Dynamics of volumetrically heated matter passing through the liquid-vapor metastable states

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Outline

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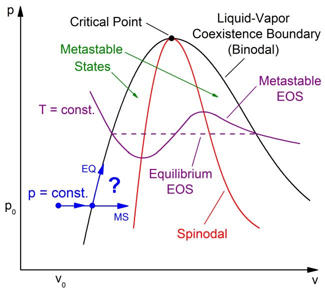
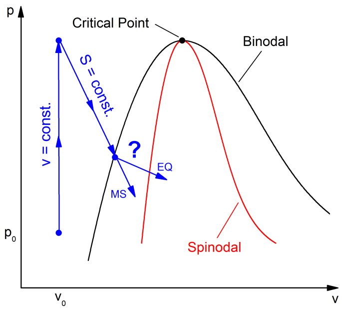
General problem in hydrodynamic simulations

Isobaric expansion



MS: Metastable EOS   EQ: Equilibrium EOS

Isochoric heating → Isentropic expansion

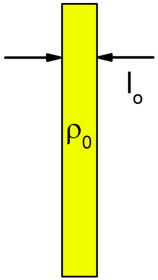


Follow metastable or use fully equilibrium EOS below the binodal?

Follow metastable EOS and use the criterion for explosive boiling!

Quasi-static thermal expansion of a planar foil

The criterion will be illustrated for a quasi-isobarically heated thin foil which expands homogeneously in density and temperature.



External pressure $p_0 > 0$

Energy deposition rate q

Quasi-isobaric expansion

$\Delta\rho/\rho \ll 1$ within $t_s = l/c_s \rightarrow$ Heating is slow!

t_s - sonic time, c_s - speed of sound

For a given q the foil can be chosen to be sufficiently thin to stay within the quasi-static regime.

EOS for SiO_2

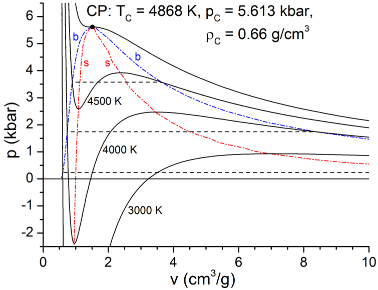
All calculations have been performed for fused silica, SiO_2.
→ Candidate for stack target experiment
→ Demonstrates the capabilities of MPQeos-JWGU

MPQeos-JWGU for SiO_2

Provides metastable and equilibrium EOS

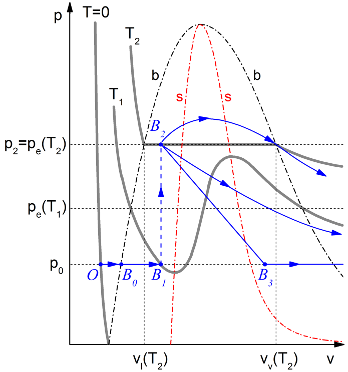
Has all characteristic features: Van-der-Waals loops, ...

Provides a realistic critical point location



Outline

General considerations



Quasi-isobaric expansion

The entire sample is represented by a single point.

Evolution of a fluid element

$O \rightarrow B_0$: Isobaric expansion

$B_0 \rightarrow B_1$: Follow MS-EOS

$B_1 \rightarrow B_2$: Explosive boiling, Transition to EQ-EOS

Explosive boiling: Local and instantaneous

Subsequent evolution $B_2 \rightarrow$?: Different trajectories are possible.

Transition constraints

The time scale of hydrodynamics and of external heating is much longer than the time scale of explosive boiling.

$\Rightarrow$ The specific internal energy ϵ and the density ρ are kept fixed.

$$\epsilon_2 = \epsilon_1 \quad \wedge \quad \rho_2 = \rho_1$$

Temperature rises!

$$\Delta T_{1\to 2} > 0$$

(can be rigorously proven)

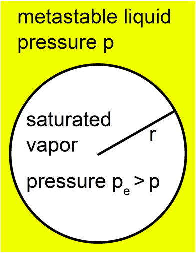
Pressure rises!

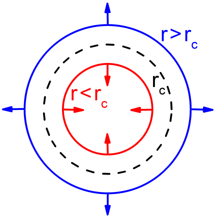
$$\Delta p_{1\to 2} > 0$$

(follows from $\Delta T_{1\to 2} > 0$)

For $p_1 = p_0 = 0.5$ kbar: $\quad T_2 \approx T_1 + 40$ K, $\quad p_2 \approx 1.6$ kbar $\approx 3p_1$

Homogeneous bubble nucleation (1/2)





Our criterion for explosive boiling is based on the theory of homogeneous nucleation!

Critical bubble parameters

Thermodynamic fluctuations $\Rightarrow$ Bubbles

$p_e(T) = p + \frac{2\sigma}{r_c} \Rightarrow$ Critical bubble radius r_c

$p_e(T)$ - saturated vapor pressure

- $r < r_c$: Surface tension σ dominates, bubble collapses
- $r > r_c$: Bubble grows

Minimum formation work: $W_c = \frac{16\pi\sigma^3}{3(p_e - p)^2}$

Homogeneous bubble nucleation (2/2)

Rate of spontaneous critical bubble creation J [cm^{-3} s^{-1}]

$J = N \left(\frac{3\sigma}{\pi m}\right)^{1/2} \exp\left(-\frac{W_c}{T}\right)$ m - molecular mass, $N = \rho/m$

$\rightarrow$ On a par with the EOS, the surface tension σ must be known!

Surface tension laws

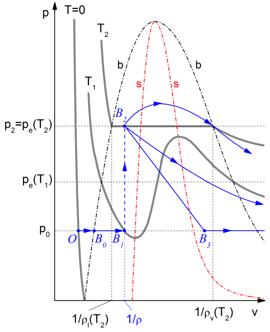
- Guggenheim-Katayama:

  $$\sigma_{GK}(T) = \sigma_m \left(\frac{T_c - T}{T_c - T_m}\right)^{11/9} \rightarrow \text{Vanishes at } T_c!$$

- Povarnitsyn et al. (vanishes at spinodal):

  $$\tilde{\sigma}(T, \rho) = \sigma_m \left(\frac{T_c - T}{T_c - T_m}\right) \left(\frac{\rho_l(T) - \rho_v(T)}{\rho_l(T_m) - \rho_v(T_m)}\right)^{2/3} \left(\frac{\rho - \rho_{l,sp}(T)}{\rho_l(T) - \rho_{l,sp}(T)}\right)^{1/2}$$

Criterion for explosive boiling



Basic assumption for the transition

Total fractional volume of overcritical bubbles $\stackrel{!}{=}$ equilibrium value ξ_v at ρ, T_2

$$0 \leq \xi_v(\rho, T) = \frac{\rho_l(T_2)-\rho}{\rho_l(T_2)-\rho_v(T_2)} \leq 1$$

$\rightarrow$ T_2 defined by $\epsilon(\rho, T) = \epsilon_{EQ}(\rho, T_2)$

$$\int_0^t J(t')V(t')\,dt' \stackrel{!}{=} \xi_v$$

Transition criterion for $W_c/T \gg 1$ $\rightarrow$ typically $W_c/T_1 \approx 15$

$$NV_c \left(\frac{3\sigma}{\pi m}\right)^{1/2} \left[\frac{d}{dt}\left(-\frac{W_c}{T}\right)\right]^{-1} \exp\left(-\frac{W_c}{T}\right) = \xi_v(\rho, T)$$

Effective boiling rate for quasi-static heating (1/2)

Effective rate of explosive boiling τ_b^{-1} [s^{-1}]

$$\tau_b^{-1} = \frac{NV_c}{\xi_v}\left(\frac{3\sigma}{\pi m}\right)^{1/2}\left[T\frac{\partial}{\partial T}\left(-\frac{W_c}{T}\right)\right]_p^{-1}\exp\left(-\frac{W_c}{T}\right)$$

Transition criterion for quasi-static heating

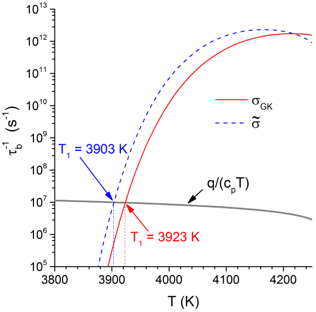
The effective rate of explosive boiling must be compared with the timescale of the quasi-static heating.

$$\tau_q^{-1} \equiv \frac{d\ln T}{dt} = \frac{q}{c_p T} = \tau_b^{-1}$$

This criterion defines the transition temperature T_1.

Since temperature is uniform in space, all fluid elements undergo the transition at the same time.

Effective boiling rate for quasi-static heating (2/2)



$p = 0.5$ kbar, $q = 10^{11}$ J/gs

Transition quantities

$T_1 = 3903 - 3923$ K

$T_2 \approx T_1 + 40$ K

$p_2 \approx 1.6$ kbar $\approx 3p_1$

Critical bubble properties

Gibbs number: $W_c/T_1 = 15$

Molecule population: $NV_c = 219$

$\rightarrow$ The theory is applicable!

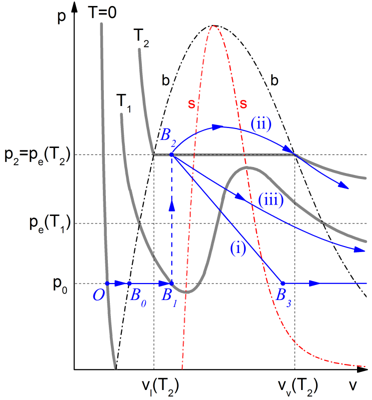
Timescale for a one-order change of the effective boiling rate

$$\Delta t \simeq \frac{c_p \Delta T_{10}}{q} \simeq \frac{\Delta T_{10}}{T}\tau_q \simeq \frac{\tau_q}{200} < 1 \text{ ns} \Rightarrow \text{ Instantaneous transition!}$$

Subsequent evolution of the two-phase states

$B_1 \rightarrow B_2$: c_s drops strongly!

Usually $c_{s2}/c_{s1} < 0.1$



$B_2 \rightarrow$?: Different trajectories

(i) - Foil boundary

$t_s = l/c_s$ may be still small.

$\Rightarrow$ Quick isentropic relaxation

$B_3 \rightarrow \ldots$: Quasi-isobaric

(ii) - Inner foil elements

$\Delta p > 0$, $\Delta T > 0$ due heating until rarefaction wave arrives.

(iii) - Intermediate case

Outline

Numerical setup

Hydro setup

Planar 1D-layer of SiO_2

100 Lagrangian cells

Application: Stack targets

Quasi-static heating

$q = 10^{11}\ \frac{\mathrm{J}}{\mathrm{gs}}$ for $t = 0 \ldots 150$ ns

$t_s = l_0/c_{s,0} \approx 2.2$ ns

Corresponds to HHT ion beam!

Initial state

MPQeos-JWGU EOS

$l_0 = 10\ \mu\mathrm{m},\ T_0 = 312$ K,

$\rho_0 = 2.2\ \frac{\mathrm{g}}{\mathrm{cm}^3},\ p_0 = 500$ bar,

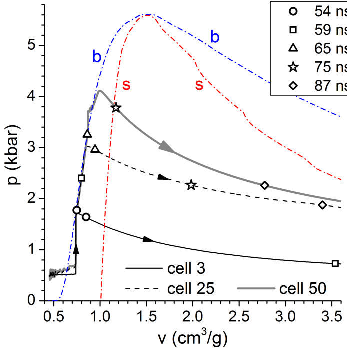
$c_{s,0} = 4.56 \times 10^5\ \frac{\mathrm{cm}}{\mathrm{s}}$

Two simulations

1. Metastable case:
   $\rightarrow$ Start with MS-EOS
   $\rightarrow$ Switch to EQ-EOS at
   $t_b = 52.95$ ns (3923 K)
2. Equilibrium case:
   $\rightarrow$ Start with EQ-EOS

Simulation results (1/2)

v-p phase plane - MS case



Cell 3: Foil boundary

Cell 25: Half distance between center and boundary

Cell 50: Foil center

Evolution after boiling

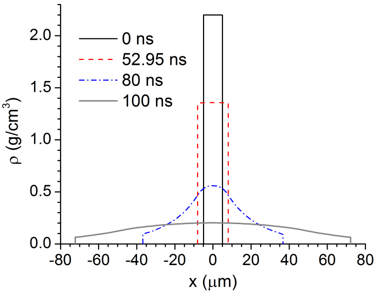
The boundary relaxes to p_0.

The center elements follow for about 20 ns the binodal until the rarefaction wave arrives!

$c_{s,MS}/c_{s,EQ} \approx 30 \ldots 3$ on binodal $\Rightarrow$ Binodal becomes an attractor!

Simulation results (2/2)

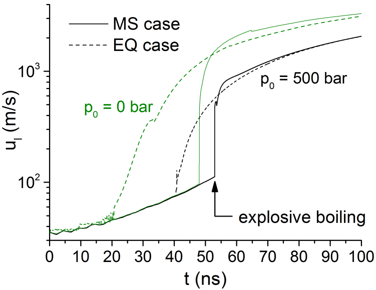
Density profiles - MS case



$t \leq t_b$: ρ homogeneous

$t > t_b$: $\rho \approx$ Gaussian

Surface velocity



Significant difference!

Jump: Measurable?

Outline

Conclusion & Outlook

- A solution to a double-valued EOS dilemma in the metastable region is proposed and stays within the purely hydro approach.
- The criterion for the instantaneous MS $\rightarrow$ EQ-EOS transition (explosive boiling) is derived.

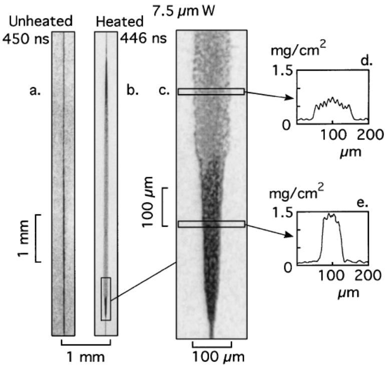
Outlook

- Full implementation in RALEF-2D needs to be considered.
- Adequate simulations of WDM experiments at HHT area and FAIR can be performed with the proposed method.
- Persistent foamlike liquid-vapor structures were observed in exploding wire cores.

Multiphase foamlike structure in exploding wires

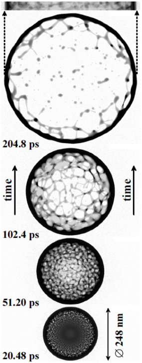
X-ray backlighter images of current induced wire explosions

S. A. Pikuz et al., Phys. Rev. Lett. 83 (1999) 21



Large scale molecular dynamics simulations

V. V. Zhakhovsky et al., will be published



Outline

MPQeos-JWGU equation-of-state model

History

MPQeos was developed by A. Kemp and J. Meyer-ter Vehn, 1998.

It is based on the "quotidian equation-of-state model (QEOS)" by R. M. More et al., 1988.

Since 2008 we improve MPQeos with the goal to provide the EOS for "arbitrary" materials, also for mixtures of elements.

Input and output quantities

Input: Density ρ_0 and bulk modulus K_0 at a reference temperature T_0 and pressure $p_0 = 0$, atomic weights A and numbers Z

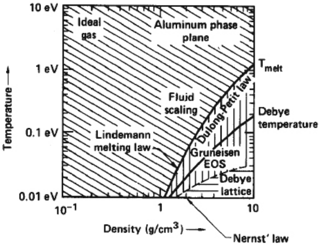
Output: Internal energy E, pressure p, Helmholtz free energy F, entropy S, charge state q, critical point, binodal, spinodal

QEOS model

The equation of state is derived from the Helmholtz free energy F.

Three contributions

1. Electronic contribution: Thomas-Fermi model
2. Ionic contribution: Analytical interpolation between Debye solid, normal solid, and liquid states
3. Bonding correction: Assures the correct values of ρ_0 and K_0 at T_0 and p_0



Drawback of QEOS

Overestimation of pressures (critical point) for $\rho < \rho_0$

Modifications in the MPQeos-JWGU model

List of improvements

- Homogeneous mixtures of elements can now be calculated.
- New numerics for the Maxwell construction
  $\Rightarrow$ Gain in accuracy and speed by a factor of 10!
- New cold curve for $\rho < \rho_0$: $\epsilon_{cold}(\rho) = A\rho^n - B\rho^m + \epsilon_{coh}$
  ϵ_{coh} - cohesive energy; n, m - fitting parameters; A, B - fixed

  E.g.: Critical point improvement for aluminum:

Experimental values:	$T_c = 5700\,\mathrm{K}$,	$p_c = 1820\,\mathrm{bar}$
Original MPQeos:	$T_c = 13487\,\mathrm{K}$,	$p_c = 23487\,\mathrm{bar}$
MPQeos-JWGU:	$T_c = 5558\,\mathrm{K}$,	$p_c = 1722\,\mathrm{bar}$

- Upcoming soon: MPQeos-JWGU will become a library.
  $\Rightarrow$ Allows direct implementation into C- and Fortran-codes

MPQeos-JWGU model users

MPQeos-JWGU is already used by working groups from

- University of Rostock, Germany
- University of Duisburg, Germany
- Ecole Polytechnique, Paris region, France
- Institute of Applied Physics and Computational Mathematics, BeiJing, China
- and in the near future also at Florida State University for simulations of Rayleigh-Taylor instability experiments at NIF

Acknowledgments & Main references

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This work is already submitted and on the verge of publication.

- V. P. Skripov, "Metastable Liquids", Wiley, New York (1974)
- M. Blander, J. L. Katz, AIChE Journal 21 (1975) 833
- R. M. More, K. H. Warren, D. A. Young, G. B. Zimmerman, Physics of Fluids 31 (1988) 3059
- A. Kemp, J. Meyer-ter-Vehn, MPQ Report 229 (1999)

Thank you for your attention!

Supplements - Quasi-static hydrodynamic solution

Long-term quasi-static solution of the hydrodynamic equations

Fluid velocity: $u(t,x) = ax$, at $x = \frac{l}{2}$: $u_l = a\frac{l}{2}$ - surface velocity

Expansion rate: $a(t) = -\frac{d \ln \rho}{dt}$

Assuming Mie-Grüneisen EOS: $a(t) = \Gamma \frac{q}{c_s^2}$

$p(\rho, \epsilon) = p_c(\rho) + \Gamma\rho\,(\epsilon - \epsilon_c(\rho))$, Γ - Grüneisen coefficient

The quasi-static solution is valid if

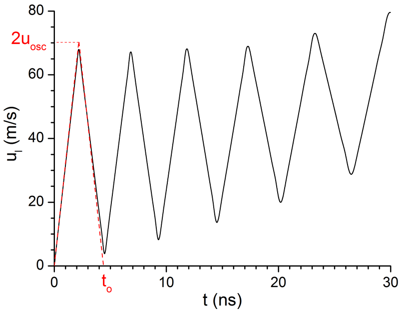
$\mathbf{at_s \ll 1}$ $\Leftrightarrow$ $\Delta\rho$ significant on time scale $\Delta t \simeq a^{-1}$

E.g. $q = 10^{11}\,\frac{\mathrm{J}}{\mathrm{gs}}$ $\Rightarrow$ $a \simeq 10^7\ \mathrm{s}^{-1}$, $at_s \lesssim 0.03$ for $l \lesssim 10\ \mu\mathrm{m}$

These conditions correspond to the energy deposition of 10 kJ/g in 100 ns (HHT ion beam).

Supplements - Quasi-elastic oscillations

At $t = 0$ the heating is turned on. $\Rightarrow$ Surface velocity oscillations!



SiO_2, $l_0 = 10\ \mu$m, $q = 10^{11}\ \frac{J}{gs}$

General hydro solution

Allows for oscillations.

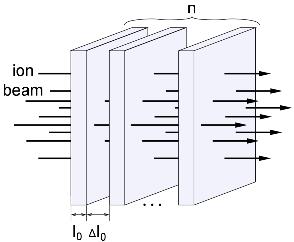
For $t \ll a^{-1}$: $u_{osc} = \frac{1}{2} a l_0$,
$t_0 = 2 l_0 / c_s$

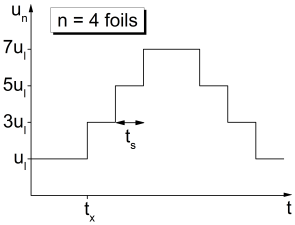
Oscillations are not wanted!

Experiment: Pre-pulse on
time scale $\Delta t \simeq a^{-1}$

Theory: $u(0, x) = a_0 x$
Linear profile at $t = 0$

Supplements - Stack target experiment





Stack targets for EOS measurements

t_x - homogenization time

$t < t_x$: Quasi-isobaric expansion

$t = t_x$: Weak shocks

$t > t_x$: Expansion by shock hydro

Measure t_x and surface temperature

$\Rightarrow$ $\alpha_p = -\rho^{-1}(\partial\rho/\partial T)_p$, $\alpha_p^* = -\rho^{-1}(\partial\rho/\partial h)_p$, $c_p = (\partial h/\partial T)_p$

Location of critical point

Non-congruent phase transitions

Supplements - Proof for $T_2 > T_1$

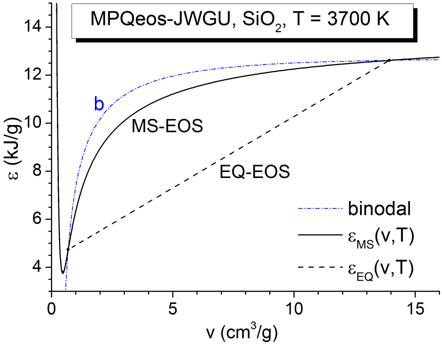
Van-der-Waals EOS

$$\epsilon_{EQ}(v, T) < \epsilon_{MS}(v, T)$$

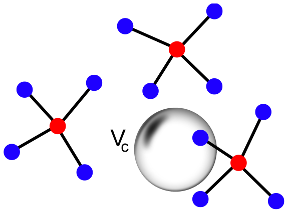
$$c_{v,EQ} = \partial\epsilon_{EQ}/\partial T > 0$$

$$\epsilon_{MS}(v, T_1) \overset{!}{=} \epsilon_{EQ}(v, T_2)$$

$$\Rightarrow T_2 > T_1$$



Supplements - Limits and constraints near the spinodal



Bubble size

$r_c = \frac{\sigma}{p_e - p} \to 0$ formally possible!

$\Rightarrow$ Restraint on molecule population:

$$NV_c \gtrsim 10 - 100$$

Nucleation rate

If $\sigma \to 0 \quad \Rightarrow \quad J = N \left(\frac{3\sigma}{\pi m}\right)^{1/2} \exp\left(-\frac{W_c}{T}\right) \to 0$

$\Rightarrow$ Restraint on preexponential factor:

$$\sigma = const. = \sigma_m = \sigma(T_m), \quad T_m \text{ - melting temperature}$$

$\sigma \to 0$: Still an open question?!

Supplements - Simulation results for the equilibrium case

v-*p* phase plane - EQ case