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

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Steffen Faik[1], Mikhail M. Basko[2,3], Anna Tauschwitz[1,2], Igor Iosilevskiy[2,4,5], Joachim A. Maruhn[1,2]

(1) ITP, Goethe-Universität, Frankfurt (2) EMMI, GSI, Darmstadt (3) ITEP, Moscow (4) JIHT-RAS, Moscow (5) MIPT, Moscow region

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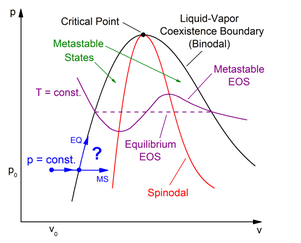
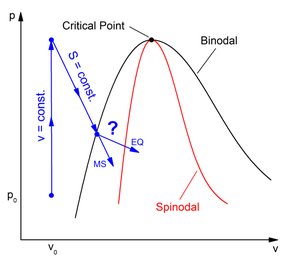
General problem in hydrodynamic simulations

Isobaric expansion



Isochoric heating → Isentropic expansion



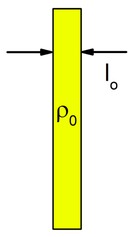
MS: Metastable EOS EQ: Equilibrium EOS

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 $t_s = l/c_s$ → 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

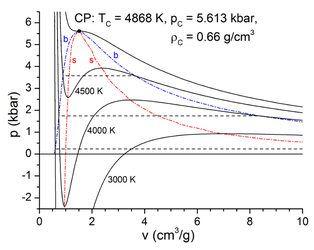
→ Demonstrates the capabilities of FEOS

FEOS for SiO_2

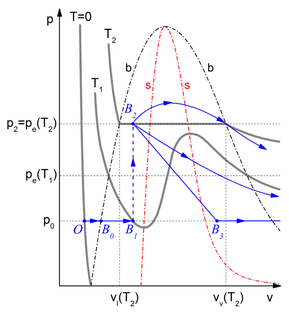
Provides metastable and equilibrium EOS

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

Provides a realistic critical point location



General considerations



Quasi-isobaric expansion

The entire sample is represented by a single point.

Evolution of a fluid element

$O \to B_0$: Isobaric expansion

$B_0 \to B_1$: Follow MS-EOS

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

Explosive boiling: Local and instantaneous

Subsequent evolution $B_2 \to ?$: 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.

⇒ 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)

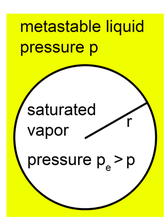
Pressure rises!

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

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

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

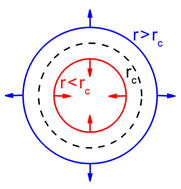
Thermodynamic fluctuations ⇒ Bubbles

$p_e(T) = p + \frac{2\sigma}{r_c}$ ⇒ 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, $N = \rho/m$

→ On a par with the EOS, the surface tension σ must be known!

Surface tension laws

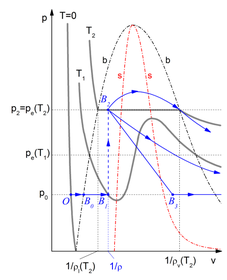
- Guggenheim-Katayama:

  $\sigma_{GK}(T) = \sigma_m \left(\frac{T_c - T}{T_c - T_m}\right)^{11/9}$ → 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

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

→ 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 $W_c/T \gg 1$ → 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

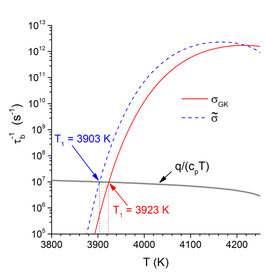
The effective rate of explosive boiling must be compared with the timescale of the quasi-static heating.

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

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: $NV_c = 219$

→ The theory is applicable!

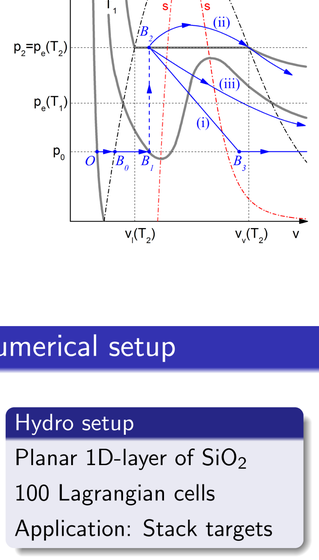
Timescale for a one-order change of the effective boiling rate

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

Subsequent evolution of the two-phase states

$B_1 \to B_2$: c_s drops strongly!

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



$B_2 \to ?$: Different trajectories

(i) - Foil boundary

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

⇒ Quick isentropic relaxation

$B_3 \to \ldots$: Quasi-isobaric

(ii) - Inner foil elements

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

(iii) - Intermediate case

Numerical setup

Hydro setup

Planar 1D-layer of SiO_2

100 Lagrangian cells

Application: Stack targets

Quasi-static heating

$q = 10^{11}$ J/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

FEOS EOS

$l_0 = 10$ μm, $T_0 = 312$ K,

$\rho_0 = 2.2$ g/cm^3, $p_0 = 500$ bar,

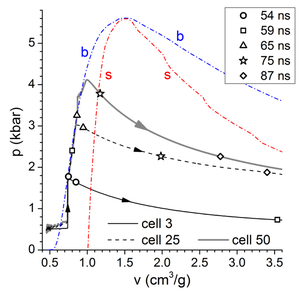
$c_{s,0} = 4.56 \times 10^5$ cm/s

Two simulations

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

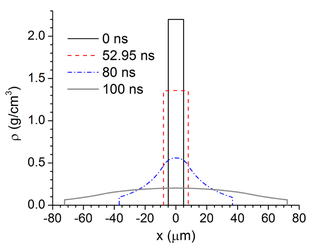
The boundary relaxes to p_0.

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 ⇒ Binodal becomes an attractor!

Simulation results (2/2)

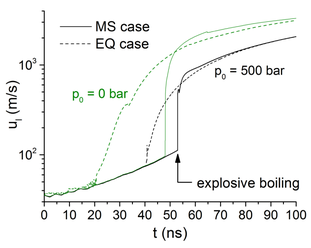
Density profiles - MS case



$t \le t_b$: ρ homogeneous

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

Surface velocity



Significant difference!

Jump: Measurable?

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 → 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.