Improvements to the FEOS Equation of State Model for Application to Hydrodynamics Simulations

J. D. Pecover, D. A. Chapman and N. P. L. Niasse

first light

Introduction

An accurate equation of state (EoS) is vital for high fidelity hydrodynamic simulations, required for modelling of HEDP and fusion experiments.

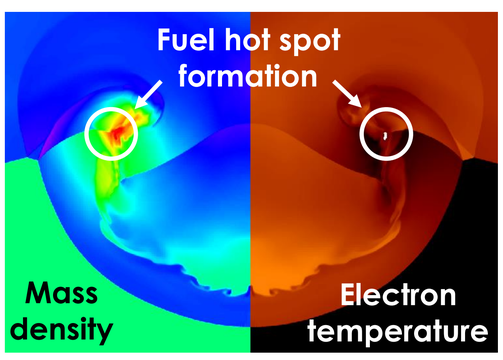

Fig. 1
Output from a cavity collapse simulation using our front-tracking hydrodynamics code Hytrac, demonstrating sharp capture of shocks and resolution of the Kelvin-Helmholtz instability.

We use FEOS [1], also used by MHD and rad-hydro codes Gorgon [2-3] and Odin; generates EoS based on small number of material properties. Builds on the QEOS formalism [4], where total EoS is split into contributions from electrons (Thomas-Fermi + solid correction) and ions (Cowan model [5]). All EoS properties are additive, ie. pressure, energy, entropy:

- $p_{tot} = p_e + p_i$
- $E_{tot} = E_e + E_i$ **(1)**
- $S_{tot} = S_e + S_i$, can be derived from the Helmholtz free energy F:

$$p = \rho^2 \frac{\partial F}{\partial \rho} \qquad E = -\frac{\partial F}{\partial T} \qquad E = F + TS \qquad \textbf{(2)}$$

- Pressure isotherms contain van der Waals loops, which must be eliminated using a Maxwell construction for use in hydrodynamics.

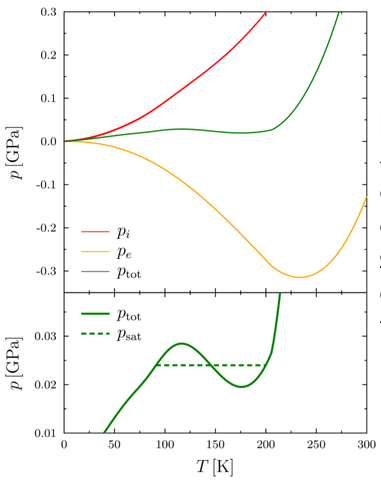

Fig. 2
47 K isotherm of deuterium, expected structures of ion, electron and total pressures.

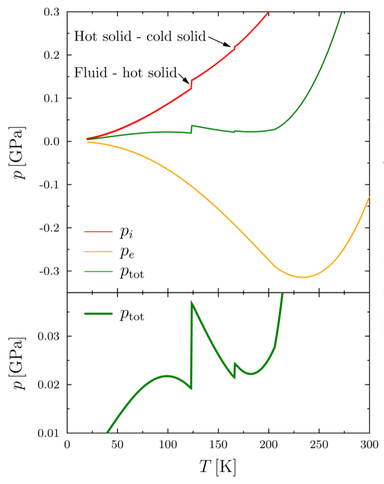

Fig. 3
47 K isotherm of deuterium, actual pressure shows discontinuities and complex loop structure.

Discontinuities cause Maxwell construction to fail, originate from ion EoS

Fixes to Cowan model

The Cowan model [5] constructs an ion Helmholtz free energy based on density-dependent melting (T_m) and Debye (Θ_D) temperatures. There are three regions: fluid, hot solid, cold solid, with joining points given by:

$$w = \frac{T_m(\rho)}{T} = 1, \text{ fluid – hot solid model join} \qquad \textbf{(3)}$$

$$u = \frac{\Theta_\mathrm{D}(\rho)}{T} = 3, \text{ hot solid – cold solid model join} \qquad \textbf{(4)}$$

- Hot and cold solid models are high and low temperature limits of the integral (originates from Debye theory):

$$f(u) = \frac{m_i}{k_\mathrm{B}T} F(u) = \frac{9}{2u^3} \int_0^u dx\, x^2 [x + 2\ln(1 - e^{-x})] \qquad \textbf{(5)}$$

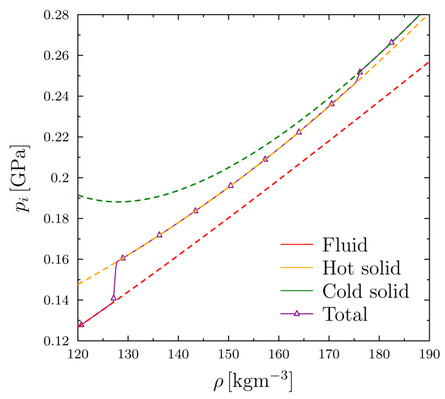

Fig. 4
Ion pressure isotherm of deuterium at 47 K, showing ion pressures returned by each part of the Cowan model and the total. The curves do not intersect, so the two transition points in the "total" curve are discontinuous.

The hot/cold solid transition can be replaced by numerical integration of Eq. 5 using Gaussian quadrature – gives the "unified solid model". Transition between unified solid and fluid models is more difficult as they are fundamentally different models. To remove the discontinuity, the hard switch (Eq. 3) is replaced with interpolation using scale factor x_0,

$$p_i = p_\mathrm{solid}\left(\exp\left[\frac{1-w^2}{x_0 w}\right] + 1\right)^{-1} + p_\mathrm{fluid}\left(\exp\left[\frac{w^2-1}{x_0 w}\right] + 1\right)^{-1} \qquad \textbf{(6)}$$

Effect of fixes using Eqs. 5 and 6 shown below for ion pressure (left) and total pressure (right). Fixes have no impact where not required.

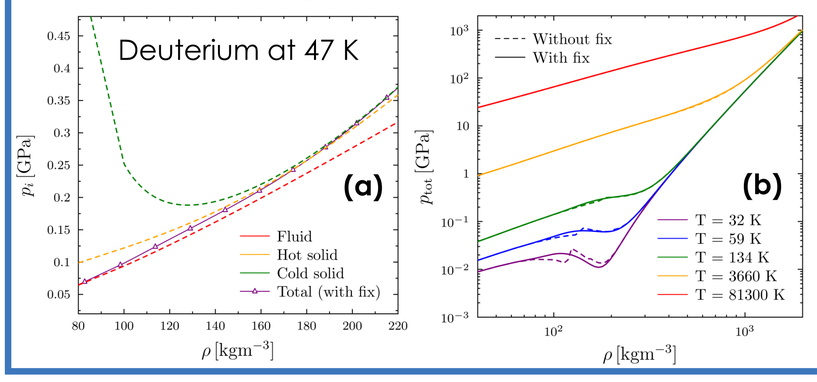

Fig. 5
(a): Ion pressure isotherm of deuterium at 47 K, showing components of the Cowan model and the smooth isotherm given by the fix.
(b): Total pressure isotherms of deuterium, showing effect of the fix at low temperature.

Experimental/DFT-MD Comparison

FEOS provides good match to Hugoniot and cold curve data for Al (Fig. 6). Isotherms of Al generally match DFT-MD data (Fig. 7), although there is discrepancy around solid density for T~1 eV. A single 10^4 K isotherm (Fig. 8) shows poor agreement until ~solid density. This coincides with region where Thomas-Fermi model over-predicts charge state compared to an improved model, the screened hydrogenic model with ℓ-splitting (SHM-ℓ) [6], resulting in an over-prediction of pressure.

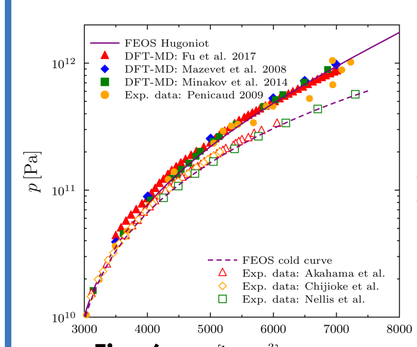

Fig. 6
Hugoniot [7] and cold curve [8] data for aluminium

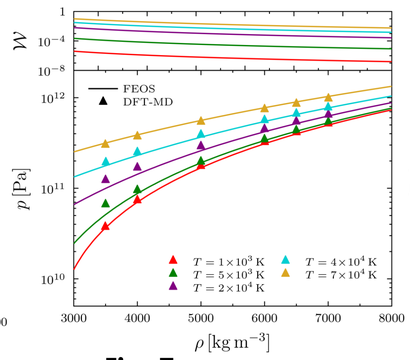

Fig. 7
(a):Isotherms of aluminium [7]

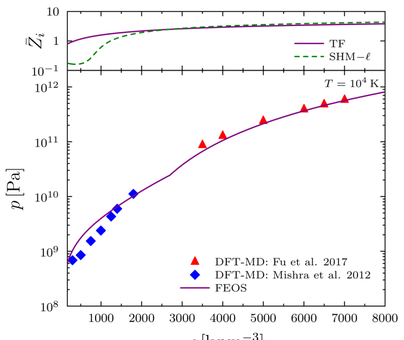

Fig. 8
(a): Single isotherm of aluminium, 10^4 K [7, 8]

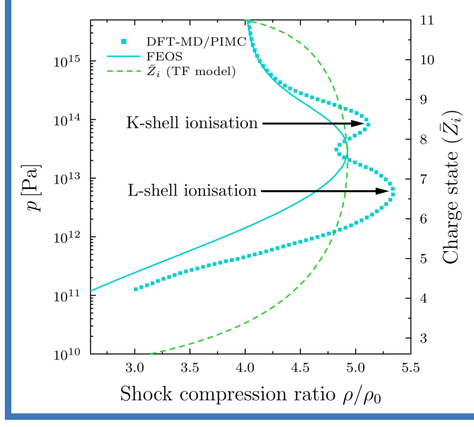

Fig. 9
Hugoniot for sodium [9] generated for FEOS around ionisation shoulder disagrees with DFT-MD data and does not reproduce the double-peaked structure. This is due to the absence of atomic shell structure and smoothing out of ionisation edges in the Thomas-Fermi model.

Conclusions and future work

The robustness of FEOS has been improved through improvement on the ion part of the QEOS model on which it relies – this has also improved accuracy in the "warm" solid regime. Priority for future work is replacement of Thomas-Fermi ionisation model and electron EoS. SHM-ℓ implemented, we also have access to SpK [10] (DCA model).

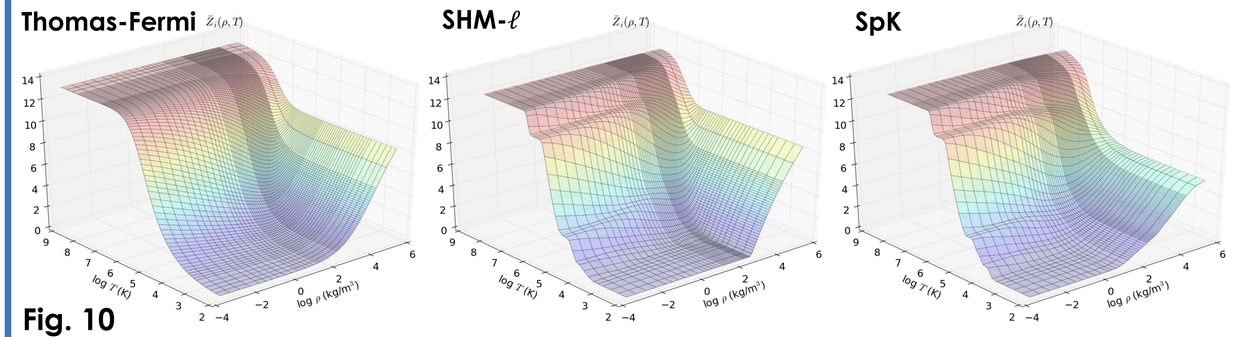

Fig. 10
Mean charge state surfaces of aluminium as functions of density, temperature. SHM-ℓ and SpK show edges and plateaux due to atomic shell structure but show differences in the pressure ionisation regime; Thomas-Fermi produces a completely smooth charge state surface.

References

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