Laser-induced cavitation bubbles: Mathematical models & simulations

Keh-Ming Shyue

Institute of Applied Mathematical Sciences
National Taiwan University
Taiwan

Joint work with Marica Pelanti at ENSTA, Paris Tech, France

In the memory of our neighbor

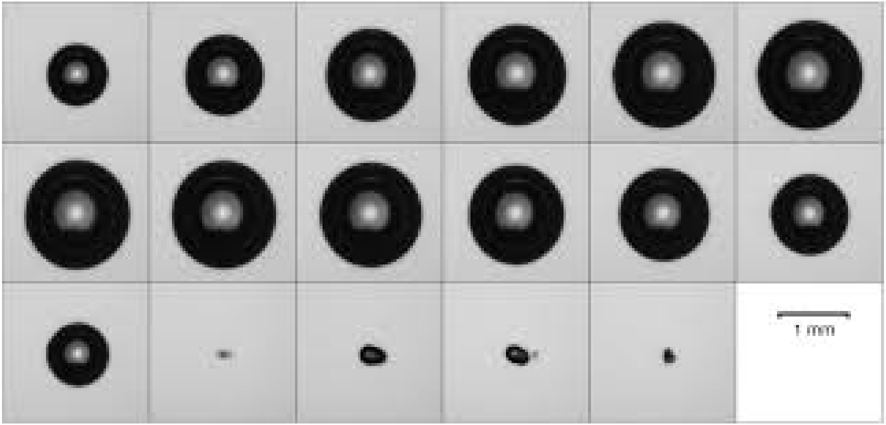
Professor Jaw-Yen Yang

NTU Qin-Tien Faculty Residence Bldg.

Model scientific problem

Expansion & collapse of laser-generated bubble

- Experimental results: Müller *et al.* (CAF 2009)



Bubble radius: Time history

Experiment vs. Keller-Miksis model

S. Müller et al. / Computers & Fluids 38 (2009) 1850–1862 1855

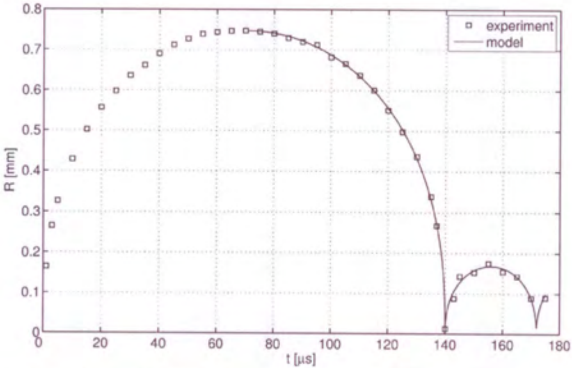
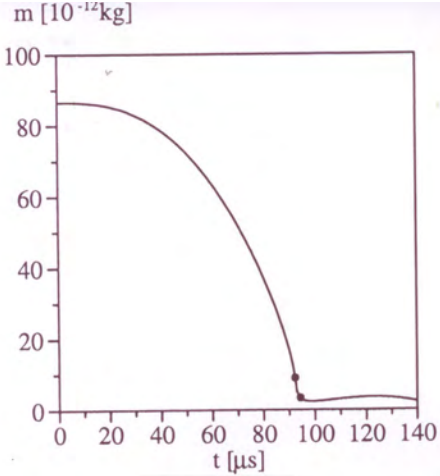


Fig. 3. The points (□) give the experimentally measured bubble radii as a function of time. The solid curve starting at maximum radius presents a numerical solution of the Keller–Miksis model with its parameters fitted to the experiment as described in the text.

Vapor mass: Time history

Akhatov *et al.* (ETFS 2002): Spherically symmetric compressible flow model with heat conduction & phase transition



Laser bubble problem: Scientific issues

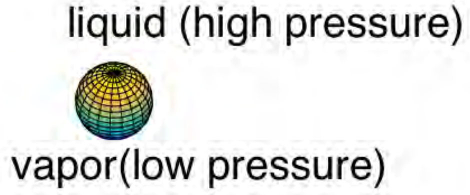
Modelling & simulation of liquid-vapor flow

1. Bubble collapse: Condensation phase
2. Bubble rebound: Evaporation phase:

Laser bubble problem: Benchmark test

Zein *et al.* , Intl J. Numer. Meth. 2013

- High pressure comprssion of spherically-symmetric water vapor (or water vapor-inert gas) bubble in liquid



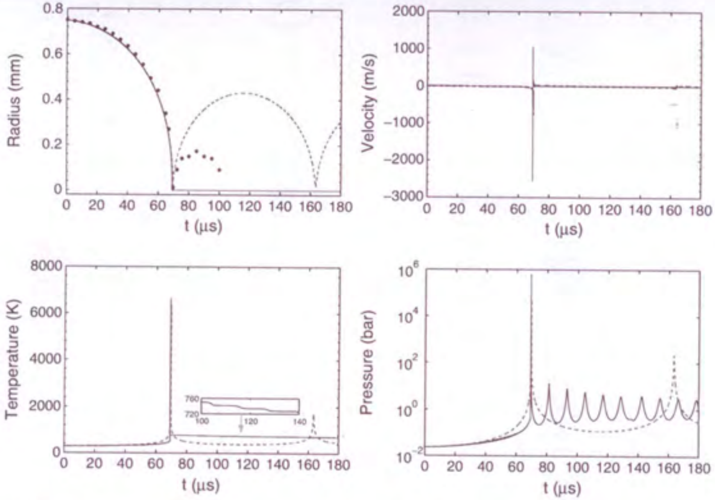
Mathematical models: Compressible 2-phase flow

Models of choice for laser bubble problems include

1. 7-equation model
   2-velocity, 2-pressure, 2-temperature, & 2-entropy
2. 6-equation model (Zein *et al.* & Müller *et al.*)
   1-velocity, 2-pressure, 2-temperature, & 2-entropy
3. 5-equation model (Müller *et al.*)
   1-velocity, 1-pressure, 2-temperature, & 2-entropy
4. 4-equation model
   1-velocity, 1-pressure, 1-temperature, & 2-entropy
5. 3-equation model
   1-velocity, 1-pressure, 1-temperature, & 1-entropy

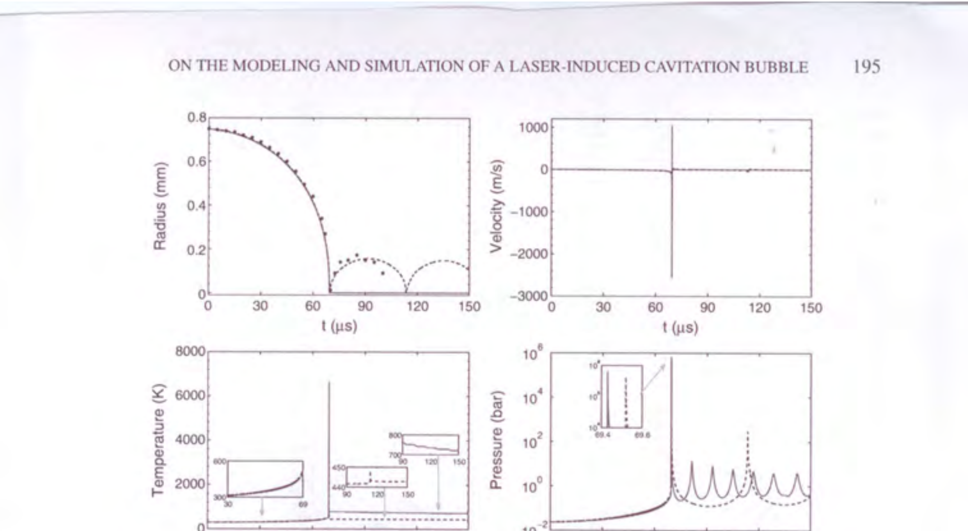
Previous result: Vapor bubble case

Zein *et al.* 2013: 6-equation for 2-phase flow with & without phase transition (no rebound after collapse with phase change)



Previous result: Gas-vapor bubble case

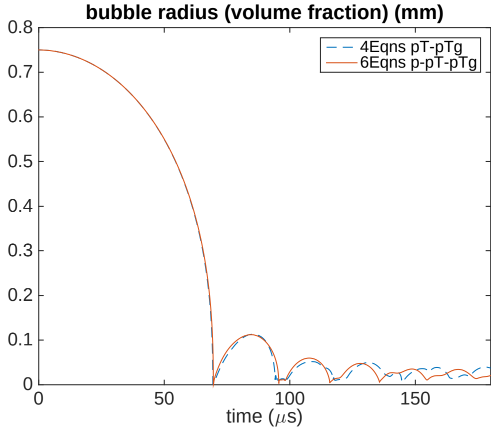
Zein *et al.* 2013: variant 6-equation for 3-phase flow with non-condensable gas (rebounds occur but disagree with experiment)



Present results: Vapor bubble case

Phase transition results of 2 different models for 2-phase flow

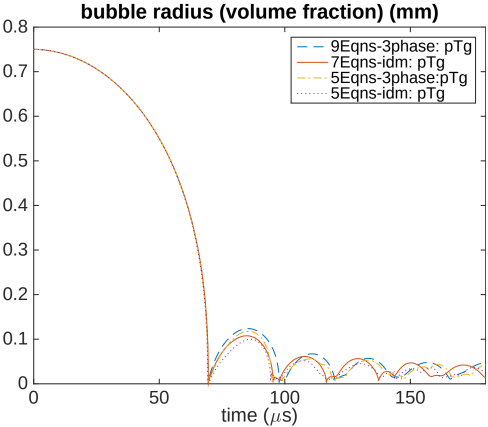
- Rebounds exist with decay of magnitude in time (agree with experiment qualitatively)



Present results: Gas-vapor bubble case

Phase transition results of 4 different models for 3-phase flow

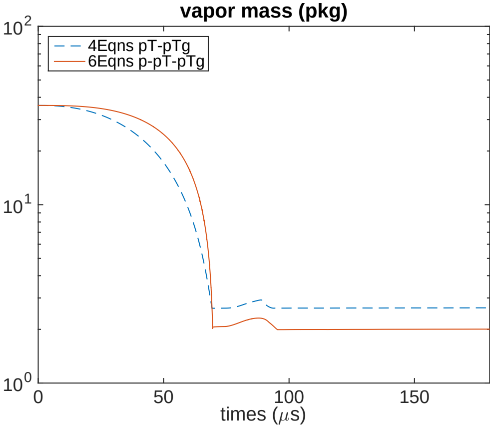
- Rebounds exist with decay of magnitude in time (agree with experiment qualitatively)
- Noncondensable O_2 with $\alpha_a = 10^{-2}$ included



Present result: Vapor bubble case

Phase transition results of 2 different models for 2-phase flow

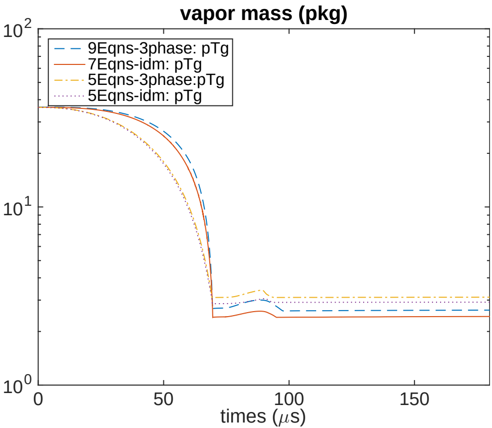
- Vapor mass decreases due to bubble collapse & increases due to rebound (agree with Akhatov's prediction qualitatively)



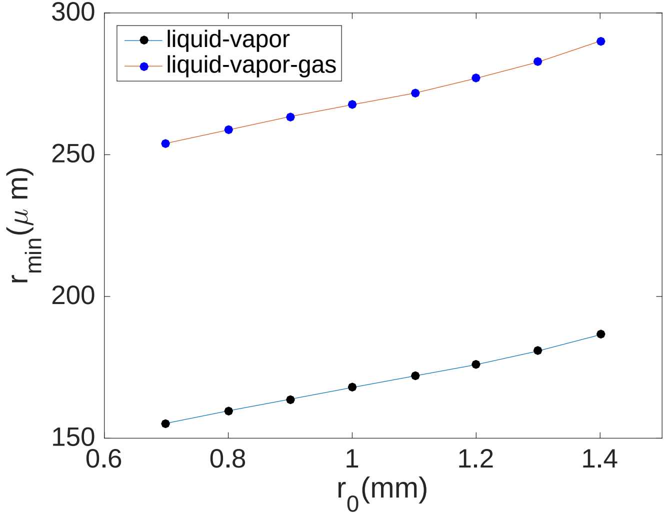
Present result: Gas-vapor bubble case

Phase transition results of 4 different models for 3-phase flow

- Gas mass decreases due to bubble collapse & increases due to rebound (agree with Akhatov's prediction qualitatively)



Initial bubble size vs. minimum bubble radius



Laser bubble problem: CPU timing

Machine: Mac with Intel(R) Xeon(R) $E5$-1620 $v2$@3.70GHz

2-phase	Mesh/R_0	CPUs	3-phase	Mesh/R_0	CPUs
4Eqns	125	3122	5Eqns	125	7703
	250	19518		250	28868
	500	72487		500	91786
6Eqns	125	4192	5Eqns-idm	125	4888
	250	24937		250	14492
	500	73649		500	56994
			9Eqns	125	6102
				250	26876
				500	101929
			7Eqns-idm	125	4625
				250	18362
				500	73366

Talk outline

Objective: Talk simple model & basic idea in numerics

Talk outline

Objective: Talk simple model & basic idea in numerics

1. Mathematical model
   - 1-velocity, 1-pressure, 1-temperature, & 2-entropy model
     - 4-equation model for 2-phase flow & its variant for 3-phase flow
   - 1-velocity, 2-pressure, 2-temperature, & 2-entropy model (referred to M. Pelanti's talk)
     - 6-equation model for 2-phase flow & its variant for 3-phase flow
2. Numerical method
   - Solver for thermo-chemical phase-change equation

Talk outline

Objective: Talk simple model & basic idea in numerics

1. Mathematical model
   - 1-velocity, 1-pressure, 1-temperature, & 2-entropy model
     - 4-equation model for 2-phase flow & its variant for 3-phase flow
   - 1-velocity, 2-pressure, 2-temperature, & 2-entropy model (referred to M. Pelanti's talk)
     - 6-equation model for 2-phase flow & its variant for 3-phase flow
2. Numerical method
   - Solver for thermo-chemical phase-change equation

Work in progress

Compressible 2-phase flow: 4-equation model

Consider 1-velocity, 1-pressure, & 1-temperature compressible 2-phase flow model with phase transition of form

$$
\begin{aligned}
\partial_t \rho + \nabla \cdot (\rho \vec{u}) &= 0 \\
\partial_t (\rho \vec{u}) + \nabla \cdot \left(\rho \vec{u} \otimes \vec{u} + p \overline{\overline{I}} \right) &= 0 \\
\partial_t (\rho E) + \nabla \cdot (\rho E \vec{u} + p \vec{u}) &= 0 \\
\partial_t (\rho Y_1) + \nabla \cdot (\rho Y_1 \vec{u}) &= \dot{m}
\end{aligned}
$$

ρ: mixture density, $\vec{u}$: velocity

p: mixture pressure, E: total energy

Y_k: mass fraction for phase k $(Y_1 + Y_2 = 1)$

$\dot{m}$: mass transfer term

Compressible 2-phase flow: 4-equation model

Consider 1-velocity, 1-pressure, & 1-temperature compressible 2-phase flow model with phase transition of form

$$
\begin{aligned}
\partial_t \rho + \nabla \cdot (\rho \vec{u}) &= 0 \\
\partial_t (\rho \vec{u}) + \nabla \cdot \left(\rho \vec{u} \otimes \vec{u} + p \overline{\overline{I}}\right) &= 0 \\
\partial_t (\rho E) + \nabla \cdot (\rho E \vec{u} + p \vec{u}) &= 0 \\
\partial_t (\rho Y_1) + \nabla \cdot (\rho Y_1 \vec{u}) &= \dot{m}
\end{aligned}
$$

ρ: mixture density, $\vec{u}$: velocity
p: mixture pressure, E: total energy
Y_k: mass fraction for phase k ($Y_1 + Y_2 = 1$)
$\dot{m}$: mass transfer term

Model closure: isobaric-isothermal, *i.e.*, p & T equilibrium without phase transition

4-equation model: Mass transfer

Assume mass transfer via thermo-chemical relaxation:

- Gibbs free energy based

$$\dot{m} = \rho\mu_g\left(g_2 - g_1\right)$$

- Mass fraction based

$$\dot{m} = \rho\mu_Y\left(Y_1^* - Y_1\right)$$

Relaxation parameter μ_k, $k = g, Y$ controls rate of "phase transition", *e.g.*, vaporization or condensation of liquid & vapor

Downar-Zapolski *et al.* : Empicical fit

$$\mu_Y = a\alpha^b\phi^c, \quad \varphi = \left|\frac{p_{\mathsf{sat}} - p}{p_c - p_{\mathsf{sat}}}\right|$$

HRM: Model as $\mu = 0$, $\nu \to \infty$ & $\theta \to \infty$

Assume frozen chemical relaxation $\mu = 0$, HRM in mechanical-thermal limit as $\nu \to \infty$ & $\theta \to \infty$ reads (Saurel *et al.* 2008, Flåtten *et al.* 2010)

$$\partial_t \rho + \nabla \cdot (\rho \vec{u}) = 0$$

$$\partial_t (\rho \vec{u}) + \nabla \cdot \left(\rho \vec{u} \otimes \vec{u} + p \overline{\overline{I}} \right) = 0$$

$$\partial_t E + \nabla \cdot (E \vec{u} + p \vec{u}) = 0$$

$$\partial_t (\rho Y_1) + \nabla \cdot (\rho Y_1 \vec{u}) = 0$$

Mechanical-thermal equilibrium speed of sound satisfies

$$\frac{1}{\rho c_{pT}^2} = \frac{1}{\rho c_p^2} + T \left(\frac{\Gamma_2}{\rho_2 c_2^2} - \frac{\Gamma_1}{\rho_1 c_1^2} \right)^2 \Bigg/ \left(\frac{1}{\alpha_1 \rho_1 c_{p1}} + \frac{1}{\alpha_2 \rho_2 c_{p2}} \right)$$

Homogeneous relaxation model (HRM)

Consider HRM for 2-phase flow of form

$$
\begin{aligned}
&\partial_t (\alpha_1\rho_1) + \nabla\cdot(\alpha_1\rho_1\vec{u}) = \mu\,(g_2 - g_1)\\
&\partial_t (\alpha_2\rho_2) + \nabla\cdot(\alpha_2\rho_2\vec{u}) = \mu\,(g_1 - g_2)\\
&\partial_t(\rho\vec{u}) + \nabla\cdot(\rho\vec{u}\otimes\vec{u}) + \nabla\,(\alpha_1 p_1 + \alpha_2 p_2) = 0\\
&\partial_t (\alpha_1 E_1) + \nabla\cdot(\alpha_1 E_1\vec{u} + \alpha_1 p_1\vec{u}) + \mathcal{B}\,(q,\nabla q) =\\
&\qquad \nu p_I\,(p_2 - p_1) + \theta T_I\,(T_2 - T_1) + \mu g_I\,(g_2 - g_1)\\
&\partial_t (\alpha_2 E_2) + \nabla\cdot(\alpha_2 E_2\vec{u} + \alpha_2 p_2\vec{u}) - \mathcal{B}\,(q,\nabla q) =\\
&\qquad \nu p_I\,(p_1 - p_2) + \theta T_I\,(T_1 - T_2) + \mu g_I\,(g_1 - g_2)\\
&\partial_t\alpha_1 + \vec{u}\cdot\nabla\alpha_1 = \nu\,(p_1 - p_2) + \mu v_I\,(g_1 - g_2)
\end{aligned}
$$

$\mathcal{B}\,(q,\nabla q)$ is non-conservative product (q: state vector)

$$
\mathcal{B} = \vec{u}\cdot\left[Y_1\nabla\,(\alpha_2 p_2) - Y_2\nabla\,(\alpha_1 p_1)\right]
$$

$\nu, \theta, \mu \to \infty$: instantaneous exchanges (relaxation effects)

1. Volume transfer via pressure relaxation: $\nu\,(p_1 - p_2)$
   - ν expresses rate toward mechanical equilibrium $p_1 \to p_2$, & is nonzero in all flow regimes of interest

2. Heat transfer via temperature relaxation: $\theta\,(T_2 - T_1)$
   - θ expresses rate towards thermal equilibrium $T_1 \to T_2$, & is nonzero only at 2-phase mixture

3. Mass transfer via thermo-chemical relaxation: $\mu\,(g_2 - g_1)$
   - μ expresses rate towards diffusive equilibrium $g_1 \to g_2$, & is nonzero only at 2-phase mixture & metastable state

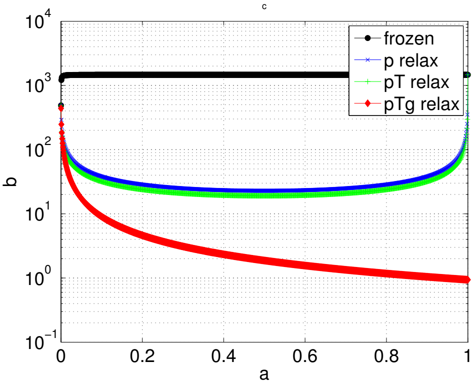
Equilibrium speed of sound

- Sound speeds follow subcharacteristic condition

$$c_{pTg} \leq c_{pT} \leq c_p \leq c_f$$

- Limit of sound speed

$$\lim_{\alpha_k \to 1} c_f = \lim_{\alpha_k \to 1} c_p = \lim_{\alpha_k \to 1} c_{pT} = c_k, \quad \lim_{\alpha_k \to 1} c_{pTg} \neq c_k$$



4-equation model: Spherically-symmetric case

For laser-induced bubble problem, equations we take are either

$$\partial_t \rho + \partial_V \left(r^2 \rho u\right) = 0$$

$$\partial_t (\rho u) + \partial_V \left(r^2 \rho u^2 + r^2 p\right) = \frac{2}{r} p$$

$$\partial_t (\rho E) + \partial_V \left(r^2 \rho E u + r^2 p u\right) = 0$$

$$\partial_t (\rho Y_1) + \partial_V \left(r^2 \rho Y_1 u\right) = \frac{1}{r^2} \dot{m}$$

where $\partial V = r^2 \partial_r$, or

$$\partial_t \rho + \partial_r (\rho u) = -\frac{2}{r} \rho u$$

$$\partial_t (\rho u) + \partial_r \left(\rho u^2 + p\right) = -\frac{2}{r} \rho u^2$$

$$\partial_t (\rho E) + \partial_r (\rho E u + p u) = -\frac{2}{r} (\rho E + p) u$$

$$\partial_t (\rho Y_1) + \partial_r (\rho Y_1 u) = -\frac{2}{r} \rho Y_1 u + \frac{1}{r^2} \dot{m}$$

Constitutive law

Assume stiffened gas equation of state (SG EOS) with

- Specific volume

$$v_k(p_k, T_k) = \frac{(\gamma_k - 1)C_{v,k}T_k}{p_k + p_{\infty,k}}$$

- Specific internal energy

$$e_k(p_k, T_k) = C_{v,k}T_k\left(\frac{p_k + \gamma_k p_{\infty,k}}{p_k + p_{\infty,k}}\right) + q_k$$

- Entropy

$$s_k(p_k, T_k) = C_{vk}\log\frac{{T_k}^{\gamma_k}}{(p_k + p_{\infty,k})^{\gamma_k - 1}} + q'_k$$

- Helmholtz free energy $a_k = e_k - T_k s_k$
- Gibbs free energy $g_k = a_k + p_k v_k$

Stiffened gas EOS parameters

Water: liquid- & vapor-phase
Air: oxygen & hydrogen (noncondensable gas)

Parameters/Phase	Liquid	Vapor	O_2	H_2
γ	2.35	1.43	1.4	1.4
p_∞ (Pa)	10^9	0	0	0
q (J/kg)	-11.6×10^3	2030×10^3	0	0
q' (J/(kg $\cdot$ K))	0	-23.4×10^3	0	0
C_v (J/(kg $\cdot$ K))	1816	1040	662	1010

Ref: Zein *et al.* , Intl J. Numer. Meth. 2013

Numerical scheme: Fractional step approach

Write model equation in compact form as

$$\partial_t q + \nabla \cdot f(q) = \psi(q) = \psi_s(q) + \psi_\mu(q)$$

Employ standard fractional step method for numerical approximation, *i.e.*,

1. Solve homogeneous equation without phase transition

   $$\partial_t q + \nabla \cdot f(q) = 0$$

   using state-of-the-art shock-capturing (diffuse-interface) method for hyperbolic conservation laws (model is hyperbolic)

2. Solve ODEs with geometric & phase transition source terms

   $$\partial_t q = \psi_s(q) + \psi_\mu(q)$$

   using standard solvers

Model closure: pT equilibrium solution

With stiffened gas EOS, it follows from

$$v = Y_1 v_1(p,T) + Y_2 v_2(p,T) \qquad (v = 1/\rho,\ v_k = 1/\rho_k)$$
$$e = Y_1 e_1(p,T) + Y_2 e_2(p,T)$$

that we have

$$v = Y_1 \frac{(\gamma_1 - 1)C_{v,1}T}{p + p_{\infty,1}} + Y_2 \frac{(\gamma_2 - 1)C_{v,2}T}{p + p_{\infty,2}}$$
$$e = Y_1 C_{v,1} T \left(\frac{p + \gamma_1 p_{\infty,1}}{p + p_{\infty,1}} \right) + Y_1 q_1 + Y_2 C_{v,2} T \left(\frac{p + \gamma_2 p_{\infty,2}}{p + p_{\infty,2}} \right) + Y_2 q_2$$

yielding single quadratic equation for p (not shown) & explicit computation of T:

$$\frac{1}{\rho T} = Y_1 \frac{(\gamma_1 - 1)C_{v1}}{p + p_{\infty,1}} + Y_2 \frac{(\gamma_2 - 1)C_{v2}}{p + p_{\infty,2}}$$

Phase change equations: pTg equilibrium solution

Suppose solution states lie in metastable region & assume infinite relaxation $\nu \to \infty$, want to find equilibrium states for p, T, & Y_1 so that $g_1 \to g_2$, yielding fulfillment of following conditions

1. Saturation condition for pressure p & temperature T

$$\mathcal{G}(p,T) := g_1(p,T) - g_2(p,T) = 0$$

2. Equilibrium condition for specific volume v

$$Y_1 v_1(p,T) + Y_2 v_2(p,T) = v$$

3. Equilibrium condition for internal energy e

$$Y_1\ e_1(p,T) + Y_2\ e_2(p,T) = e$$

or for specific enthalpy h defined by $h_k = e_k + pv_k$

$$Y_1 h_1(p,T) + Y_2 h_2(p,T) = h$$

pTg equilibrium solution

From saturation condition for equilibrium p & T:

$$\mathcal{G}(p, T) = 0$$

& equilibrium conditions 2 & 3 above: *i.e.*, either

$$\mathcal{H}(p, T) = \frac{v - v_2(p, T)}{v_1(p, T) - v_2(p, T)} - \frac{e - e_2(p, T)}{e_1(p, T) - e_2(p, T)} = 0$$

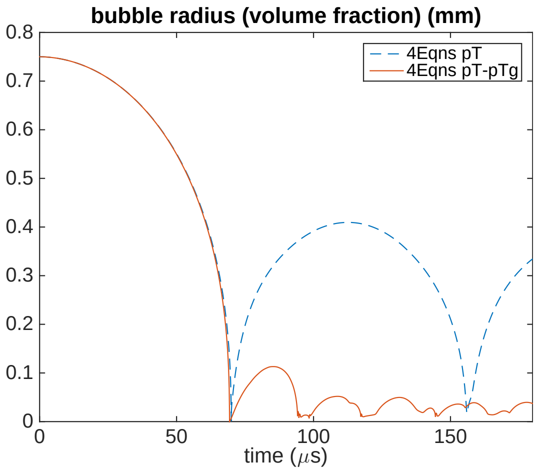
or

$$\mathcal{H}(p, T) = \frac{v - v_2(p, T)}{v_1(p, T) - v_2(p, T)} - \frac{h(p) - h_2(p, T)}{h_1(p, T) - h_2(p, T)} = 0$$

we have 2 equations $\mathcal{G} = 0$ & $\mathcal{H} = 0$ for 2 unknowns p & T which can be solved by employing root-finding method iteratively

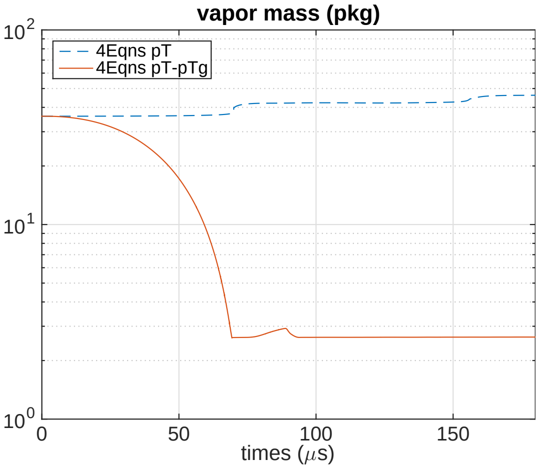
Benchmark laser bubble test: Bubble radius

Less rebounds without phase transition



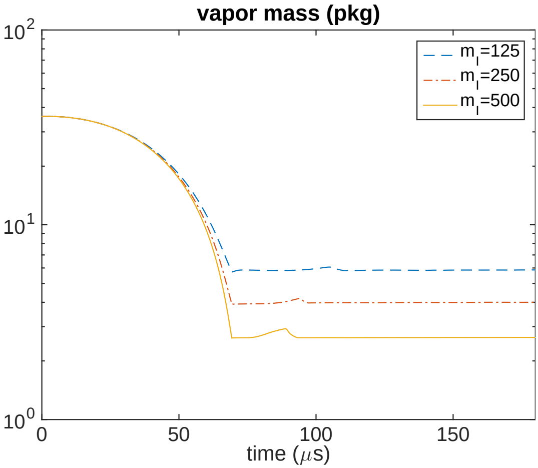
Benchmark laser bubble test: Vapor mass

Vapor mass increases without phase transition



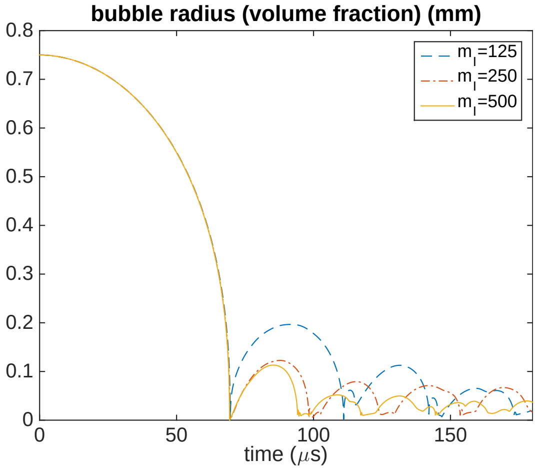
Vapor mass: Mesh refinement test

Vapor mass decreases more as mesh is refined



Bubble radius: Mesh refinement test

More rebounds as mesh is refined with smaller bubble-radius amplitude



Compressible 3-phase flow: 5-equation model

Extension of 4-equation p-T model from 2-phase to 3-phase flow takes form

$$
\begin{aligned}
\partial_t(\alpha_v\rho_v) + \nabla\cdot(\alpha_v\rho_v\vec{u}) &= \dot{m} \\
\partial_t(\alpha_l\rho_l) + \nabla\cdot(\alpha_l\rho_l\vec{u}) &= -\dot{m} \\
\partial_t(\alpha_a\rho_a) + \nabla\cdot(\alpha_a\rho_a\vec{u}) &= 0 \quad (\text{non-condensible}) \\
\partial_t(\rho\vec{u}) + \nabla\cdot\left(\rho\vec{u}\otimes\vec{u}) + p\bar{\bar{I}}\right) &= 0 \\
\partial_t(\rho E) + \nabla\cdot(\rho E\vec{u} + p\vec{u}) &= 0
\end{aligned}
$$

With given EOS for each phase, mixture pressure p & temperature T can be computed from

$$
\begin{aligned}
v &= Y_v v_v(p,T) + Y_l v_l(p,T) + Y_a v_a(p,T) \\
e &= Y_v e_v(p,T) + Y_l e_l(p,T) + Y_a e_a(p,T)
\end{aligned}
$$

Mass transfer term $\dot{m}$ takes same relaxation form as before

Phase change equations: pTg solution

Suppose solution state lies in metastable region & assume infinite relaxation $\nu \to \infty$, want to find equilibrium states for p, T, & Y_v so that $g_v \to g_l$, yielding fulfillment of following conditions

1. Saturation condition for pressure p & temperature T

$$\mathcal{G}(p, T) := g_v(p, T) - g_l(p, T) = 0$$

2. Equilibrium condition for specific volume v

$$Y_v v_v(p, T) + Y_l v_l(p, T) + Y_a v_a(p, T) = v$$

3. Equilibrium condition for specific enthalpy h

$$Y_v h_v(p, T) + Y_l h_l(p, T) + Y_a h_a(p, T) = h$$

4. Equilibrium condition for mass fraction $Y_v + Y_l$

$$Y_v + Y_l = 1 - Y_a$$

3-phase 5-equation model: pTg solution

From saturation condition for equilibrium p & T:

$$\mathcal{G}(p, T) = 0$$

& equlibrium conditions 2, 3, & 4 above:

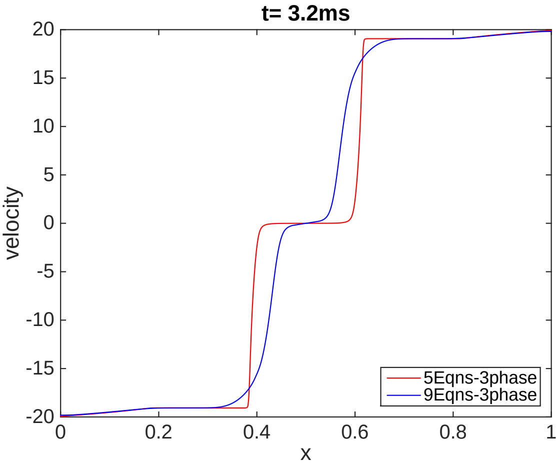
$$\mathcal{H}(p, T) := \frac{v - Y_a v_a(p, T) - (1 - Y_a)\, v_l(p, T)}{v_v(p, T) - v_l(p, T)} - \frac{h(p, T) - Y_a h_a(p, T) - (1 - Y_a)\, h_l(p, T)}{h_v(p, T) - h_l(p, T)} = 0$$

we have 2 equations for 2 unknowns p & T which can be solved by employing root-finding method iteratively

Cavitation test: Numerical validation

Velocity at time $t = 3.2$ms

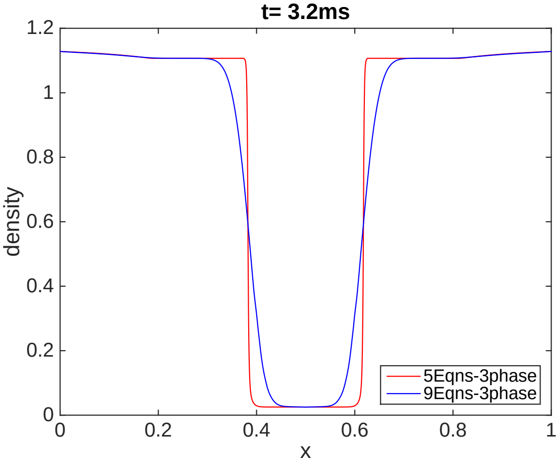
- Existence of 4 (2 rerefaction & 2 evaporation) wave structures



Cavitation test: Numerical validation

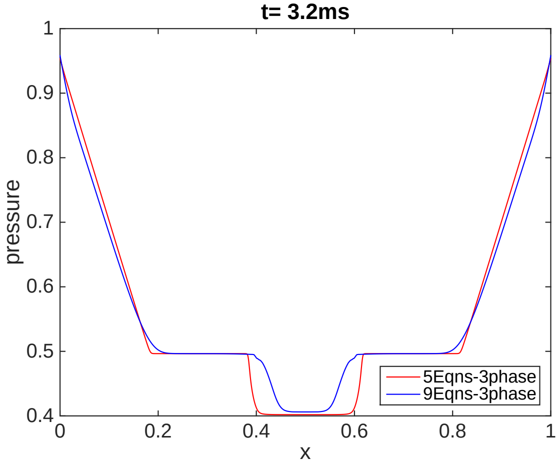
Total density at time $t = 3.2$ms

- 5-equation model gives sharper resolution for evaporation wave than 9-equation model



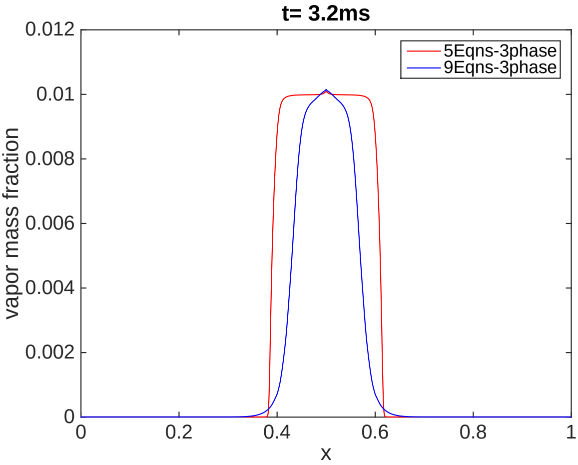
Cavitation test: Numerical validation

Pressure at time $t = 3.2$ms



Cavitation test: Numerical validation

Vapor mass fraction at time $t = 3.2$ms



3-phase flow: 5-equation ideal-mixing model

Assume ideal mixing of air & vapor, *i.e.*, each component behaves as ideal gas alone & occupies entire gas mixture

Ideal-mixing (2-phase) version of 3-phase 5-equation model is

$$\partial_t \left(\alpha_l \rho_l\right) + \nabla \cdot \left(\alpha_l \rho_l \vec{u}\right) = \dot{m}$$

$$\partial_t \left(\alpha_g \rho_v\right) + \nabla \cdot \left(\alpha_g \rho_v \vec{u}\right) = -\dot{m}$$

$$\partial_t \left(\alpha_g \rho_a\right) + \nabla \cdot \left(\alpha_g \rho_a \vec{u}\right) = 0 \quad \text{(non-condensible)}$$

$$\partial_t (\rho \vec{u}) + \nabla \cdot \left(\rho \vec{u} \otimes \vec{u}) + p\overline{\overline{I}}\right) = 0$$

$$\partial_t \left(\rho E\right) + \nabla \cdot \left(\rho E \vec{u} + p\vec{u}\right) = 0$$

Mixture density ρ & gas mass fraction Y_g are defined by

$$\rho = \alpha_l \rho_l + \alpha_g \rho_g, \quad \rho_g = \rho_a + \rho_v$$

$$Y_g = Y_v + Y_a = \frac{\alpha_g \rho_g}{\alpha_l \rho_l + \alpha_g \rho_g}, \quad \alpha_l + \alpha_g = 1$$

Model closure: pT equilibrium solution

Given Y_g, v, & e, model admit single p & T fulfilling

$$(1 - Y_g)\, v_l(p, T) + Y_g v_g(p, T) = v$$
$$(1 - Y_g)\, e_l(p, T) + Y_g e_g(p, T) = e$$

with EOS parameters for v_g & e_g known a priori

Aforementioned pT equilibrium solver for 2-phase 4-equation model is applicable here

5-equation ideal-mixing: EOS parameters

Assume SG EOS for each fluid phase k, $k = l$, v, a

Assume $T_g = T_v = T_a$ & $p_g = p_v + p_a$, we have

$$C_{v,g} = \frac{\rho_v}{\rho_g} C_{v,v} + \frac{\rho_a}{\rho_g} C_{v,a}$$

$$q_g = \frac{\rho_v}{\rho_g} q_v + \frac{\rho_a}{\rho_g} q_a$$

$$p_{\infty,g} = p_{\infty,v} + p_{\infty,a}$$

$$\gamma_g C_{v,g} = \frac{\rho_v}{\rho_g} \gamma_v C_{v,v} + \frac{\rho_a}{\rho_g} \gamma_a C_{v,a}$$

5-equation ideal-mixing: pTg equilibrium solution

Given v, e, & Y_a, want to find equilibrium states for p, T, & Y_v so that following conditions are satisfied

1. Saturation condition for pressure p & temperature T

$$\mathcal{G}(p, T) := g_l(p, T) - g_v(p, T) = 0$$

2. Equilibrium condition for specific volume v

$$(1 - Y_a - Y_v)\, v_l(p, T) + (Y_a + Y_v)\, v_g(p, T) = v$$

3. Equilibrium condition for specific enthalpy h

$$(1 - Y_a - Y_v)\, h_l(p, T) + (Y_a + Y_v)\, h_g(p, T) = h$$

5-equation ideal-mixing model: binary diffusion

With binary diffusion included, 3-phase 5-equation model with ideal mixings reads

$$\partial_t (\alpha_l \rho_l) + \nabla \cdot (\alpha_l \rho_l \vec{u}) = \dot{m}$$

$$\partial_t (\alpha_g \rho_v) + \nabla \cdot (\alpha_g \rho_v \vec{u}) = -\dot{m} + \nabla \cdot \left(\alpha_g \rho_g \varepsilon_{va} \nabla \left(\frac{\rho_v}{\rho_g} \right) \right)$$

$$\partial_t (\alpha_g \rho_a) + \nabla \cdot (\alpha_g \rho_a \vec{u}) = \nabla \cdot \left(\alpha_g \rho_g \varepsilon_{va} \nabla \left(\frac{\rho_a}{\rho_g} \right) \right)$$

$$\partial_t (\rho \vec{u}) + \nabla \cdot \left(\rho \vec{u} \otimes \vec{u}) + p \overline{\overline{I}} \right) = 0$$

$$\partial_t (\rho E) + \nabla \cdot (\rho E \vec{u} + p \vec{u}) = 0$$

ε_{va}: binary diffusion coefficient

Employ fractional step approach for numerical treatment of binary diffusion terms

4-phase flow: 6-equation ideal-mixing model

In problems with 2 different non-condensable gas, say O_2 & H_2, 4-phase flow model with ideal-mixing takes

$$\partial_t\left(\alpha_l\rho_l\right)+\nabla\cdot\left(\alpha_l\rho_l\vec{u}\right)=\dot{m}$$

$$\partial_t\left(\alpha_g\rho_v\right)+\nabla\cdot\left(\alpha_g\rho_v\vec{u}\right)=-\dot{m}$$

$$\partial_t\left(\alpha_g\rho_{a_1}\right)+\nabla\cdot\left(\alpha_g\rho_{a_1}\vec{u}\right)=0 \quad \text{(non-condensible)}$$

$$\partial_t\left(\alpha_g\rho_{a_2}\right)+\nabla\cdot\left(\alpha_g\rho_{a_2}\vec{u}\right)=0 \quad \text{(non-condensible)}$$

$$\partial_t(\rho\vec{u})+\nabla\cdot\left(\rho\vec{u}\otimes\vec{u})+p\overline{\overline{I}}\right)=0$$

$$\partial_t\left(\rho E\right)+\nabla\cdot\left(\rho E\vec{u}+p\vec{u}\right)=0$$

Mixture density ρ & gas mass fraction Y_g are defined by

$$\rho=\alpha_l\rho_l+\alpha_g\rho_g, \quad \rho_g=\rho_v+\rho_{a_1}+\rho_{a_2}$$

$$Y_g=Y_v+Y_{a_1}+Y_{a_2}=\frac{\alpha_g\rho_g}{\alpha_l\rho_l+\alpha_g\rho_g}, \quad \alpha_l+\alpha_g=1$$

6-equation ideal-mixing: EOS parameters

Assume SG EOS for each fluid phase k, $k = l$, v, a_1, a_2

Assume $T_g = T_v = T_{a_1} = T_{a_2}$ & $p_g = p_v + p_{a_1} + p_{a_2}$, we have

$$
\begin{aligned}
C_{v,g} &= \frac{\rho_v}{\rho_g} C_{v,v} + \frac{\rho_{a_1}}{\rho_g} C_{v,a_1} + \frac{\rho_{a_2}}{\rho_g} C_{v,a_2} \\
q_g &= \frac{\rho_v}{\rho_g} q_v + \frac{\rho_{a_1}}{\rho_g} q_{a_1} + \frac{\rho_{a_2}}{\rho_g} q_{a_2} \\
p_{\infty,g} &= p_{\infty,v} + p_{\infty,a_1} + p_{\infty,a_2} \\
\gamma_g C_{v,g} &= \frac{\rho_v}{\rho_g} \gamma_v C_{v,v} + \frac{\rho_{a_1}}{\rho_g} \gamma_{a_1} C_{v,a_1} + \frac{\rho_{a_2}}{\rho_g} \gamma_{a_2} C_{v,a_2}
\end{aligned}
$$

Analogously, EOS parameters for mixture of $m \geq 2$ different non-condensable gas can be defined easily

6-equation ideal-mixing: pTg equilibrium solution

Given v, e, Y_{a_1}, & Y_{a_2}, want to find equilibrium states for p, T, & Y_v so that following conditions are satisfied

1. Saturation condition for pressure p & temperature T

$$\mathcal{G}(p, T) := g_l(p, T) - g_v(p, T) = 0$$

2. Equilibrium condition for specific volume v

$$(1 - Y_{a_1} - Y_{a_2} - Y_v)\, v_l(p, T) + (Y_{a_1} + Y_{a_2} + Y_v)\, v_g(p, T) = v$$

3. Equilibrium condition for specific enthalpy h

$$(1 - Y_{a_1} - Y_{a_2} - Y_v)\, h_l(p, T) + (Y_{a_1} + Y_{a_2} + Y_v)\, h_g(p, T) = h$$

5-phase flow: 7-equation ideal-mixing model

In problems with 2 different non-condensable gas, say O_2 & H_2, & additional solid or fluid-like phase, 5-phase flow model with ideal-mixing for gas & immiscible for other phase takes

$$
\begin{aligned}
\partial_t\left(\alpha_l \rho_l\right)+\nabla \cdot\left(\alpha_l \rho_l \vec{u}\right) &= \dot{m} \\
\partial_t\left(\alpha_g \rho_v\right)+\nabla \cdot\left(\alpha_g \rho_v \vec{u}\right) &= -\dot{m} \\
\partial_t\left({\color{blue}\alpha_g \rho_{a_1}}\right)+\nabla \cdot\left(\alpha_g \rho_{a_1} \vec{u}\right) &= 0 \quad \text{(non-condensible)} \\
\partial_t\left({\color{blue}\alpha_g \rho_{a_2}}\right)+\nabla \cdot\left(\alpha_g \rho_{a_2} \vec{u}\right) &= 0 \quad \text{(non-condensible)} \\
\partial_t\left({\color{red}\alpha_s \rho_s}\right)+\nabla \cdot\left(\alpha_s \rho_s \vec{u}\right) &= 0 \quad \text{(solid phase)} \\
\partial_t(\rho \vec{u})+\nabla \cdot\left(\rho \vec{u} \otimes \vec{u})+p \overline{\overline{I}}\right) &= 0 \\
\partial_t\left(\rho E\right)+\nabla \cdot\left(\rho E \vec{u}+p \vec{u}\right) &= 0
\end{aligned}
$$

Phase transition closure ?

Bubbly flow in liquid

Iordanski-Kogarko-Wijngaarden model for bubbly flow in liquid takes

$$\partial_t \rho + \partial_x (\rho u) = 0$$

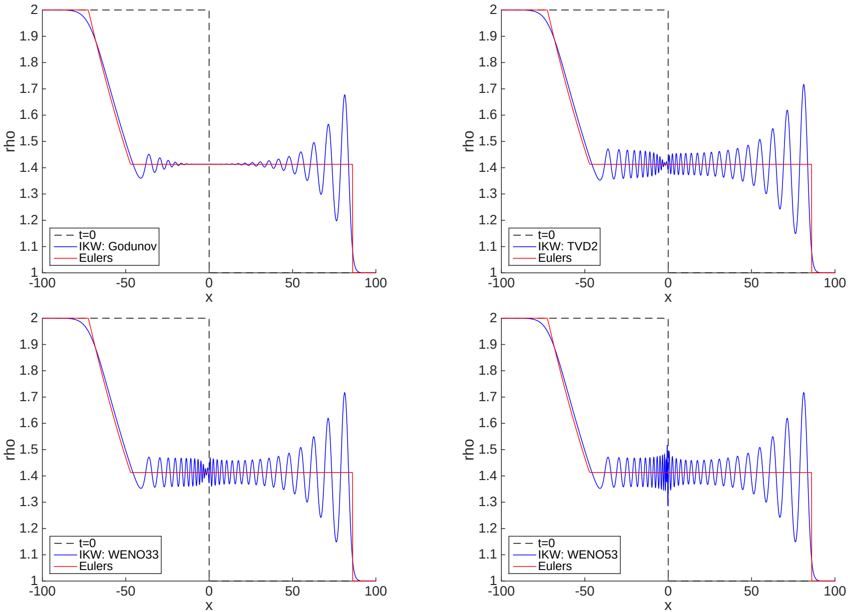
$$\partial_t (\rho K) + \partial_x (\rho K u + p_g(R)) = \partial_x \left(\frac{a^2 \rho_l}{18 \rho^3 R^4} (\partial_x u)^2 \right)$$

with generalized velocity K defined by

$$K = u - \partial_x \left(\frac{a \rho_l}{3 \rho R} \partial_x u \right).$$

Here $\rho = \alpha_l \rho_l + \alpha_g \rho_g$, u, p_g, R denote mixture density, velocity, gas pressure, & bubble radius, respectively. Variables α_k & ρ_k are in turn volume fraction & phasic density of fluid phase k for $k = l$ (liquid phase), g (gas phase); $\alpha_l + \alpha_g = 1$

Dambreak problem: IKW model



Thank you