Homogeneous relaxation models & methods for compressible three-phase flow & more

I: Reduced 4-equation based models

Keh-Ming Shyue

Institute of Applied Mathematical Sciences
National Taiwan University

May 8-12, 2017, CSRC, Beijing, China

Outline

Objective: Talk simple model & basic idea in numerics

Outline

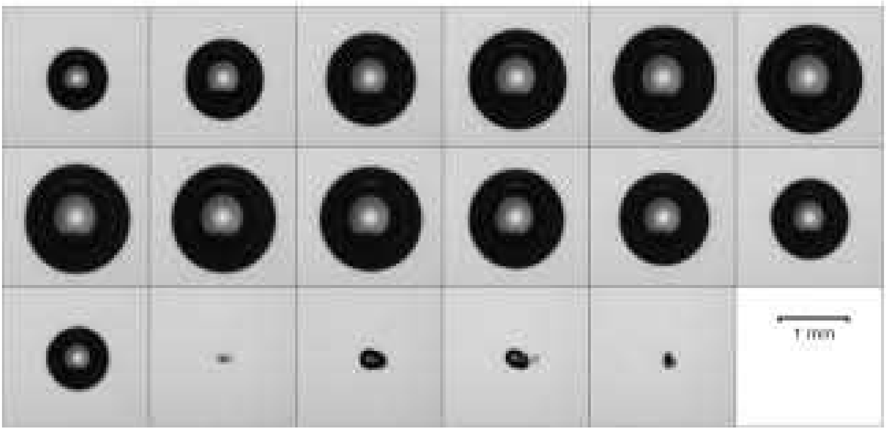
Objective: Talk simple model & basic idea in numerics

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
     - 6-equation model for 2-phase flow & its variant for 3-phase flow
2. Numerical method
   - Solver for thermo-chemical phase-change equation

Model problem

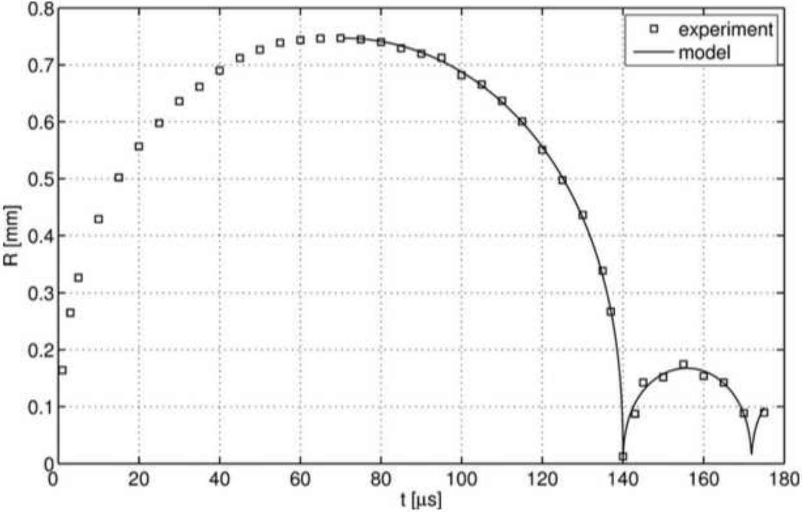
Expansion & collapse of laser-generated bubble

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



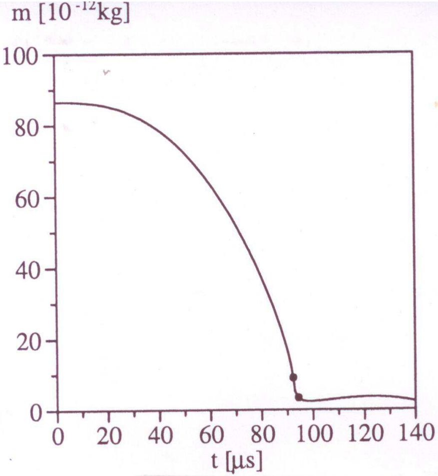
Bubble radius: Time history

Experiment vs. Keller-Miksis model



Vapor mass: Time history

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



Laser bubble problem: Scientific issues

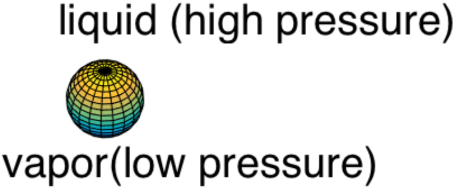
Modelling & simulation of liquid-vapor flow

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)

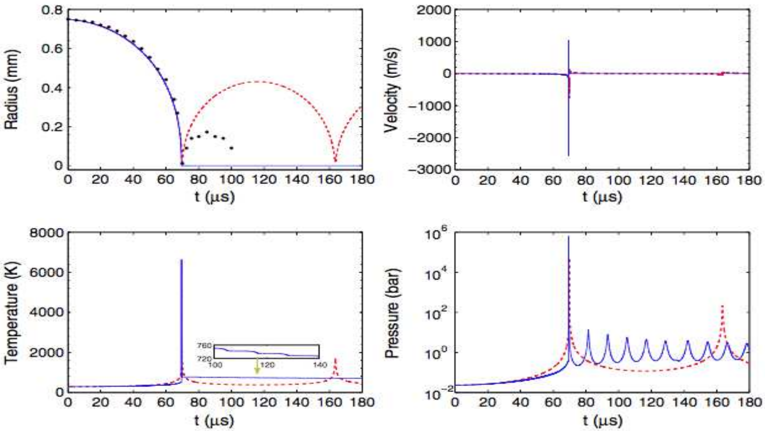


Figure 7. The collapsing vapor bubble results with mass transfer (solid line) compared with those without mass transfer (dashed line). The computed radii are compared with the experimental data (dots). $N_I = 500$ cells, $T_v = 293$ K and $p_v = 2339$ Pa.

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)

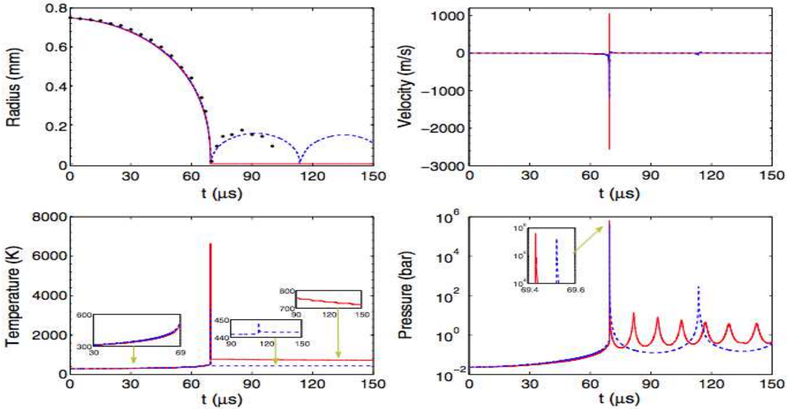
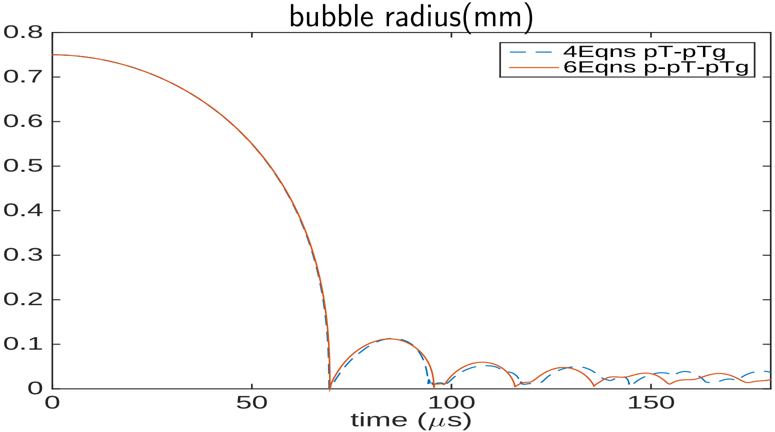


Figure 17. Bubble results with mass transfer, comparison between the results of vapor bubble (solid line) with gas-vapor bubble (dashed line). The computed radii are compared with the experimental data (dots). Computations are made with $N_I = 500$ cells, initial state inside the bubble: $T = 293$ K and $p = 2339$ Pa. The noncondensable gas is hydrogen with a mass fraction of 1%.

Present results: Vapor bubble case

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

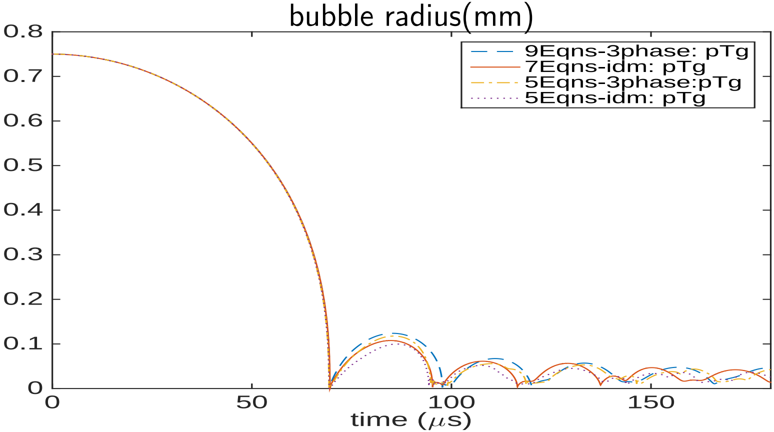
- Rebounds exist with decay of magnitude in time (agree with experiment qualitatively)



Present results: Gas-vapor bubble case

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

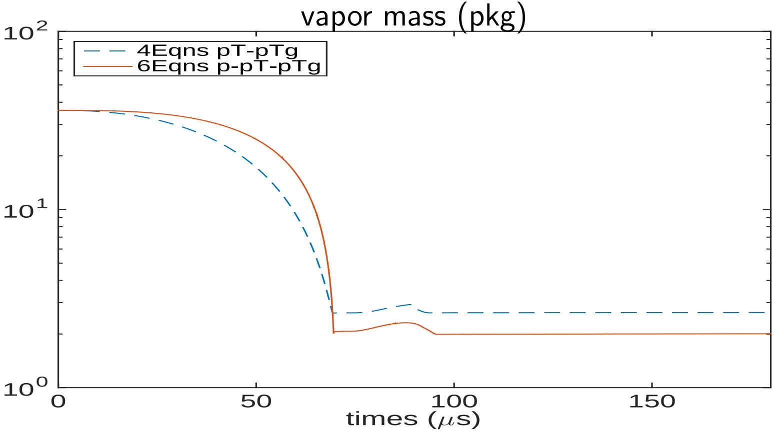
- Rebounds exist with decay of magnitude in time (agree with experiment qualitatively)
- Noncondensable O_2 with $\alpha_a = 10^{-2}$ included



Present result: Vapor bubble case

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

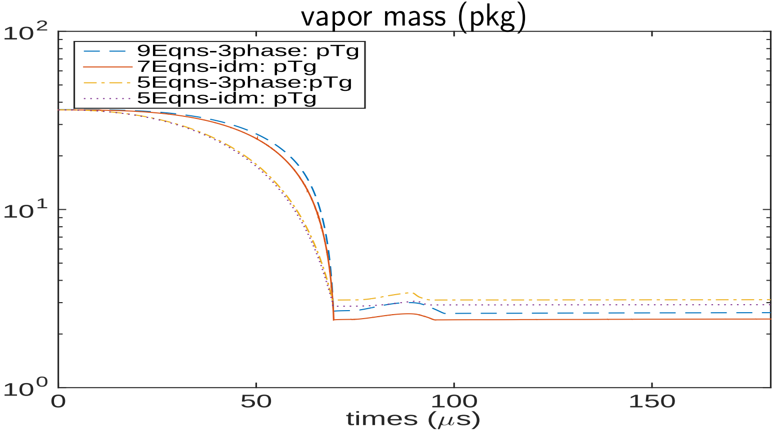
- Vapor mass decreases due to bubble collapse & increases due to rebound (agree with Akhatov's prediction qualitatively)



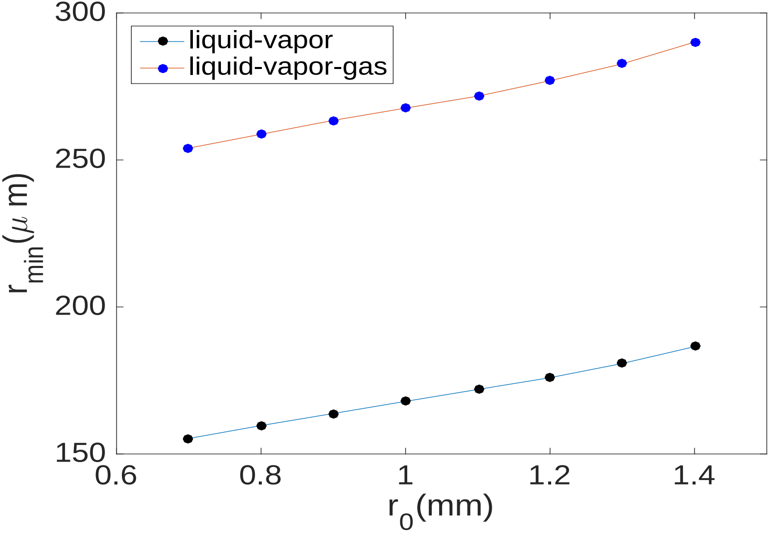
Present result: Gas-vapor bubble case

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

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

Reduced 4-equation model: Mass transfer

Assume mass transfer via thermo-chemical relaxation:

- Gibbs free energy based

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

- Mass fraction based

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

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

Downar-Zapolski *et al.* : Empicical fit

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

4-equation model: Without phase transition

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)

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

Mechanical-thermal equilibrium speed of sound satisfies

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

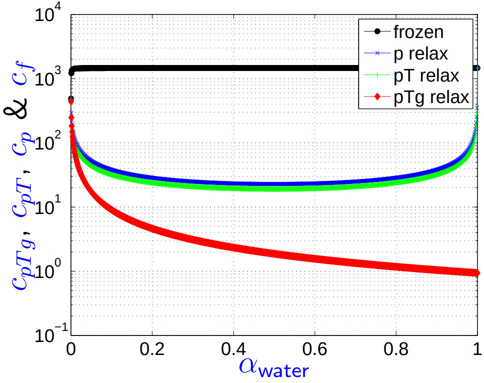
Equilibrium speed of sound

- Sound speeds follow subcharacteristic condition

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

- Limit of sound speed

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



4-equation model: Spherically-symmetric case

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

$$
\begin{aligned}
\partial_t \rho + \partial_V \left(r^2 \rho u\right) &= 0 \\
\partial_t \left(\rho u\right) + \partial_V \left(r^2 \rho u^2 + r^2 p\right) &= \frac{2}{r} p \\
\partial_t \left(\rho E\right) + \partial_V \left(r^2 \rho E u + r^2 p u\right) &= 0 \\
\partial_t \left(\rho Y_1\right) + \partial_V \left(r^2 \rho Y_1 u\right) &= \frac{1}{r^2} \dot{m}
\end{aligned}
$$

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

$$
\begin{aligned}
\partial_t \rho + \partial_r \left(\rho u\right) &= -\frac{2}{r} \rho u \\
\partial_t \left(\rho u\right) + \partial_r \left(\rho u^2 + p\right) &= -\frac{2}{r} \rho u^2 \\
\partial_t \left(\rho E\right) + \partial_r \left(\rho E u + p u\right) &= -\frac{2}{r} \left(\rho E + p\right) u \\
\partial_t \left(\rho Y_1\right) + \partial_r \left(\rho Y_1 u\right) &= -\frac{2}{r} \rho Y_1 u + \frac{1}{r^2} \dot{m}
\end{aligned}
$$

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 sources

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

   using suitable 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 $h_k = e_k + p v_k$

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

pTg equilibrium solution

From saturation condition for equilibrium p & T:

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

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

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

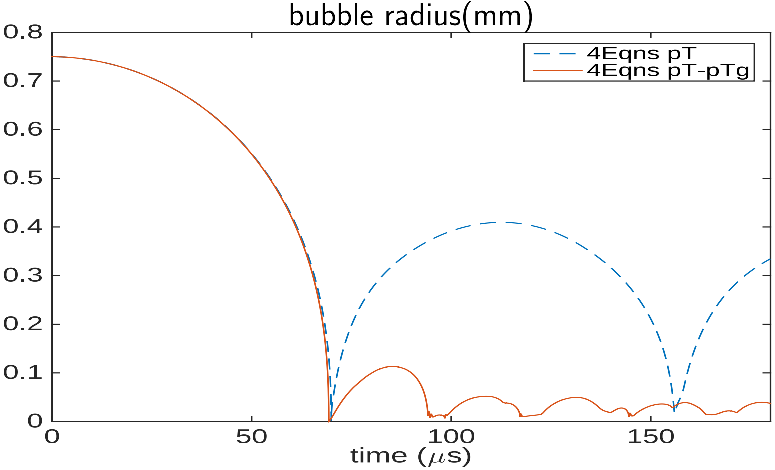
or

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

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

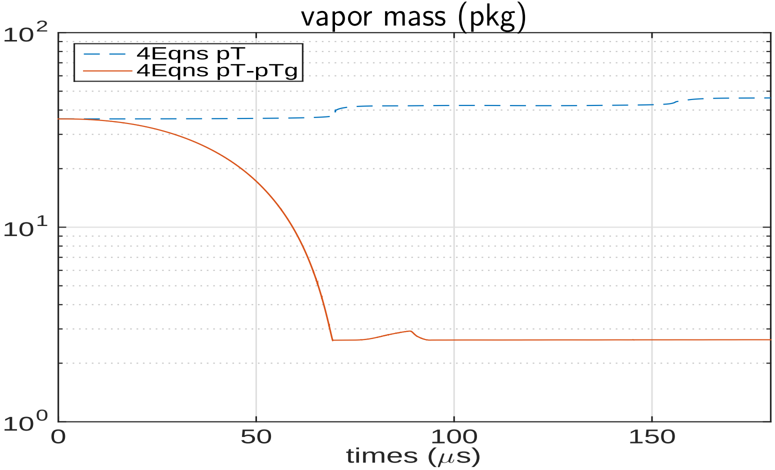
Benchmark laser bubble test: Bubble radius

Less rebounds without phase transition



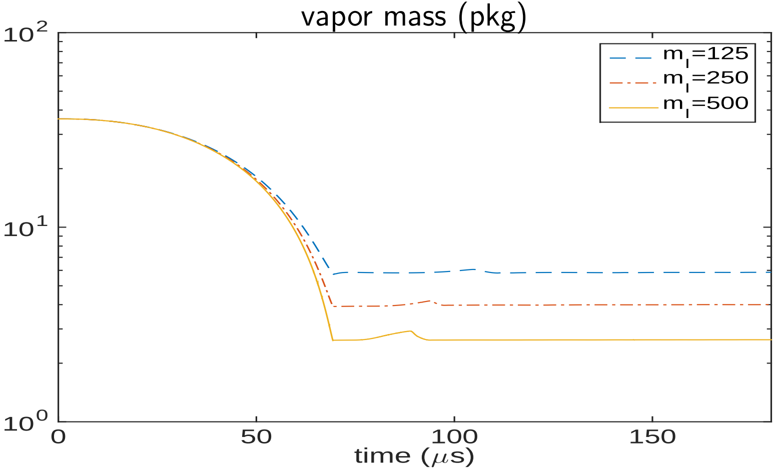
Benchmark laser bubble test: Vapor mass

Vapor mass increases without phase transition



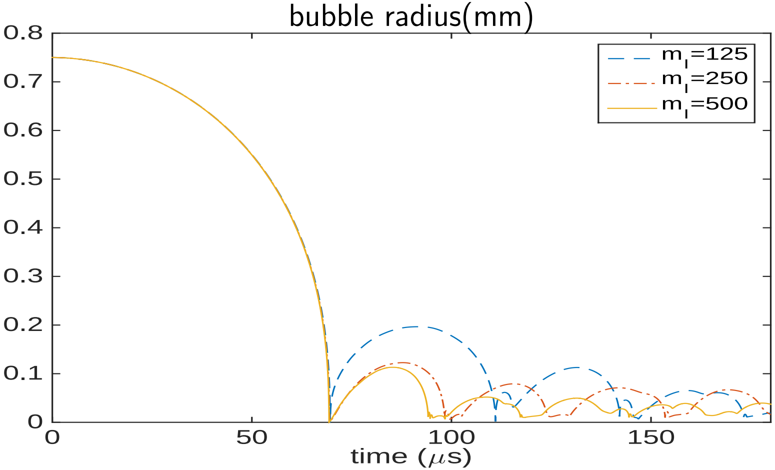
Vapor mass: Mesh refinement test

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

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

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

$$v = Y_v v_v(p,T) + Y_l v_l(p,T) + Y_a v_a(p,T)$$
$$e = Y_v e_v(p,T) + Y_l e_l(p,T) + Y_a e_a(p,T)$$

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:

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

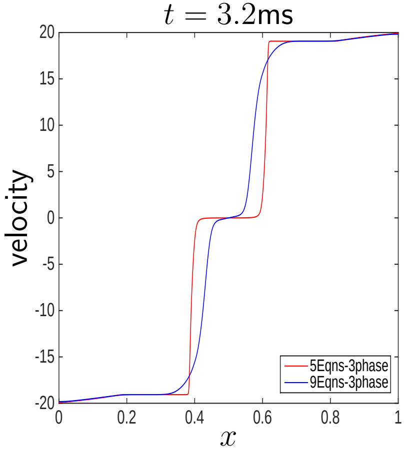
& equlibrium conditions 2, 3, & 4 above:

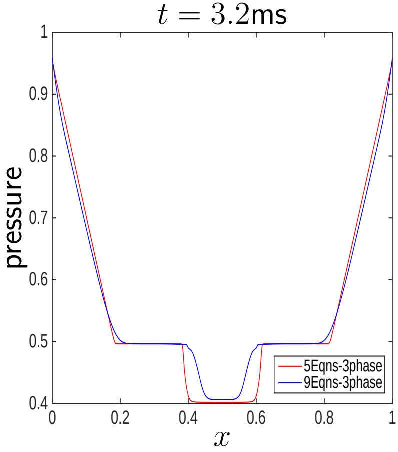
$$\mathcal{H}(p, T) := \frac{v - Y_a v_a(p, T) - (1 - Y_a)\, v_l(p, T)}{v_v(p, T) - v_l(p, T)} - \frac{h(p, T) - Y_a h_a(p, T) - (1 - Y_a)\, h_l(p, T)}{h_v(p, T) - h_l(p, T)} = 0$$

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

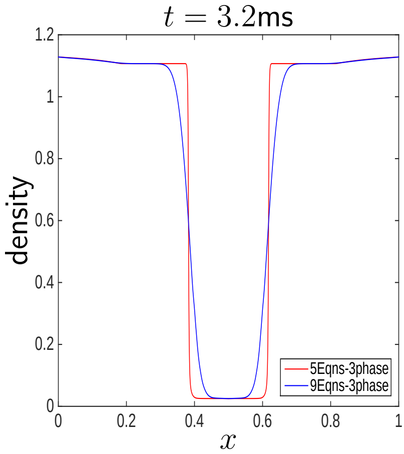
Cavitation test: Numerical validation

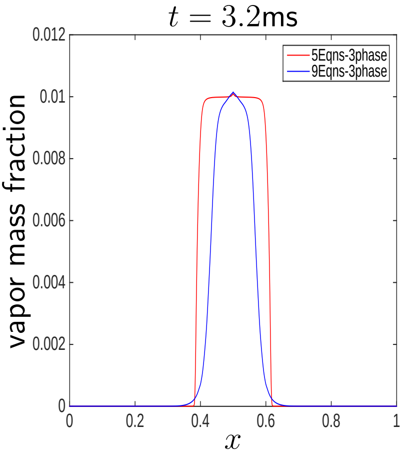
- Existence of 4 (2 rerefaction & 2 evaporation) wave structures





Cavitation test: Numerical validation





Cavitation test: Numerical validation

Taken from Pelanti, Shyue, FIFlåtten (HYP 2016)

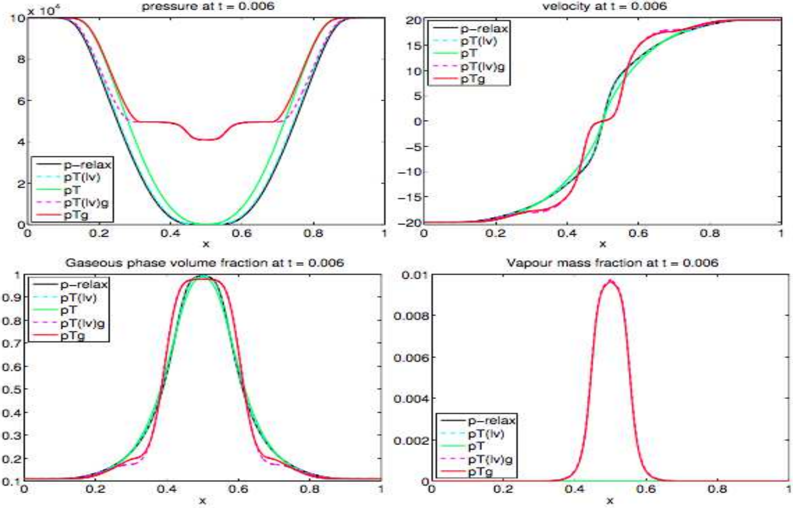


Fig. 1 Numerical results for the pressure, velocity, total gas volume fraction, and vapor mass fraction for the water cavitation tube test.

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

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

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

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

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

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

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 (see below)

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

$$
\begin{aligned}
C_{v,g} &= \frac{\rho_v}{\rho_g} C_{v,v} + \frac{\rho_a}{\rho_g} C_{v,a} \\
q_g &= \frac{\rho_v}{\rho_g} q_v + \frac{\rho_a}{\rho_g} q_a \\
p_{\infty,g} &= p_{\infty,v} + p_{\infty,a} \\
\gamma_g C_{v,g} &= \frac{\rho_v}{\rho_g} \gamma_v C_{v,v} + \frac{\rho_a}{\rho_g} \gamma_a C_{v,a}
\end{aligned}
$$

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

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

Underwater explosion: Flat solid wall

Taken from Pelanti, Shyue, FIFlåtten (HYP 2016)

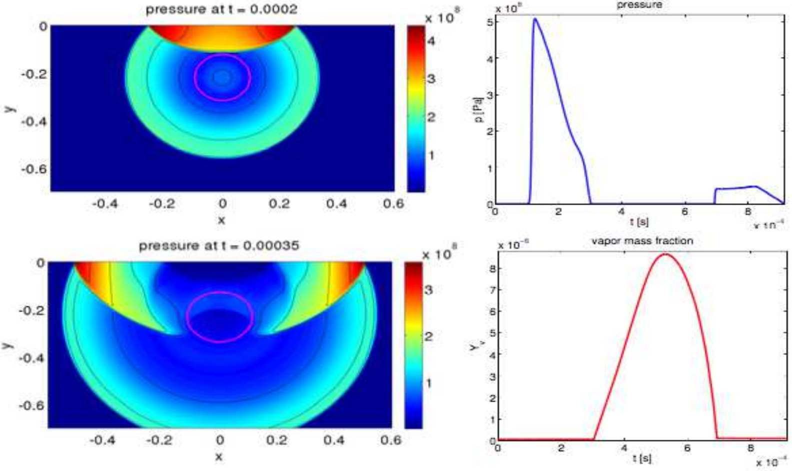


Fig. 2 Numerical results for the UNDEX experiment. Left: pressure field at time $t = 0.2$ ms (top) and $t = 0.35$ ms (bottom). The thick solid circle line indicates the water/bubble interface. Right: Pressure history (top) and vapor mass fraction history (bottom) at the point $(0,0)$ at the center of the wall.

Underwater explosion: Free surface