An improved low-temperature equation of state model for integrated IFE target-chamber response simulations

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Overview

Abstract

A new quotidian equation of state model (QEOS) has been developed to perform integrated inertial fusion energy (IFE) target explosion-chamber response simulations. This QEOS model employs a scaled binding energy model for the ion EOS and utilizes both *n*- and *ℓ*-splitting for determining the ionization state and electron EOS. This QEOS model, named BADGER, can perform both local thermodynamic equilibrium (LTE) and non-LTE EOS calculations. BADGER has been integrated with the 1-D radiation hydrodynamics code BUCKY to simulate the chamber response of an exploding indirect-drive deuterium-tritium (DT) target, xenon gas-filled chamber and tungsten first-wall armor. The simulated system is a prototypical configuration for the LIFE reactor study being conducted by Lawrence Livermore National Laboratory (LLNL).

Overview of the Problem

Typically radiation hydrodynamics codes rely on tabulated equation of state (EOS) models to determine the values of the state variables of the materials in the problem domain while the simulation is in progress. While table lookups are computationally fast, there are several drawbacks to relying on tabulated data. First, tabulated data by definition only resolve a finite set of temperature and density points. This necessitates that the program calling on the data tables perform interpolation to estimate the state variable values at intermediate locations in temperature and density space. Generally interpolation is only valid in regions where these data are smoothly-varying as functions of temperature and density. Second, since data tables only resolve a finite set of number density and temperature points, there is always the possibility of a radiation hydrodynamics code "running off of the end of the table," requesting data outside the bounds of the table. Also, "bad data points" are problematic for hydrodynamics codes. These points can result from numerical errors or points in the model where a spurious value is returned. Finally, and perhaps most importantly, is that relying on externally-generated data tables puts the users of a radiation hydrodynamics code at the mercy of the producers of the data tables.

The Solution: BADGER, the In-line Equation of State Library

The solution to the problems highlighted above is making available a software library that can perform in-line calculations of ionization and state variable quantities. BADGER is a Fortran equation of state code that calculates two-temperature ($T_i \neq T_e$) data and the mean ionization state of an arbitrary material composed of elements or isotopes up to a Z of 86 (radon). Material definitions are passed to the BADGER library in MCNP material identifier format ($ZZAAA$) and fractional abundance. The material identifier format allows BADGER to differentiate between natural elements and isotopes in a mixture. For example, a material identifier of 6000 is elemental carbon, whereas a material identifier of 2003 represents the isotope ^{3}He. If an element is defined instead of an isotope, BADGER automatically calculates the isotopic composition . Once the mixtures are defined, a number density for the total mixture, electron and ion temperatures are passed to the library. With these few pieces of input data BADGER can calculate EOS and ionization data for every isotope in the mixture. The EOS and ionization models used were developed using an assumption of local thermodynamic equilibrium (LTE). Non-LTE data are computed using a Busquet equivalent-temperature model. Using the assumption of thermodynamic consistency, the EOS value of the mixture is simply the sum of its isotopic constituents. The primary limitation of the library is that it assumes that the isotopes of the material are only self-interacting. Overcoming this limitation is a subject of active research. Since BADGER uses dynamic memory allocation, the number of components of a mixture or the total number of mixtures solved is only limited by the RAM available on the system where it is installed.

Since BADGER is a software library, an end user can either call the library directly from a code and use the results in-line or write a wrapper program that generates tabular data in any format that the user wishes. This poster is intended to give an overview of the equation of state models used by BADGER and present example data generated by the library.

Support for This Research

This code was developed to support the Fusion Technology Institute's collaborative effort with Lawrence Livermore National Laboratory on the LIFE inertial confinement fusion reactor design study, subcontract № B587835.

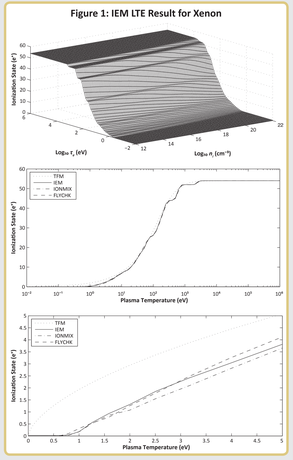
Material Ionization Model

Individual Electron Accounting Ionization Model (IEM)

The individual electron accounting ionization model used by BADGER is an adaptation of the extended Saha equation with principal (n) and angular (ℓ) quantum number electron shell degeneracy. This model was originally published by Faussurier et al using a screened hydrogenic approach [1]. IEM replaces the shell-averaged electron ionization potential and quantum numbers with the individual electron values published by Carlson [2]. Using the individual electron values provides better resolution of the average charge state at low temperatures, an important feature for the cold plasmas typically found in gas-filled ICF reactor chambers.

The IEM result for xenon was verified against the FLYCHK code from LLNL and the IONMIX code from the University of Wisconsin — Madison [3, 4]. Figure 1 shows the calculated xenon ionization as a function of density and temperature and the verification comparison for the both full temperature range and the cold plasma region. The middle and bottom plots are for xenon at a density of 10^{18} cm^{-3}, and include the Thomas-Fermi ionization result for comparison.

Figure 1: IEM LTE Result for Xenon

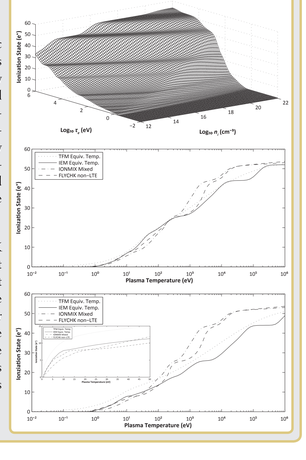


Busquet Equivalent Temperature Method for non-LTE Plasmas

The IEM was developed based on a local thermodynamic equilibrium (LTE) screened-hydrogenic model. While LTE is usually an appropriate approximation for very cold (~eV), very hot (>10 MeV) or very dense (>10^{24} cm^{-3}) plasmas, in general plasmas exhibit non-LTE behavior. Most methods of calculating non-LTE plasma ionization involve complex detailed transition array reaction rate calculations, which are prohibitively expensive for an in-line EOS code. BADGER uses an analytic-fit Busquet equivalent temperature method to get around this problem [5]. The Busquet analytic-fit implemented in the code has a range of validity of 10^{18}–10^{24} cm^{-3}.

The non-LTE model was verified against non-LTE FLYCHK and IONMIX calculations, as shown in Figure 2. The top plot shows the non-LTE ionization for xenon using the Busquet temperature equivalent method. The middle plot shows the comparison between the three codes and Thomas-Fermi for 10^{18} cm^{-3}. The bottom plot shows a comparison between the three codes and Thomas-Fermi for 10^{16} cm^{-3}. This is outside the range of validity for the Busquet method, but the results are "good enough" to be used for IFE chamber calculations, as shown in the inset plot.

Figure 2: IEM non-LTE Result for Xenon



Ion and Electron EOS Models

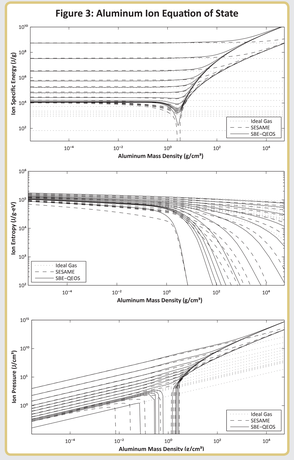
Ion Quotidian Equation of State (QEOS) with Scaled Binding Energies (SBE)

The ion equation of state model used by BADGER is an adaptation of the QEOS method developed by More et al at LLNL [6]. This model divides the material up into three regions: a "cold" solid (T_i<3T_{Debye}), a "warm" solid (3T_{Debye} < T_i < T_{melt}), and a fluid (T_i>T_{melt}). For each of these regions a scaling function, $f(u, w)$, and its derivative, $f'(u,w)$, are used to determine the values of the state variables. Here $u = T_{\text{Debye}}/T_i$ and $w = T_{\text{melt}}/T_i$ where the Debye and melting temperatures are functions of density.

BADGER uses the SBE modification to QEOS developed by Bhattacharya and Srivastava where the semi-empirical functions that determine the u and w functions are replaced by a scaled binding energy function and its derivatives whose polynomial coefficients are determined by the experimental values for cohesive energy, bulk modulus and bulk modulus pressure derivative [7].

The BADGER ion equation of state model was verified against an aluminum SESAME equation of state table [8]. The plots in Figure 3 show every fourth non-zero isotherm in the SESAME data file and the corresponding values from BADGER and what a simple ideal gas model would predict.

Figure 3: Aluminum Ion Equation of State

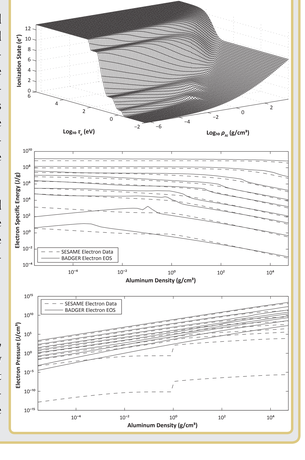


Electron Equation of State Model

The electron equation of state model used in BADGER is based on a Helmholtz free energy minimization method developed by Faussurier et al. In this model, the total Helmholtz free energy is calculated as the sum of the contributions due to free electron Coulomb field interactions, ionization potential lowering and ionization energy ($F_e = F_{\text{free}} + F_{\text{ion-sphere}} + F_e$). From this result one subtracts the zero-temperature result to obtain the final Helmholtz free energy. The Helmholtz free energy minimized differentials with respect to density and temperature yield the remaining state variable functions.

The BADGER electron equation of state model was verified against an aluminum SESAME equation of state table. The plots in Figure 4 show every fourth non-zero isotherm in the SESAME data file and the corresponding values from BADGER using an LTE ionization state model.

Figure 4: Aluminum Electron Equation of State



Conclusion

The combination of individual electron accounting ionization, SBE-QEOS ion equation of state and Helmholtz free energy minimization electron equation of state models yield a robust EOS library that is capable of calculating state variable quantities on the fly with results that are comparable to much more established models.

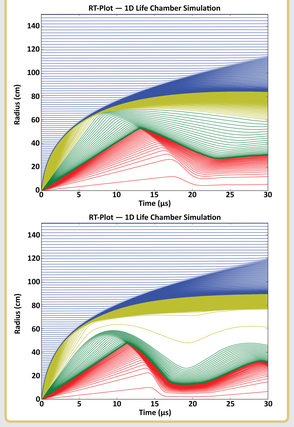
Using BADGER in Integrated IFE Simulations

Integrated ICF target-chamber calculations using the BADGER EOS Library

As a preliminary test of the BADGER library, 1-D lagrangian simulations were performed using the COOPER radiation hydrodynamics code [9]. The problem simulated is that of an integrated ICF target and xenon gas-filled chamber. Figure 5 shows the radius-vs.-time (RT) plot for the LIFE chamber. In these plots DT is shown in red, ablator in green, gold in gold and xenon in blue. The top plot shows the simulation result when using the IONMIX EOS tables and the bottom plot shows the result when using tables generated using the BADGER EOS library. For these simulations, high-density xenon was used as a proxy material for gold since IONMIX is unable to calculate gold EOS data.

These results demonstrate the difference between using an ideal gas model (IONMIX) vs. a detailed EOS (BADGER). The BADGER EOS predicts less compression of the gold layer by the exploding capsule, while the outer extent of the hohlraum plus its contents do not extend any further out into the xenon (both expand to roughly 90 cm). These results confirm that while BADGER produces results that are comparable to an ideal gas EOS model, the high-density plasma exhibits non-ideal effects. The COOPER results are preliminary, additional simulations will be performed using modified zoning to resolve the interface between the hohlraum and the ablator.

Figure 5: Integrated ICF target-chamber simulation using the COOPER radiation hydrodynamics code



Ackowldedgement

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