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A Review of Equation-of-State Models for Inertial Confinement Fusion Materials☆

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ABSTRACT

Material equation-of-state (EOS) models, generally providing the pressure and internal energy for a given density and temperature, are required to close the equations of hydrodynamics. As a result they are an essential piece of physics used to simulate inertial confinement fusion (ICF) implosions. Historically, EOS models based on different physical/chemical pictures of matter have been developed for ICF relevant materials such as the deuterium (D_2) or deuterium-tritium (DT) fuel, as well as candidate ablator materials such as polystyrene (CH), glow-discharge polymer (GDP), beryllium (Be), carbon (C), and boron carbide (B_4C). The accuracy of these EOS models can directly affect the reliability of ICF target design and understanding, as shock timing and material compressibility are essentially determined by what EOS models are used in ICF simulations. Systematic comparisons of current EOS models, benchmarking with experiments, not only help us to understand what the model differences are and why they occur, but also to identify the state-of-the-art EOS models for ICF target designers to use. For this purpose, the first Equation-of-State Workshop, supported by the US Department of Energy's ICF program, was held at the Laboratory for Laser Energetics (LLE), University of Rochester on 31 May–2nd June, 2017. This paper presents a detailed review on the findings from this workshop: (1) 5–10% model-model variations exist throughout the relevant parameter space, and can be much larger in regions where ionization and dissociation are occurring, (2) the D_2 EOS is particularly uncertain, with no single model able to match the

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available experimental data, and this drives similar uncertainties in the CH EOS, and (3) new experimental capabilities such as Hugoniot measurements around 100 Mbar and high-quality temperature measurements are essential to reducing EOS uncertainty.

1. Introduction

Accurate equation of state (EOS) models, relating the thermodynamic state variables of a material, are essential to materials science, plasma and high energy density physics, and warm dense matter studies since they are required to enforce the conservation laws in multiphysics simulations [1]. In high energy density physics applications, the EOS must describe the material response over huge ranges of conditions covering the full variety of phases from crystalline or amorphous solid to ionized plasma. The large range of conditions and their extreme nature make it impossible to completely explore the EOS experimentally and so researchers must rely on theoretical calculations, benchmarked against experiments at a few (T, ρ) points. Where data do not exist, confidence in EOS models can be built by comparing calculations from fundamentally different approaches. This process is essential to the development of reliable EOS models.

In inertial confinement fusion (ICF) experiments, the EOS plays an essential role in determining the overall implosion performance (measured by the total fusion yield). The EOS determines the overall drive efficiency through the ablation pressure and hydrodynamic coupling efficiency to the deuterium-tritium fuel [2], the timing of shock waves [3–6] driven through the target, the growth rates of hydrodynamic instabilities [7–10], and the compressibility of both the fuel and ablator [11]. As a result the EOS is an essential piece of ICF design calculations; in turn, ongoing ICF experiments have stimulated very rapid developments in state-of-the-art EOS simulations and experiments. In a 2016 white paper detailing the major challenges to ICF research commissioned by the US Department of Energy's National Nuclear Security Administration (DOE-NNSA) [12], it was recommended that the EOS community should hold a series of workshops with the aim of investigating the uncertainties in current EOS models and determining the challenges. To respond to that call, the first in a series of equation-of-state workshops, supported by the DOE's ICF program, was held at the Laboratory for Laser Energetics (LLE), University of Rochester on 31 May–2nd June, 2017. The aim of this paper is to present a detailed review on the findings from this workshop, which focussed on fundamental EOS issues with respect to ICF modeling. They are summarized here:

1. Model-model variations of 5–10% are present throughout the temperatures and densities of interest to ICF, and are significantly larger in regions where ionization and dissociation is taking place,
2. In several cases, models that agree well in P-ρ space have significantly different temperatures, making temperature data extremely useful for constraining models,
3. The deuterium EOS is quite uncertain, with no single model able to match all of the available data around 1 Mbar, and none of the frequently-used ICF EOS tables are in agreement with first-principles approaches. State-of-the-art experimental and theoretical results are in much better agreement, and so the prospect of new high-precision D_2 EOS tables is encouraging,
4. The lack of a precise experimental platform capable of reaching > 100 Mbar leads to significant uncertainties in ablator EOSs, in particular in the peak compression region where model variations can be large.

The paper is organized as follows: In Section 2 we give a brief discussion of ICF experiments and motivate our choice of comparison cases; in Section 3 we briefly introduce the rich set of theoretical approaches used to build modern EOS tables. In Section 4 we describe the workshop format and the data submissions we received. In Sections 5–8 we present comparisons of theoretical calculations and experimental data for 4 ICF-relevant materials: deuterium, beryllium, carbon and polystyrene. Finally in Section 9 we summarize our findings and discuss the perspectives for the EOS and ICF communities.

2. Material conditions of interest to ICF research

In ICF [13], an external driver delivers kinetic energy (through material ablation or the $v \times B$ force) to a shell of dense material filled with hydrogen-isotope (deuterium-tritium, DT) fusion fuel, causing it to implode. The DT fuel is compressed and heated to stimulate a self-sustaining fusion burn. Current ICF experiments focus on three approaches, characterized by the nature of the drive: 'direct drive' experiments in which a spherical plastic shell is directly illuminated by a high energy (MJ class) laser [14,15], 'indirect drive' experiments in which laser energy is first converted to a bath of quasi-thermal X-rays [16,17], and magnetically driven experiments in which a cylinder of material is magnetically imploded using high (MA) electric current [18–20]. Under shock compression and subsequent radial convergence, both the DT and ablator materials can experience extreme pressures ranging from millions to hundreds of billions atmospheres (Mbar - 100 GBar) making this a particular challenge for EOS models.

Table 1 shows the conditions at some selected points during an ICF implosion. The first shock is very important in setting the fuel entropy and determining the density profile of the mass driver as it implodes. This makes the principle Hugoniot of ICF materials at pressures of 1–10 Mbar very important, as well as the release isentropes from those pressures. Conditions behind the first shock are 1–10 eV and several times compressed (densities of several g/cm^3), while conditions in the ablation region are somewhat hotter and decompressed. At stagnation the central DT 'hotspot' reaches multi-keV temperatures and densities of $\sim 50 - 100$ g/cm^3 while the surrounding DT is at $\sim 100 - 500$ eV and $\sim 300 - 1000$ g/cm^3. The plasma conditions for ablators are similar to the DT ice layer. The precise trajectory taken during the implosion is very important in determining the final neutron yield; in this work we will attempt to address the wide ranging EOS quantities between these points as well as the principal Hugoniot.

3. Equation-of-state calculations & tables

Simulations of ICF implosions are most often done using hydrodynamics codes. In this context, the EOS is required to close the conservation equations at all (T, ρ) points in the simulation. It is not computationally feasible to have large-scale simulation codes also calculate material properties like the EOS 'on-the-fly', and so it has become common practice to generate EOS data in tabular form which can be interpolated by hydrodynamics codes as required. The state-of-the-art approach is to perform a large (as large as possible given computational constraints) set of first principles calculations of various types in order

Table 1
Conditions at some selected points during an ICF implosion

Location	DT	Ablators
First shock	0.6–1.0 g/cm^3 1–10 eV	3–10 g/cm^3 1–10 eV
In-flight	5–10 g/cm^3 10–50 eV	5–10 g/cm^3 10–50 eV
Stagnating	300–1000 g/cm^3 100–500 eV	200–500 g/cm^3 100–500 eV
Hotspot	50–100 g/cm^3 1–10 keV	-