IMPROVEMENTS TO ANEOS FOR MULTIPLE PHASE TRANSITIONS G. S. Collins[1], H. J. Melosh[2]
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Introduction: Accurate equations of state are of vital importance in impact calculations. Robust predictions of impact melt and vapour volumes require sophisticated equation of state representation, including accurately determined phase boundaries and two-phase regions. ANEOS is a complex computer program for calculating equations of state, developed at Sandia National Laboratories [1, 2] and recently modified and improved for geological materials [3]. Its advantages over simpler analytical equations of state include thermodynamic consistency, definition of phase boundaries, a better treatment of vapour and calculation of both temperature and entropy.

Although ANEOS is the most accurate equation of state package that is widely used in impact modelling, it is not without limitations. An important weakness in the treatment of the compressed region is that only one high-pressure solid phase transition can be included and it is accounted for by modifying the cold compression term alone [3, 4]. This implies that the experimentally observed dependence of phase transition pressure on temperature cannot be reproduced [3] and that the thermal expansion coefficient of the high pressure phase is the same as the low pressure phase [5], which can make it difficult to define realistic initial conditions in impact simulations where gravitational overburden pressures are significant, such as in giant planetary collisions. The fixed-pressure phase transformation also makes it difficult to locate the liquid/solid phase boundary. As a result, in the current version of ANEOS, liquid and solid states cannot be distinguished when a high-pressure phase transformation is included, and temperatures above the melt temperature are overestimated as latent heat of melting is not subtracted from the internal energy [3, 4].

Improvements to ANEOS and iSALE: Here we describe modifications to the ANEOS code to overcome these limitations and incorporate the improvements into the iSALE impact hydrocode package. In a first step, we added new routines to (a) locate and store in a table the liquid/solid phase boundaries in combination with the existing method for defining a solid/solid phase transition; and (b) given a specified density and temperature, use the liquid/solid transition table to identify the phase and calculate the mixed phase state if necessary. This in-memory table method, which mirrors the approach used by ANEOS to locate the vapour transition, allows a (slower) more robust search algorithm to be used to locate the melt phase boundaries during the initial construction of the table, without reducing the effi-

ciency of subsequent calls to ANEOS. However, as ANEOS is typically used to construct equation of state tables for subsequent use in hydrocodes (rather than called directly from the hydrocode) the raw efficiency of a call to ANEOS is not of paramount importance. Linear interpolation is used to locate the phase boundary between points in the table and the lever-arm rule is used to compute the thermodynamic state in the mixed phase region. When used in conjunction with a solid-solid phase transition, the tabulated melt curve is modified in the double mixed phase region by assuming a linear density-temperature relationship along the liquid and solid curves across the mixed-phase low- and high-pressure-solid region. This approach has been successfully employed in the construction of equation of state tables for quartz (SiO_2; not shown) and forsterite (Mg_2SiO_4; Fig. 1).
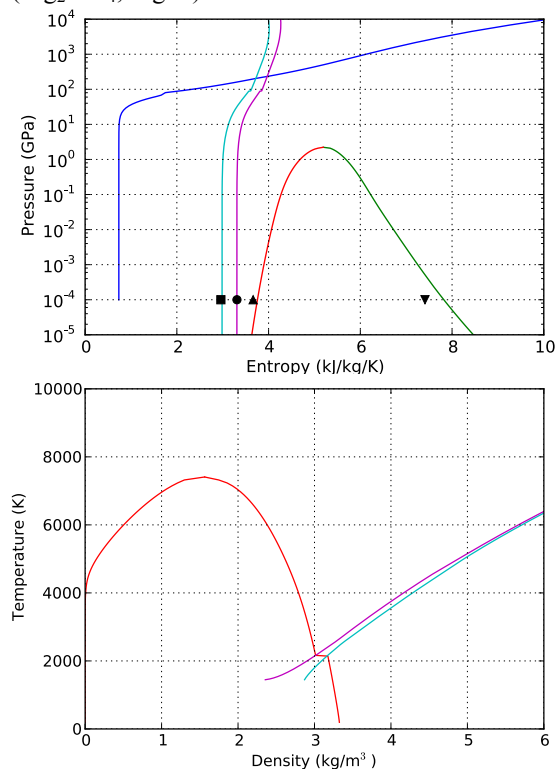

Figure 1: ANEOS-derived equation of state for Mg_2SiO_4 with solid-solid and melt phase transitions in pressure-entropy space (top) and density-temperature space (bottom), showing Hugoniot (blue), liquid-vapour curve (red), and the incipient- (cyan) and complete-melting curves (magenta). The 1-bar entropies for incipient melting (square), complete melting (circle), incipient vaporization (right triangle) and complete vaporization (inverted triangle) after [6] were used as constraints, along with experimental data [7, 8].

In a second, on-going step, following the success of recent multiphase equation of state development [e.g., 9] we are modifying ANEOS so that it treats high-pressure phase(s) as separate materials, with different thermodynamic constants. Phase boundaries are determined using a thermodynamic equilibrium approach analogous to that currently used to define the solid/liquid phase transition. As with our modified melt transition method, the solid-solid phase transition information is stored in a table for subsequent use by ANEOS. Linear interpolation is used to locate the phase boundary between points in the table and the lever-arm rule is used to compute the thermodynamic state in the mixed phase region.

To exploit the improvements made to ANEOS in this work, we have modified the iSALE hydrocode [10] to generate in-memory equation of state tables using ANEOS during problem start-up and to include entropy in the tables from which phase information can be deduced.

Discussion: The omission of the melt transition in ANEOS-derived equation of state tables has been an important limitation of many previous impact-modeling studies [e.g., 11]. Neglecting the latent heat of melting implies that post-shock temperatures above the melt temperature are overestimated, and accurate melt volumes are difficult to calculate. Using new ANEOS parameters for forsterite that include both a solid-solid phase transition (old method) and a melt transition (with a high melt temperature of 2163 K, appropriate for pure forsterite), together with the epsilon-alpha porous compaction model, we calculated post-shock temperature as a function of peak shock pressure for forsterite with a range of different initial porosities (0-50%). Post-shock temperatures above the melt transition can be overestimated by as much as 660 K, which corresponds to a difference in shock pressure of 5-25 GPa, depending on initial porosity.
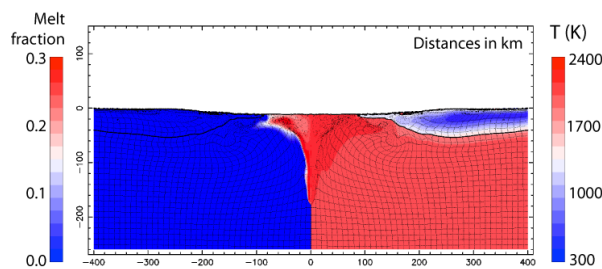

Figure 2 Melt fraction (computed from entropy; left) and final temperature (right) distribution beneath a simulated lunar impact basin (52-km impactor diameter; 15-km/s impact velocity; 40-km crustal thickness; 35-K/km thermal gradient) using the SiO_2 (crust) and Mg_2SiO_4 (mantle; impactor) ANEOS equations of state with melting.

Inclusion of the melt transition also allows melt fraction to be estimated directly during an impact simulation from the specific entropy (Fig. 2). In addition to improving the accuracy of melt-volume calculations, this will allow melt fraction to be used as a variable in rheological models of partially molten material. Simulations of large impact crater formation on early planetary surfaces depend sensitively on the rheology of the hot planetary interior and additional impact-related heating. Current approaches tend to reduce the shear strength of the target to zero at the point of incipient melting; however, material with a melt fraction <0.5 likely provides substantial viscous resistance to flow, which needs to be accounted for in future impact simulations.

Outlook: The improvements to ANEOS described here address long-standing limitations of the software that will aid the construction of accurate equation of state tables and improve future planetary impact simulations. However, recent experiments have highlighted a further limitation of ANEOS [12, 13], which fails to correctly predict the entropy on the Hugoniot with the consequence that the shock pressure of vaporization is overestimated. Future efforts will focus on addressing this shortcoming, as well as mixture-model approaches for developing more realistic whole-rock equations of state by combining single-mineral equations of state, such as those developed for SiO_2 and Mg_2SiO_4.

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