

'5-Phase' EOS: A Tabular H₂O EOS for Shock Physics Codes

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The current table version is 8.0 (first public release).

Terms of Use

- 1) The table is available for non-commercial use.
- 2) Users are expected to validate hydrocode calculations using the tabular EOS for their particular application. The table has only been used and tested for specific applications.
- 3) Users are asked not to redistribute the table. Please direct queries for the table to Sarah in order to maintain a distribution list for corrections/additions/clarifications.
- 4) All extended abstracts, reports, and papers that use the 5-Phase H₂O EOS should cite the appendix in:
Senft, L. E., and S. T. Stewart. Impact Crater Formation in Icy Layered Terrains on Mars. *Meteoritics and Planetary Science*, 43 (12), 1993-2013, 2008.

Description of the Table

The 5-Phase H₂O tabular equation of state model includes ice Ih, ice VI, ice VII, liquid, and vapor. Although there are many more phases of H₂O, only these 5 are identified on the shock Hugoniot of ice Ih [Stewart and Ahrens, 2005]. A more detailed description of the models used in each portion of the phase space is found in the appendix of Senft and Stewart [2008]. The table follows experimentally determined phase boundaries except for the artificial ice Ih-ice VI boundary and the adjacent liquid boundary.

SESAME style equations of state are tables of pressure, energy (and optionally entropy) on a density-temperature grid. The distributed table uses 275 density points (0 to 5 g cm⁻³) and 218 temperature points (0 to 200,000 K) in a combination of linear and logarithmic sections to resolve each phase and phase boundaries. Refer to the plots of the table.

There are two versions of the table:

- 1) With tension regions for ice Ih and liquid (for dynamic calculations)
- 2) Without tension regions (for static/equilibrium calculations)

The tension regions are extensions of the pure ice Ih or liquid equation of state into the bulk density phase boundary occupied by the equilibrium mixtures of ice Ih-vapor and liquid-vapor. The tension regions are tabulated to -100 MPa to allow for failure model iterations beyond the estimated (approx.) -10 MPa dynamic tensile strength of ice Ih [Ahrens, et al., 2009] and liquid [Boteler and Sutherland, 2004]. There is a discontinuity at the -100 MPa edge of the tension region and the vapor mixed phase regions.

The table is available as a Sandia-style SESAME table that is compatible with the CTH code and as a set of IDL binary '.sav' files. The units in the IDL files are temperature in K, density in kg m⁻³, pressure in MPa, internal energy in kJ/kg, entropy in kJ/kg/K. The IDL files contain:

- 2D arrays that contain energy, pressure, and entropy (earr, parr, sarr) on the density-temperature grid (1D darr and tarr; 2D dijarr and tijarr)
- a character array that identifies the phase(s) at each grid point (phasearr)
- arrays describing the phase boundaries: melting, sublimation, and vapor curves and artificial ice Ih-VI boundary

The SESAME file reference state is liquid water at 298 K and 1 bar. The material ID number is 3. SESAME file units are K, GPa, g cm⁻³, MJ/kg, MJ/kg/K. Both ascii and binary files are included.

Known Issues:

- Sound speeds calculated within phase boundaries (where $dP/d\rho \sim 0$) will be unrealistically small. This is a particular problem in the artificially large region of density space between ice Ih and ice VI.
- The ice Ih sublimation curve has extremely low vapor pressures below about 150 K [Feistel and Wagner, 2007]. The tabulated vapor pressure is linearly extrapolated to zero pressure between 0 and 150 K to prevent floating point errors. As a result, below 150 K, vapor is not tabulated; only the 3 solid ice polymorphs are tabulated. Furthermore, for these solid phases, the values in the table below 150 K are extrapolated beyond the experimental data sets that defined their individual equations of state models.
- There are small discontinuities in the table at low temperatures as the equations of state are extrapolated to 0 K: e.g., a small kink in entropy in the ice VII field at 251 K.

Requests:

- Please notify Sarah of any errors or problems with the table.
- Please send requests for changes or development of the table to Sarah.
- In some cases, users may need to determine if their result is sensitive to the artificial ice Ih-ice VI boundary. Alternate tables may be generated with different locations of this boundary if desired.

References

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- Boteler, J. M., and G. T. Sutherland (2004), Tensile failure of water due to shock wave interactions, *J. Appl. Phys.*, 96 (11), 6919-6924, doi: 10.1063/1.1810635.
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Bibliography of work using the 5-Phase H₂O EOS

- Senft, L. E., and S. T. Stewart (2008), Impact Crater Formation in Icy Layered Terrains on Mars, *Meteorit. Planet. Sci.*, 43 (12), 1993-2013.
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- Kraus, R. G., S. T. Stewart, Scaling Laws for Impact Induced Melting and Vaporization of H₂O Ice, *Icarus*, in prep., 2010.