indicated. Half the fuel volume lies closer to the wall than this point. The circles surrounding the point indicate the mean free path for thermal ions (red circle) and Gamow peak energy ions (green circle). The case for 2 keV ion temperature (left) requires the zoomed-in image to even see the radii, while at 10 keV temperature (right), although the thermal ions are still not reaching the wall, a high fraction of the Gamow peak ions do. This picture illustrates how Knudsen layer effect operates in practice. At ignition temperatures (as low as 2 keV in some systems), no effect will be seen. But as fusion proceeds to the higher temperatures of propagating burn (10 keV and above), one can expect efficient escape of fusing ions, resulting in significant reduction of fusion reactivity and therefore a reduction in fusion yield.

We have developed a simple theory of the Knudsen tail effect by employing a kinetic spatial diffusion model, wherein the diffusion coefficient depended on particle energy and the diffusion operator was replaced by a local loss term of the same magnitude. We could then obtain a kinetic equation for the tail ion distribution function, and an approximate WKB solution for a modified ion distribution function that no longer has a Maxwellian shape. Thus tail depletion depends on the so-called Knudsen number, which is the ratio of thermal mean free path to distance from the wall. From the modified distribution function one sees that while the Knudsen number may be small, strong energy dependence of the modified distribution can make ion losses significant for energies around the Gamow peak.

From the modified distribution a fusion reactivity can be computed that is now a function of Knudsen number. The result is that we obtain a non-local reactivity that depends on distance from the wall as well as local ion temperature.

Simulations of ICF Capsule Implosion Experiments on OMEGA

We implemented this simple model in a radiation-hydrodynamics code and performed simulations of implosions of DT-filled ICF capsules conducted at the OMEGA laser[2] during 2005 to 2011. The implosions were selected to be highly diverse, spanning 2 1/2 orders of magnitude in observed yield and a factor of four in observed ion temperature. Fuel gas molar composition ranged from T:D = 0.55:1 to T:D = 585:1, more than three orders of magnitude. Several of the capsules were the deuterated-shell implosions and corresponding *reference* implosions analyzed by Wilson et al.[3]; these capsules give unambiguous evidence for ion-species mixing at the scale of an ion mean free path (*atomic mix*). Since it is clear that to explain the deuterated shell yield requires mix, we use the Dimonte[4] mix model (already in the code), either alone or in combination with the new Knudsen model.

The model contained two parameters, the mix initial scale length and the fraction of absorbed laser energy, that were varied to best fit the 11 shots simulated. The Knudsen model was used without adjustable parameters. We used a normalized error metric to measure the deviation of simulation from experiment as determined by the three measured quantities: ion temperature, DT neutron yield, and bang time (time of peak neutron production rate). For each model, several hundred one-dimensional

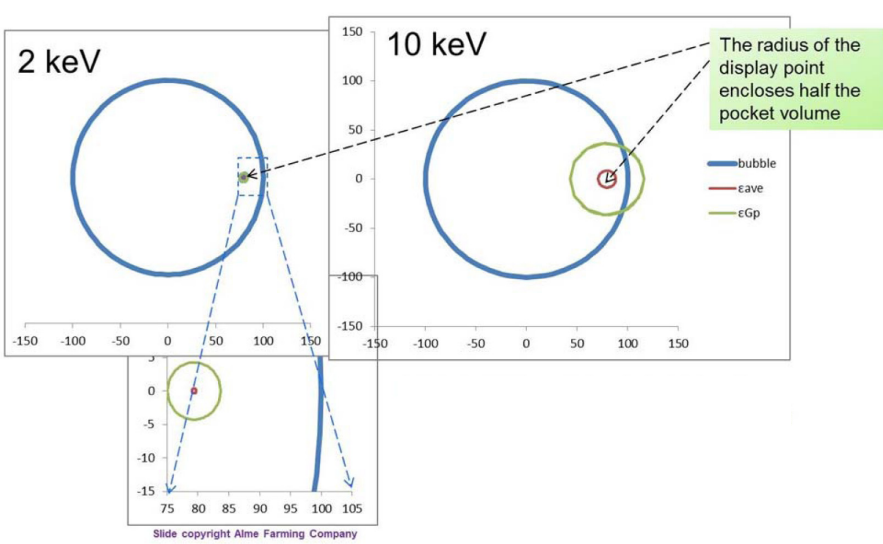

Figure 2. 100 um radius spherical cavity of burning DT plasma at 5 gm/cm^3 is shown. Cavities of 2 keV and 10 keV plasma temperatures are compared.

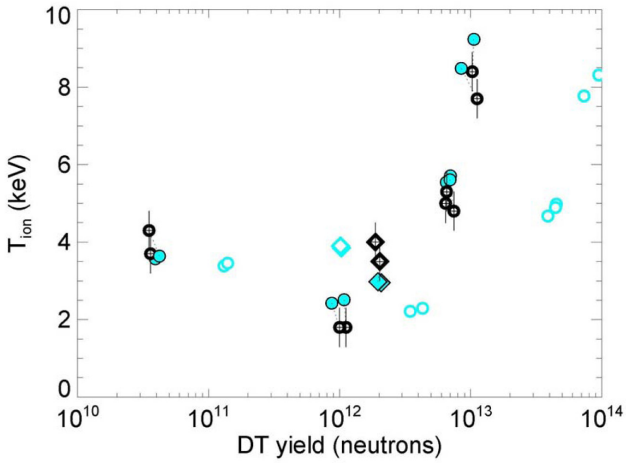

Figure 3. Comparison of observed (black symbols) and simulated (blue symbols) DT neutron yields and ion temperatures for the OMEGA capsules discussed in the text. Open blue symbols show "nominal" simulations. Filled blue symbols show simulations using Knudsen/mix model. Circles indicate ordinary plastic-shell capsules. Diamonds show deuterated-shell capsules. Knudsen/mix model gives markedly improved agreement with observations, compared to nominal.

simulations were run for each of the 11 capsules in Figure 3, spanning a grid varying the two input parameters: mix scale length and fractional laser source. We then identified the values of the input parameters giving the smallest value of the error metric, averaged over all of the capsules in Figure 3. The result was that for the Knudsen/mix model, the error metric had a minimum value of about 2 standard deviations for a mix scale length of 0.15 μm, while for the mix model alone, the error metric had a minimum value of about 4 standard deviations at a mix scale length of 0.4 μm. In other words, the Knudsen/mix model explained the observations about two times better than the mix model alone.

For the hotter implosions, most of the observed yield reduction is accounted for by the Knudsen model. For cooler implosions, most of the yield reduction comes from mix, and the yield increase seen for the deuterated shells also comes from mix. Our Knudsen/mix model handles all of this variation automatically and naturally. The improved agreement between observations and simulations given by the Knudsen/mix model, compared to the mix model alone, is significant, indicating the greater explanatory and predictive power of the Knudsen/mix model.

In summary, we believe the Knudsen layer effect on reactivity to be an important new piece of physics in fusion burn that helps resolve the long standing enigma of over-prediction of yield. Much work needs be done to compute the effect accurately in complex geometry and with a much more detailed treatment of the wall interaction with the high energy fuel ions, and this work is currently in progress.

References

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[2]T.R. Boehly et al., Opt. Commun. 133, 495, 1997.

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Awards and Highlights

Woman Physicist of the Month

The American Physical Society's (APS's) Committee on the Status of Women in Physics (CSWP) awarded Dr. Jolie Cizewski of Rutgers University the Woman Physicist of the Month for November 2012. CSWP began this program to recognize female physicists who have positively impacted other individuals' lives and careers. Dr. Cizewski, a well-respected member of the low energy nuclear physics community and principal investigator at the Stewardship Science Academic Alliances Program Center of Excellence at Rutgers University for the past 10 years, has a long history of doing just that. She works to better the careers of and provide professional opportunities for the many undergraduate and graduate students and post doctoral researchers she mentors.

2012 Excellence in Fusion Engineering Award

Fusion Power Associates (FPA) presented Mark Herrmann of Sandia National Laboratories with its 2012 Excellence in Fusion Engineering Award during the annual meeting in December 2012. He was recognized for his "many technical contributions to inertial fusion capsule design, his leadership of the Sandia high-energy-density physics program and his earlier contributions to magnetic fusion while at the Princeton Plasma Physics Laboratory." Each year, FPA presents awards to individuals in the early stages of their careers "who have shown both technical accomplishment and the potential to become exceptionally influential leaders in the fusion field."

In addition, Herrmann was elected a Fellow by the American Physical Society in September 2012. His award reads: "For innovative technical advances and exceptional leadership in the areas of inertial confinement fusion target design and magnetically driven high-energy-density science." The citation will be published in the March 2013 issue of *APS News*.

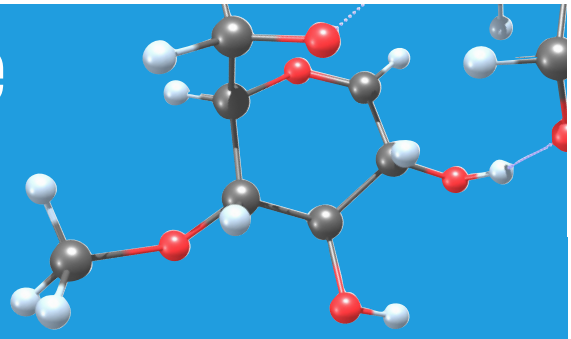
2013 Computational Science Graduate Fellowship (CSGF) Annual Meeting

Save the date for the 2013 CSGF Annual Meeting to be held Thursday, July 25 through Saturday, July 27 at the Crystal Gateway Marriott in Arlington, Virginia. Visit http://www.krellinst.org/csgf/conf for more information.

2013 Stewardship Science Graduate Fellowship (SSGF) Annual Meeting

Save the date for the 2013 SSGF Symposium to be held Tuesday, June 25 through Thursday, June 27 at the Inn & Spa at Loretto in Santa Fe, New Mexico. Visit http://www.krellinst.org/ssgf/conf in the spring of 2013 for more information.

Computational Science Graduate Fellowship



The Department of Energy Computational Science Graduate Fellowship (DOE CSGF) program provides outstanding benefits and opportunities to students pursuing doctoral degrees in fields of study that utilize high performance computing to solve complex problems in science and engineering.

BENEFITS:

- $36,000 yearly stipend
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This is an equal opportunity program and is open to all qualified persons without regard to race, gender, religion, age, physical disability or national origin.

Department of Energy National Nuclear Security Administration

Stewardship Science Graduate Fellowship

The Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship (DOE NNSA SSGF) program provides outstanding benefits and opportunities to students pursuing a Ph.D. in areas of interest to stewardship science, such as properties of materials under extreme conditions and hydrodynamics, nuclear science, or high energy density physics. The fellowship includes a 12-week research experience at Lawrence Livermore National Laboratory, Los Alamos National Laboratory or Sandia National Laboratories.

BENEFITS

- $36,000 yearly stipend
- Payment of full tuition and required fees
- $1,000 yearly academic allowance
- Yearly conferences
- 12-week research practicum
- Renewable up to four years

APPLY ONLINE

The DOE NNSA SSGF program is open to senior undergraduates or students in their first or second year of graduate study. Access application materials and additional information at:

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