A mixture-energy-consistent numerical method for compressible two-phase flow with interfaces, cavitation, and evaporation waves

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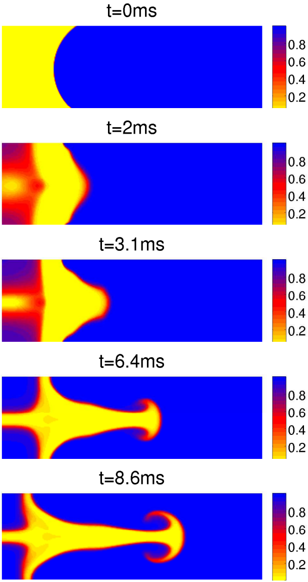
Outline

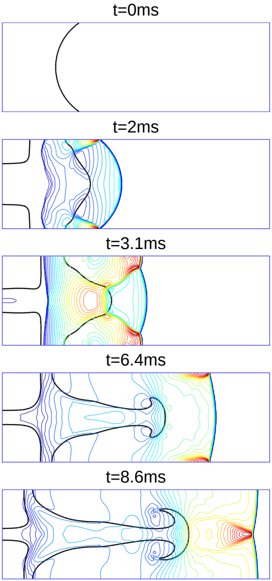
1. Model problems
2. Constitutive law
   - Saturation curve for metastable liquids
3. Compressible 2-phase flow model
   - Homogeneous relaxation model (HRM)
   - Reduced 5-equation model
4. Numerical scheme
   - Finite volume method
   - Stiff relaxation solver
5. Numerical examples

Cavitating Richtmyer-Meshkov problem

Gas volume fraction

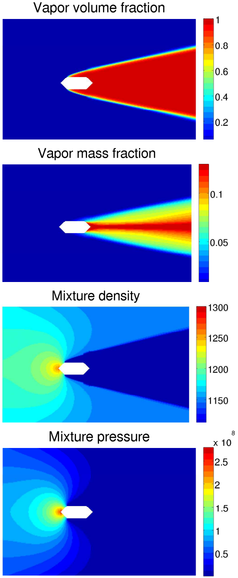


Mixture pressure

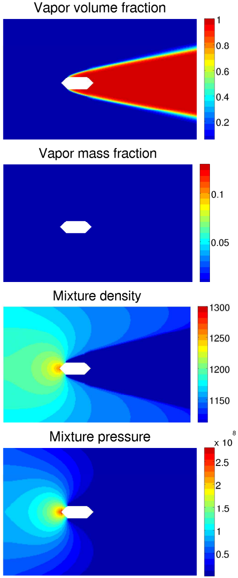


High-speed underwater projectile

With thermo-chemical relaxation

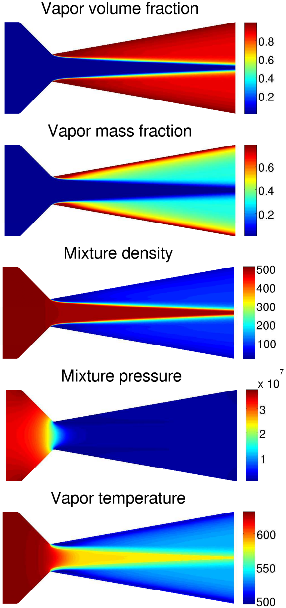


No thermo-chemical relaxation

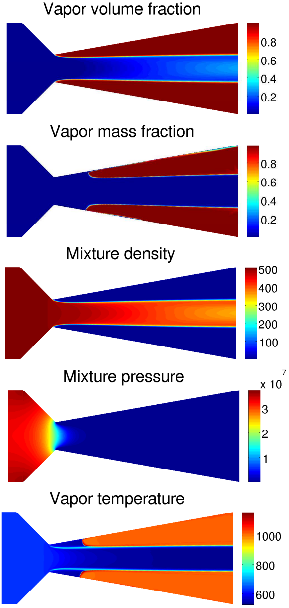


High-pressure fuel injector

With thermo-chemical relaxation



No thermo-chemical relaxation



Constitutive law

Stiffened gas equation of state (SG EOS) with

- Pressure

$$p_k(e_k, \rho_k) = (\gamma_k - 1)\rho_k \left(e_k - \eta_k\right) - \gamma_k p_{\infty k}$$

- Temperature

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

- Entropy

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

- Helmholtz free energy $a_k = e_k - T_k s_k$
- Gibbs free energy $g_k = a_k + p_k v_k, \quad v_k = 1/\rho_k$

Constitutive law: SG EOS parameters

Ref: Le Metayer *et al.* , Intl J. Therm. Sci. 2004

Fluid	Water	
Parameters/Phase	Liquid	Vapor
γ	2.35	1.43
p_∞ (Pa)	10^9	0
η (J/kg)	-11.6×10^3	2030×10^3
η' (J/(kg $\cdot$ K))	0	-23.4×10^3
C_v (J/(kg $\cdot$ K))	1816	1040

Fluid	Dodecane	
Parameters/Phase	Liquid	Vapor
γ	2.35	1.025
p_∞ (Pa)	4×10^8	0
η (J/kg)	-775.269×10^3	-237.547×10^3
η' (J/(kg $\cdot$ K))	0	-24.4×10^3
C_v (J/(kg $\cdot$ K))	1077.7	1956.45

Constitutive law: Saturation curves

Assume two phases in diffusive equilibrium with equal Gibbs free energies ($g_1 = g_2$), saturation curve for phase transitions is

$$\mathcal{G}(p,T) = \mathcal{A} + \frac{\mathcal{B}}{T} + \mathcal{C}\log T + \mathcal{D}\log(p+p_{\infty 1}) - \log(p+p_{\infty 2}) = 0$$

$$\mathcal{A} = \frac{C_{p1} - C_{p2} + \eta_2' - \eta_1'}{C_{p2} - C_{v2}}, \qquad \mathcal{B} = \frac{\eta_1 - \eta_2}{C_{p2} - C_{v2}}$$

$$\mathcal{C} = \frac{C_{p2} - C_{p1}}{C_{p2} - C_{v2}}, \qquad \mathcal{D} = \frac{C_{p1} - C_{v1}}{C_{p2} - C_{v2}}$$

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$$\mathcal{C} = \frac{C_{p2} - C_{p1}}{C_{p2} - C_{v2}}, \qquad \mathcal{D} = \frac{C_{p1} - C_{v1}}{C_{p2} - C_{v2}}$$

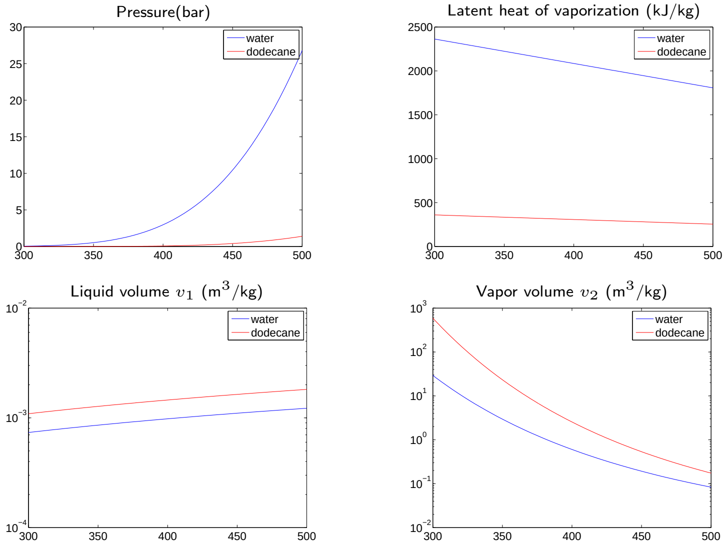
or, from $dg_1 = dg_2$, we get Clausius-Clapeyron equation

$$\frac{dp(T)}{dT} = \frac{L_h}{T(v_2 - v_1)}$$

$L_h = T(s_2 - s_1)$: latent heat of vaporization

Constitutive law: Saturation curves (Cont.)

Saturation curves for water & dodecane in $T \in [298, 500]$K



Homogeneous relaxation model (HRM)

Consider HRM for 2-phase flow of form

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

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

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

Homogeneous relaxation model (Cont.)

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

1. Volume transfer via pressure relaxation: $\mu\,(p_1 - p_2)$
   - μ 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: $\nu\,(g_2 - g_1)$
   - ν expresses rate towards diffusive equilibrium $g_1 \to g_2$, & is nonzero only at 2-phase mixture & metastable state $T_{\text{liquid}} > T_{\text{sat}}$

Homogeneous relaxation model (Cont.)

HRM model in compact form

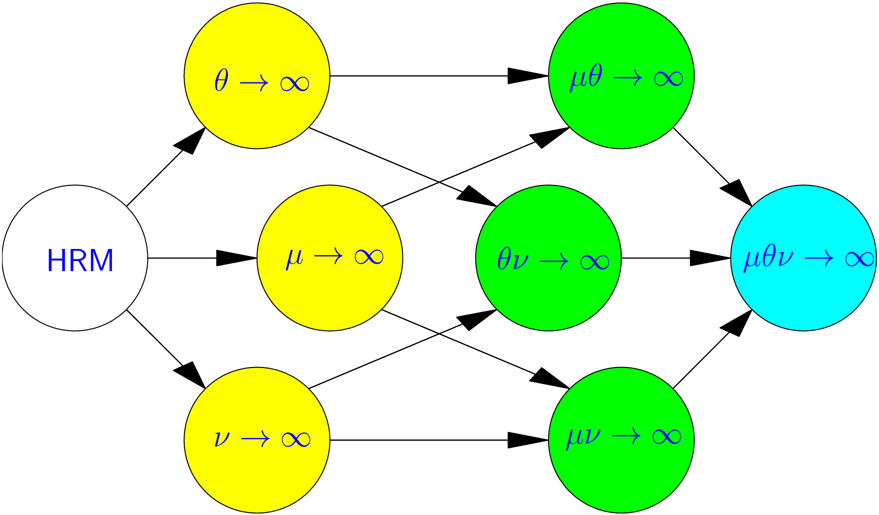
$$\partial_t q + \nabla \cdot f(q) + w\left(q, \nabla q\right) = \psi_\mu(q) + \psi_\theta(q) + \psi_\nu(q)$$

where

$$\begin{aligned}
q &= \left[\alpha_1,\ \alpha_1\rho_1,\ \alpha_2\rho_2,\ \rho\vec{u},\ \alpha_1 E_1,\ \alpha_2 E_2,\ \alpha_1\right]^T \\
f &= \left[\alpha_1\rho_1\vec{u},\ \alpha_2\rho_2\vec{u},\ \rho\vec{u}\otimes\vec{u} + (\alpha_1 p_1 + \alpha_2 p_2) I_N,\right. \\
&\qquad \left.\alpha_1\left(E_1 + p_1\right)\vec{u},\ \alpha_2\left(E_2 + p_2\right)\vec{u},\ 0\right]^T \\
w &= \left[0,\ 0,\ 0,\ \mathcal{B}\left(q, \nabla q\right),\ -\mathcal{B}\left(q, \nabla q\right),\ \vec{u}\cdot\nabla\alpha_1\right]^T \\
\psi_\mu &= \left[0,\ 0,\ 0,\ \mu p_I\left(p_2 - p_1\right),\ \mu p_I\left(p_1 - p_2\right),\ \mu\left(p_1 - p_2\right)\right]^T \\
\psi_\theta &= \left[0,\ 0,\ 0,\ \theta T_I\left(T_2 - T_1\right),\ \theta T_I\left(T_1 - T_2\right),\ 0\right]^T \\
\psi_\nu &= \left[\nu\left(g_2 - g_1\right),\ \nu\left(g_1 - g_2\right),\ 0,\ \nu g_I\left(g_2 - g_1\right),\right. \\
&\qquad \left.\nu g_I\left(g_1 - g_2\right),\ \nu v_I\left(g_1 - g_2\right)\right]^T
\end{aligned}$$

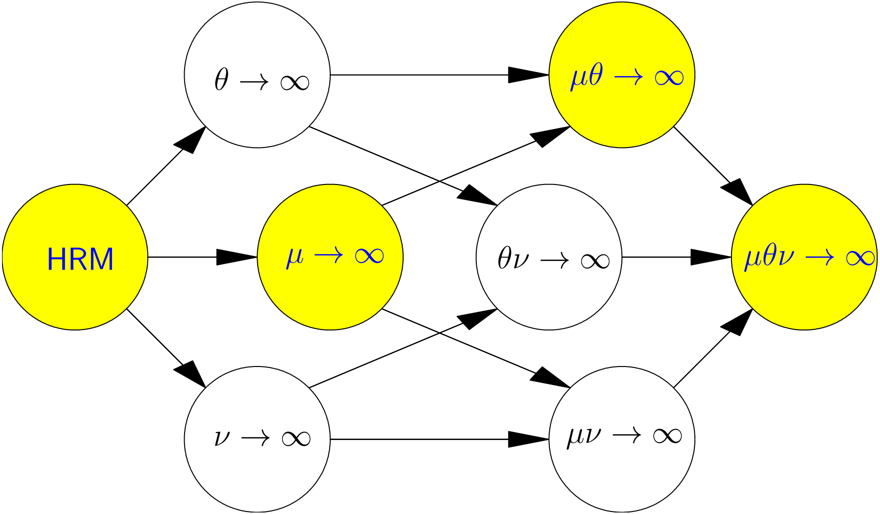
Homogeneous relaxation model (Cont.)

Flow hierarchy in HRM: H. Lund (SIAP 2012)



Homogeneous relaxation model (Cont.)

Consider HRM limits as $\mu \to \infty$, $\mu\theta \to \infty$, & $\mu\theta\nu \to \infty$



HRM: Reduced model as $\theta = \nu = 0$ & $\mu \to \infty$

Assume frozen thermal & chemical relaxation, HRM reduces to

$$
\begin{aligned}
&\partial_t \left(\alpha_1 \rho_1\right) + \nabla \cdot \left(\alpha_1 \rho_1 \vec{u}\right) = 0 \\
&\partial_t \left(\alpha_2 \rho_2\right) + \nabla \cdot \left(\alpha_2 \rho_2 \vec{u}\right) = 0 \\
&\partial_t (\rho \vec{u}) + \nabla \cdot \left(\rho \vec{u} \otimes \vec{u}\right) + \nabla \left(\alpha_1 p_1 + \alpha_2 p_2\right) = 0 \\
&\partial_t \left(\alpha_1 E_1\right) + \nabla \cdot \left(\alpha_1 E_1 \vec{u} + \alpha_1 p_1 \vec{u}\right) + \mathcal{B}\left(q, \nabla q\right) = \mu p_I \left(p_2 - p_1\right) \\
&\partial_t \left(\alpha_2 E_2\right) + \nabla \cdot \left(\alpha_2 E_2 \vec{u} + \alpha_2 p_2 \vec{u}\right) - \mathcal{B}\left(q, \nabla q\right) = \mu p_I \left(p_1 - p_2\right) \\
&\partial_t \alpha_1 + \vec{u} \cdot \nabla \alpha_1 = \mu \left(p_1 - p_2\right)
\end{aligned}
$$

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&\partial_t (\rho \vec{u}) + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) + \nabla \left(\alpha_1 p_1 + \alpha_2 p_2\right) = 0 \\
&\partial_t \left(\alpha_1 E_1\right) + \nabla \cdot \left(\alpha_1 E_1 \vec{u} + \alpha_1 p_1 \vec{u}\right) + \mathcal{B}\left(q, \nabla q\right) = \mu p_I \left(p_2 - p_1\right) \\
&\partial_t \left(\alpha_2 E_2\right) + \nabla \cdot \left(\alpha_2 E_2 \vec{u} + \alpha_2 p_2 \vec{u}\right) - \mathcal{B}\left(q, \nabla q\right) = \mu p_I \left(p_1 - p_2\right) \\
&\partial_t \alpha_1 + \vec{u} \cdot \nabla \alpha_1 = \mu \left(p_1 - p_2\right)
\end{aligned}
$$

Take formal asymptotic expansion ansatz

$$q = q^0 + \varepsilon q^1 + \cdots$$

Find equilibrium equation for q^0 as $\mu = 1/\varepsilon \to \infty$ ($\varepsilon \to 0^+$)

Reduced model: Asymptotic analysis as $\mu \to \infty$

Define material derivative

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \vec{u} \cdot \nabla$$

Rewrite energy & volume-fraction equations in form

$$\frac{dp_1}{dt} + \rho_1 c_1^2 \nabla \cdot \vec{u} = \frac{\rho_1 c_{I1}^2}{\alpha_1} \frac{1}{\varepsilon} (p_2 - p_1)$$
$$\frac{dp_2}{dt} + \rho_2 c_2^2 \nabla \cdot \vec{u} = \frac{\rho_2 c_{I2}^2}{\alpha_2} \frac{1}{\varepsilon} (p_1 - p_2)$$
$$\frac{d\alpha_1}{dt} = \frac{1}{\varepsilon} (p_1 - p_2)$$

Assume formal asymptotic expansion as

$$\alpha_1 = \alpha_1^0 + \varepsilon \alpha_1^1 + \cdots$$
$$p_k = p_k^0 + \varepsilon p_k^1 + \cdots \quad \text{for } k = 1, 2$$

Reduced model: Asymptotic analysis (Cont.)

We get

$$\frac{d}{dt}\left(p_1^0+\varepsilon p_1^1+\cdots\right)+\rho_1 c_1^2\nabla\cdot\vec{u}=$$
$$\frac{\rho_1 c_{I1}^2}{\alpha_1}\frac{1}{\varepsilon}\left[\left(p_2^0-p_1^0\right)+\varepsilon\left(p_2^1-p_1^1\right)+\cdots\right]$$
$$\frac{d}{dt}\left(p_2^0+\varepsilon p_2^1+\cdots\right)+\rho_2 c_2^2\nabla\cdot\vec{u}=$$
$$\frac{\rho_2 c_{I2}^2}{\alpha_2}\frac{1}{\varepsilon}\left[\left(p_1^0-p_2^0\right)+\varepsilon\left(p_1^1-p_2^1\right)+\cdots\right]$$
$$\frac{d}{dt}\left(\alpha_1^0+\varepsilon\alpha_1^1+\cdots\right)=\frac{1}{\varepsilon}\left[\left(p_1^0-p_2^0\right)+\varepsilon\left(p_1^1-p_2^1\right)+\cdots\right]$$

Reduced model: Asymptotic analysis (Cont.)

Collecting equal power of ε, we have

- $O(1/\varepsilon)$

$$p_1^0 = p_2^0 = p^0 \quad \Longrightarrow p_I^0 = p^0, \quad c_{Ik}^{0^2} = c_k^{0^2}$$

- $O(1)$

$$\frac{dp^0}{dt} + \rho_1^0 c_1^{0^2} \nabla \cdot \vec{u} = \frac{\rho_1^0 c_1^{0^2}}{\alpha_1^0} \left(p_2^1 - p_1^1\right)$$

$$\frac{dp^0}{dt} + \rho_2^0 c_2^{0^2} \nabla \cdot \vec{u} = \frac{\rho_2^0 c_2^{0^2}}{\alpha_2^0} \left(p_1^1 - p_2^1\right)$$

$$\frac{d\alpha_1^0}{dt} = p_1^1 - p_2^1$$

Reduced model: Asymptotic analysis (Cont.)

Subtracting former two equations, we find

$$\left(\rho_1^0 c_1^{0^2} - \rho_2^0 c_2^{0^2}\right) \nabla \cdot \vec{u} = \left(\frac{\rho_1^0 c_1^{0^2}}{\alpha_1^0} + \frac{\rho_2^0 c_2^{0^2}}{\alpha_2^0}\right) \left(p_2^1 - p_1^1\right)$$

i.e.,

$$\frac{d\alpha_1^0}{dt} = p_1^1 - p_2^1 = \left(\frac{\rho_2^0 c_2^{0^2} - \rho_1^0 c_1^{0^2}}{\rho_1^0 c_1^{0^2}/\alpha_1^0 + \rho_2^0 c_2^{0^2}/\alpha_2^0}\right) \nabla \cdot \vec{u}$$

Reduced model as $\theta = \nu = 0$ & $\mu \to \infty$ (Cont.)

Thus, as $\theta = 0$, $\nu = 0$ & $\mu \to \infty$ leading order approximation of RHM model becomes so-called reduced 5-equation model (*e.g.*, Kapila *et al.* 2001, Murrone *et al.* 2005)

$$
\begin{aligned}
&\partial_t (\alpha_1 \rho_1) + \nabla \cdot (\alpha_1 \rho_1 \vec{u}) = 0 \\
&\partial_t (\alpha_2 \rho_2) + \nabla \cdot (\alpha_2 \rho_2 \vec{u}) = 0 \\
&\partial_t (\rho \vec{u}) + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) + \nabla p = 0 \\
&\partial_t E + \nabla \cdot (E \vec{u} + p \vec{u}) = 0 \\
&\partial_t \alpha_1 + \vec{u} \cdot \nabla \alpha_1 = \left(\frac{\rho_2 c_2^2 - \rho_1 c_1^2}{\rho_1 c_1^2 / \alpha_1 + \rho_2 c_2^2 / \alpha_2} \right) \nabla \cdot \vec{u}
\end{aligned}
$$

Mixture pressure $p = p(\rho e, \rho_1, \rho_2, \alpha_1)$ determined from algebraic equation (linear one with SG EOS)

$$
\rho e = \alpha_1 \rho_1 e_1(p, \rho_1) + \alpha_2 \rho_2 e_2(p, \rho_2)
$$

p relaxation: Subcharacteristic condition

Mechanical equilibrium sound speed $c_p \leq c_f$ (frozen speed)

$$\frac{1}{\rho c_p^2} = \sum_{k=1}^{2} \frac{\alpha_k}{\rho_k c_k^2} \quad \& \quad \rho c_f^2 = \sum_{k=1}^{2} \alpha_k \rho_k c_k^2$$

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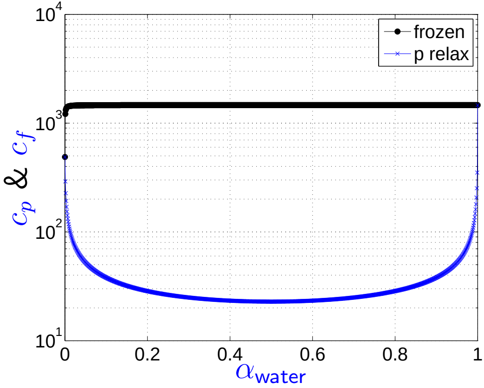
$$\frac{1}{\rho c_p^2} = \sum_{k=1}^{2} \frac{\alpha_k}{\rho_k c_k^2} \quad \& \quad \rho c_f^2 = \sum_{k=1}^{2} \alpha_k \rho_k c_k^2$$



Non-monotonic c_p leads to stiffness in equations & difficulties in numerical solver, *e.g.*, positivity-preserving in volume fraction

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

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

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

Mechanical-thermal equilibrium speed of sound satisfies

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

HRM: Limit model as $z \to \infty$, $z = \mu$, θ, & ν

As all relaxation parameters go to infinity; $z \to \infty$, $z = \mu$, θ, & ν, limit system of HRM is homogeneous equilibrium model (HEM) that follows standard mixture Euler equation

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

This gives local resolution at interface only

Speed of sound satisfies

$$
\frac{1}{\rho c_{pTg}^2} = \frac{1}{\rho c_p^2} + T \left[\frac{\alpha_1 \rho_1}{C_{p1}} \left(\frac{d s_1}{d p} \right)^2 + \frac{\alpha_2 \rho_2}{C_{p2}} \left(\frac{d s_2}{d p} \right)^2 \right]
$$

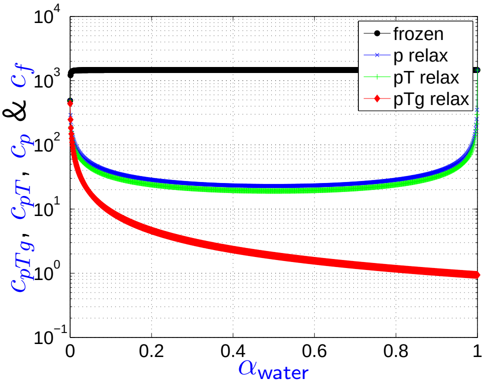
Equilibrium speed of sound: Comparison

- Sound speeds follow subcharacteristic condition

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

- Limit of sound speed

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



5-equation model: liquid-vapor phase transition

Modelling phase transition in metastable liquids Saurel *et al.* (JFM 2008) proposed

$$\partial_t(\alpha_1\rho_1) + \nabla\cdot(\alpha_1\rho_1\vec{u}) = \dot{m}$$

$$\partial_t(\alpha_2\rho_2) + \nabla\cdot(\alpha_2\rho_2\vec{u}) = -\dot{m}$$

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

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

$$\partial_t\alpha_1 + \nabla\cdot(\alpha_1\vec{u}) = \alpha_1\frac{\bar{K}_s}{K_s^1}\nabla\cdot\vec{u} + \frac{1}{q_I}Q + \frac{1}{\rho_I}\dot{m}$$

$$\bar{K}_s = \left(\frac{\alpha_1}{K_s^1} + \frac{\alpha_2}{K_s^2}\right)^{-1}, \quad K_s^\iota = \rho_\iota c_\iota^2$$

$$q_I = \left(\frac{K_s^1}{\alpha_1} + \frac{K_s^2}{\alpha_2}\right) \Big/ \left(\frac{\Gamma_1}{\alpha_1} + \frac{\Gamma_2}{\alpha_2}\right), \quad Q = \theta(T_2 - T_1)$$

$$\rho_I = \left(\frac{K_s^1}{\alpha_1} + \frac{K_s^2}{\alpha_2}\right) \Big/ \left(\frac{c_1^2}{\alpha_1} + \frac{c_2^2}{\alpha_2}\right), \quad \dot{m} = \nu(g_2 - g_1)$$

5-equation model (Cont.)

- Mathematically, 5-equation model approaches to same relaxation limits as HRM, but is difficult to solve numerically to ensure solution to be feasible

5-equation model (Cont.)

- Mathematically, 5-equation model approaches to same relaxation limits as HRM, but is difficult to solve numerically to ensure solution to be feasible
- Saurel *et al.* (JCP 2009) & Zein *et al.* (JCP 2010) proposed HRM based on phasic internal energy as alternative way to solve 5-equation model

HRM: Phasic-internal-energy-based

HRM based on phasic internal energy formulation of Saurel *et al.* (JCP 2009) & Zein *et al.* (JCP 2010) is

$$\partial_t (\alpha_1 \rho_1) + \nabla \cdot (\alpha_1 \rho_1 \vec{u}) = \nu (g_2 - g_1)$$
$$\partial_t (\alpha_2 \rho_2) + \nabla \cdot (\alpha_2 \rho_2 \vec{u}) = \nu (g_1 - g_2)$$
$$\partial_t (\rho \vec{u}) + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) + \nabla (\alpha_1 p_1 + \alpha_2 p_2) = 0$$
$$\partial_t (\alpha_1 \rho_1 e_1) + \nabla \cdot (\alpha_1 \rho_1 e_1 \vec{u}) + \alpha_1 p_1 \nabla \cdot \vec{u} = \mu p_I (p_2 - p_1) + \theta T_I (T_2 - T_1) + \nu g_I (g_2 - g_1)$$
$$\partial_t (\alpha_2 \rho_2 e_2) + \nabla \cdot (\alpha_2 \rho_2 e_2 \vec{u}) + \alpha_2 p_2 \nabla \cdot \vec{u} = \mu p_I (p_1 - p_2) + \theta T_I (T_1 - T_2) + \nu g_I (g_1 - g_2)$$
$$\partial_t \alpha_1 + \vec{u} \cdot \nabla \alpha_1 = \mu (p_1 - p_2) + \nu v_I (g_2 - g_1)$$

To ensure conservation of mixture total energy include

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

HRM: Phasic-total-energy-based

Numerically more advantageous to use HRM based on phasic-total-energy formulation than phasic-internal-energy one; for ease of devise mixture-energy-consistent discretization Pelanti & Shyue (JCP 2014), *i.e.*,

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

Relaxation scheme

To find approximate solution of HRM, in each time step, fractional-step method is employed:

1. Non-stiff hyperbolic step
   Solve hyperbolic system without relaxation sources
   $$\partial_t q + \nabla \cdot f(q) + w\left(q, \nabla q\right) = 0$$
   using state-of-the-art solver over time interval Δt

2. Stiff relaxation step
   Solve system of ordinary differential equations
   $$\partial_t q = \psi_\mu(q) + \psi_\theta(q) + \psi_\nu(q)$$
   in various flow regimes under relaxation limits

Relaxation scheme (Cont.)

Definition (mixture-energy consistent)

(i) Mixture total energy conservation consistency

$$E^0 = E^{0,\mathrm{C}}$$

where $E^0 = (\alpha_1 E_1)^0 + (\alpha_2 E_2)^0$

(ii) Relaxed pressure consistency

$$e^{0,\mathrm{C}} = \alpha_1^* e_1 \left(p^*, \frac{(\alpha_1 \rho_1)^0}{\alpha_1^*} \right) + \alpha_2^* e_2 \left(p^*, \frac{(\alpha_2 \rho_2)^0}{\alpha_2^*} \right),$$

where $e^{0,\mathrm{C}} = E^{0,\mathrm{C}} - \frac{(\rho \vec{u})^0 \cdot (\rho \vec{u})^0}{2\rho^0}$

Method proposed here with phasic-total-energy formulation is mixture-energy consistent

Non-stiff hyperbolic step: Mapped grid method

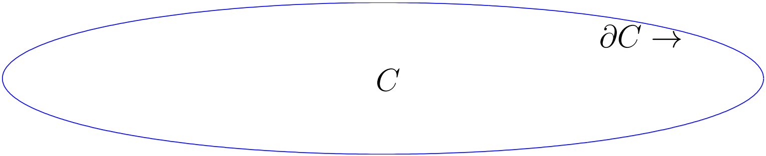
Consider solution of model system

$$\partial_t q + \nabla \cdot f(q) + w\left(q, \nabla q\right) = 0$$

in 2D general non-rectangular geometry
Model in integral form over any control volume C is

$$\frac{d}{dt}\int_C q \; d\Omega = -\int_{\partial C} f(q) \cdot \vec{n} \; ds - \int_C w\left(q, \nabla q\right) \; d\Omega$$

where $\vec{n}$ is outward-pointing normal vector at boundary ∂C



Hyperbolic step: Mapped grid (Cont.)

Then finite volume method on control volume C reads

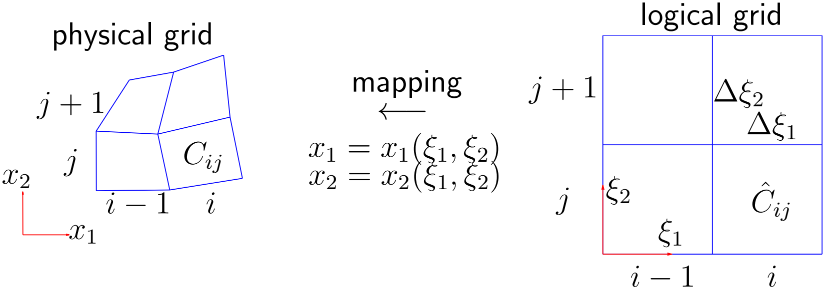
$$Q^{n+1} = Q^n - \frac{\Delta t}{\mathcal{M}(C)} \sum_{j=1}^{N_s} h_j \breve{F}_j - \Delta t W^* \mathcal{M}(C)$$

- $Q^n := \int_C q(z, t_n)\, dz / \mathcal{M}(C)$
- $\mathcal{M}(C)$ measure (area in 2D or volume in 3D) of C
- N_s number of sides
- h_j length of j-th side (in 2D) or area of cell edge (in 3D) measured in physical space
- $\breve{F}_j$ numerical approximation to normal flux in average across j-th side of grid cell
- W^* cell average of w in cell C

Hyperbolic step: Mapped grid (Cont.)

Assume mapped (*i.e.*, logically rectangular) grid in 2D, we get

$$
\begin{aligned}
Q_{ij}^{n+1} = Q_{ij}^{n} - \frac{\Delta t}{\kappa_{ij}\Delta\xi_1}\left(F^1_{i+\frac{1}{2},j} - F^1_{i-\frac{1}{2},j}\right) - \\
\frac{\Delta t}{\kappa_{ij}\Delta\xi_2}\left(F^2_{i,j+\frac{1}{2}} - F^2_{i,j-\frac{1}{2}}\right) - \Delta t W^*_{ij}\Delta\xi_1\Delta\xi_2
\end{aligned}
$$

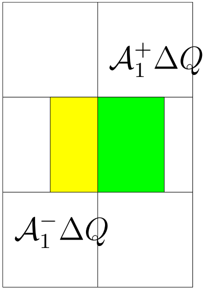


$\kappa_{ij} = \mathcal{M}(C_{ij})/\Delta\xi_1\Delta\xi_2$

Mapped grid method: Wave propagation (Cont.)

Godunov-type in wave propagation form is

$$Q_{ij}^{n+1} = Q_{ij}^{n} - \frac{\Delta t}{\kappa_{ij}\Delta\xi_1}\left(\mathcal{A}_1^+\Delta Q_{i-\frac{1}{2},j} + \mathcal{A}_1^-\Delta Q_{i+\frac{1}{2},j}\right) - \frac{\Delta t}{\kappa_{ij}\Delta\xi_2}\left(\mathcal{A}_2^+\Delta Q_{i,j-\frac{1}{2}} + \mathcal{A}_2^-\Delta Q_{i,j+\frac{1}{2}}\right)$$



- fluctuations $\mathcal{A}_1^+\Delta Q_{i-\frac{1}{2},j}$, $\mathcal{A}_1^-\Delta Q_{i+\frac{1}{2},j}$, $\mathcal{A}_2^+\Delta Q_{i,j-\frac{1}{2}}$, & $\mathcal{A}_2^-\Delta Q_{i,j+\frac{1}{2}}$: Solve one-dimensional Riemann problems in direction normal to cell edges
- W_{ij}^* may be included in fluctuations

Mapped grid mtehod: Wave propagation (Cont.)

Speeds & limited of waves are used to calculate second order correction:

$$Q_{ij}^{n+1} := Q_{ij}^{n+1} - \frac{\Delta t}{\kappa_{ij}\Delta\xi_1}\left(\widetilde{\mathcal{F}}^1_{i+\frac{1}{2},j} - \widetilde{\mathcal{F}}^1_{i-\frac{1}{2},j}\right) - \frac{\Delta t}{\kappa_{ij}\Delta\xi_2}\left(\widetilde{\mathcal{F}}^2_{i,j+\frac{1}{2}} - \widetilde{\mathcal{F}}^2_{i,j-\frac{1}{2}}\right)$$

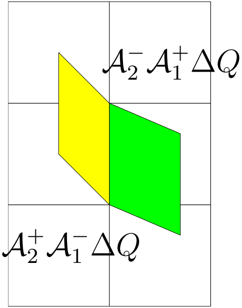
For example, at cell edge $(i-\frac{1}{2},j)$ correction flux takes

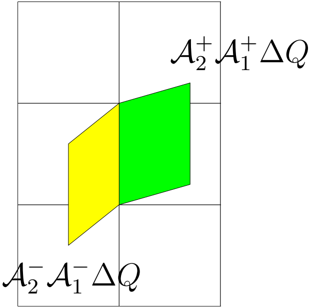
$$\widetilde{\mathcal{F}}^1_{i-\frac{1}{2},j} = \frac{1}{2}\sum_{k=1}^{N_w}\left|\lambda^{1,k}_{i-\frac{1}{2},j}\right|\left(1 - \frac{\Delta t}{\kappa_{i-\frac{1}{2},j}\Delta\xi_1}\left|\lambda^{1,k}_{i-\frac{1}{2},j}\right|\right)\widetilde{\mathcal{W}}^{1,k}_{i-\frac{1}{2},j}$$

$\kappa_{i-\frac{1}{2},j} = (\kappa_{i-1,j} + \kappa_{ij})/2$, $\widetilde{\mathcal{W}}^{1,k}_{i-\frac{1}{2},j}$ is limited waves to avoid oscillations near discontinuities

Mapped grid method: Wave propagation (Cont.)

Transverse wave propagation is included to ensure second order accuracy & also improve stability





Mapped grid method: Wave propagation (Cont.)

Method can be shown to be quasi conservative & stable under a variant of CFL (Courant-Friedrichs-Lewy) condition

$$\Delta t \max_{i,j,k} \left(\frac{\left|\lambda^{1,k}_{i-\frac{1}{2},j}\right|}{\kappa_{i_p,j}\Delta\xi_1}, \frac{\left|\lambda^{2,k}_{i,j-\frac{1}{2}}\right|}{\kappa_{i,j_p}\Delta\xi_2} \right) \le 1,$$

$$i_p = i \quad \text{if } \lambda^{1,k}_{i-\frac{1}{2},j} > 0 \quad \& \quad i-1 \quad \text{if } \lambda^{1,k}_{i-\frac{1}{2},j} < 0$$

Mapped grid method: Wave propagation (Cont.)

Semi-discrete wave propagation method takes form

$$\partial_t Q(t) = \mathcal{L}(Q(t))$$

where in 2D

$$\mathcal{L}(Q_{ij}(t) = -\frac{1}{\kappa_{ij}\Delta\xi_1}\left(\mathcal{A}_1^+\Delta Q_{i-\frac{1}{2},j} + \mathcal{A}_1^-\Delta Q_{i+\frac{1}{2},j} + \mathcal{A}_1\Delta Q_{ij}\right) - \frac{1}{\kappa_{ij}\Delta\xi_2}\left(\mathcal{A}_2^+\Delta Q_{i,j-\frac{1}{2}} + \mathcal{A}_2^-\Delta Q_{i,j+\frac{1}{2}} + \mathcal{A}_2\Delta Q_{ij}\right)$$

ODEs are integrated in time using strong stability-preserving (SSP) multistage Runge-Kutta, *e.g.*, 3-stage 3rd-order

$$Q^* = Q^n + \Delta t\mathcal{L}\left(Q^n\right)$$

$$Q^{**} = \frac{3}{4}Q^n + \frac{1}{4}Q^* + \frac{1}{4}\Delta t\mathcal{L}\left(Q^*\right)$$

$$Q^{n+1} = \frac{1}{3}Q^n + \frac{2}{3}Q^* + \frac{2}{3}\Delta t\mathcal{L}\left(Q^{**}\right)$$

Relaxation scheme: Stiff solvers

1. Algebraic-based approach
   - Saurel *et al.* (JFM 2008), Zein *et al.* (JCP 2010), LeMartelot *et al.* (JFM 2013), Pelanti-Shyue (JCP 2014)
   - Impose equilibrium conditions directly, without making explicit of interface states p_I, g_I,...
2. Differential-based approach
   - Saurel *et al.* (JFM 2008), Zein *et al.* (JCP 2010)
   - Impose differential of equilibrium conditions, require explicit of interface states p_I, g_I,...
3. Optimization-based approach (for mass transfer only)
   - Helluy & Seguin (ESAIM: M2AN 2006), Faccanoni *et al.* (ESAIM: M2AN 2012)

p relaxation: Algebraic approach

Assume frozen thermal & thermo-chemical relaxation, *i.e.*, $\theta = 0$ & $\nu = 0$, look for solution of ODEs in limit $\mu \to \infty$

$$
\begin{aligned}
\partial_t \left(\alpha_1 \rho_1\right) &= 0 \\
\partial_t \left(\alpha_2 \rho_2\right) &= 0 \\
\partial_t \left(\rho \vec{u}\right) &= 0 \\
\partial_t \left(\alpha_1 E_1\right) &= \mu p_I \left(p_2 - p_1\right) \\
\partial_t \left(\alpha_2 E_2\right) &= \mu p_I \left(p_1 - p_2\right) \\
\partial_t \alpha_1 &= \mu \left(p_1 - p_2\right)
\end{aligned}
$$

under mechanical equilibrium with equal pressure

$$p_1 = p_2 = p$$

p relaxation (Cont.)

We find easily

$$\alpha_k \rho_k = \alpha_{k0} \rho_{k0}, \quad \rho = \rho_0, \quad \vec{u} = \vec{u}_0, \quad E = E_0, \quad e = e_0$$
$$\partial_t \left(\alpha E\right)_k = \partial_t \left(\alpha \rho e\right)_k = -p_I \partial_t \alpha_k, \qquad k = 1, 2$$

p relaxation (Cont.)

We find easily

$$\alpha_k\rho_k = \alpha_{k0}\rho_{k0}, \quad \rho = \rho_0, \quad \vec{u} = \vec{u}_0, \quad E = E_0, \quad e = e_0$$
$$\partial_t\left(\alpha E\right)_k = \partial_t\left(\alpha\rho e\right)_k = -p_I\partial_t\alpha_k, \qquad k = 1, 2$$

Integrating latter equation & using $\alpha_k\rho_k = \alpha_{k0}\rho_{k0}$ leads to

$$e_k\left(p_k, \rho_k\right) - e_{k0} + \bar{p}_I\left(\frac{1}{\rho_k} - \frac{1}{\rho_{k0}}\right) = 0$$

This gives condition for ρ_k in p, $k = 1, 2$, if assume *e.g.*, $\bar{p}_I = (p_I^0 + p)/2$, & impose mechanical equilibrium in EOS

p relaxation (Cont.)

Combining that with saturation condition for volume fraction

$$\frac{\alpha_1 \rho_1}{\rho_1(p)} + \frac{\alpha_2 \rho_2}{\rho_2(p)} = 1$$

leads to algebraic equation (quadratic one with SG EOS) for relaxed pressure p

With that, ρ_k, α_k can be determined & state vector q is updated from current time to next

pT relaxation

Now assume frozen thermo-chemical relaxation $\nu = 0$, look for solution of ODEs in limits μ & $\theta \to \infty$

$$
\begin{aligned}
\partial_t \left(\alpha_1 \rho_1\right) &= 0 \\
\partial_t \left(\alpha_2 \rho_2\right) &= 0 \\
\partial_t \left(\rho \vec{u}\right) &= 0 \\
\partial_t \left(\alpha_1 E_1\right) &= \mu p_I \left(p_2 - p_1\right) + \theta T_I \left(T_2 - T_1\right) \\
\partial_t \left(\alpha_2 E_2\right) &= \mu p_I \left(p_1 - p_2\right) + \theta T_I \left(T_1 - T_2\right) \\
\partial_t \alpha_1 &= \mu \left(p_1 - p_2\right)
\end{aligned}
$$

under mechanical-thermal equilibrium conditons

$$
\begin{aligned}
p_1 = p_2 = p \\
T_1 = T_2 = T
\end{aligned}
$$

pT relaxation (Cont.)

As before, for $k = 1, 2$, states remain in equilibrium are

$$\alpha_k \rho_k = \alpha_{k0} \rho_{k0}, \quad \rho = \rho_0, \quad \vec{u} = \vec{u}_0, \quad E = E_0, \quad e = e_0$$

Lead to equilibrium in mass fraction $Y_k = \alpha_k \rho_k / \rho = Y_{k0}$

pT relaxation (Cont.)

As before, for $k = 1, 2$, states remain in equilibrium are

$$\alpha_k \rho_k = \alpha_{k0} \rho_{k0}, \quad \rho = \rho_0, \quad \vec{u} = \vec{u}_0, \quad E = E_0, \quad e = e_0$$

Lead to equilibrium in mass fraction $Y_k = \alpha_k \rho_k / \rho = Y_{k0}$

Impose mechanical-thermal equilibrium to

1. Saturation condition

$$\frac{\alpha_1 \rho_1}{\rho_1(p, T)} + \frac{\alpha_2 \rho_2}{\rho_2(p, T)} = 1$$

or

$$\frac{Y1}{\rho_1(p, T)} + \frac{Y_2}{\rho_2(p, T)} = \frac{1}{\rho}$$

pT relaxation (Cont.)

Impose mechanical-thermal equilibrium to

1. Saturation condition

$$\frac{Y1}{\rho_1(p,T)} + \frac{Y_2}{\rho_2(p,T)} = \frac{1}{\rho}$$

2. Equilibrium of internal energy

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

Give 2 algebraic equations for 2 unknowns p & T

pT relaxation (Cont.)

Impose mechanical-thermal equilibrium to

1. Saturation condition

$$\frac{Y1}{\rho_1(p,T)} + \frac{Y_2}{\rho_2(p,T)} = \frac{1}{\rho}$$

2. Equilibrium of internal energy

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

Give 2 algebraic equations for 2 unknowns p & T

For SG EOS, it reduces to single quadratic equation for p & explicit computation of T:

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

pTg relaxation

Look for solution of ODEs in limits $\mu,\ \theta,\ \&\ \nu \to \infty$

$$\begin{aligned}
\partial_t \left(\alpha_1 \rho_1\right) &= \nu \left(g_2 - g_1\right) \\
\partial_t \left(\alpha_2 \rho_2\right) &= \nu \left(g_1 - g_2\right) \\
\partial_t \left(\rho \vec{u}\right) &= 0 \\
\partial_t \left(\alpha_1 E_1\right) &= \mu p_I \left(p_2 - p_1\right) + \theta T_I \left(T_2 - T_1\right) + \nu \left(g_2 - g_1\right) \\
\partial_t \left(\alpha_2 E_2\right) &= \mu p_I \left(p_1 - p_2\right) + \theta T_I \left(T_1 - T_2\right) + \nu \left(g_1 - g_2\right) \\
\partial_t \alpha_1 &= \mu \left(p_1 - p_2\right) + \nu v_I \left(g_2 - g_1\right)
\end{aligned}$$

under mechanical-thermal-chemical equilibrium conditons

$$\begin{aligned}
p_1 &= p_2 = p \\
T_1 &= T_2 = T \\
g_1 &= g_2
\end{aligned}$$

pTg relaxation (Cont.)

In this case, states remain in equilibrium are

$$\rho = \rho_0, \quad \rho\vec{u} = \rho_0\vec{u}_0, \quad E = E_0, \quad e = e_0$$

but $\alpha_k\rho_k \neq \alpha_{k0}\rho_{k0}$ & $Y_k \neq Y_{k0}$, $k = 1, 2$

Impose mechanical-thermal-chemical equilibrium to

1. Saturation condition for temperature

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

2. Saturation condition for volume fraction

$$\frac{Y_1}{\rho_1(p, T)} + \frac{Y_2}{\rho_2(p, T)} = \frac{1}{\rho}$$

3. Equilibrium of internal energy

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

pTg relaxation (Cont.)

From saturation condition for temperature

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

we get T in terms of p, while from

$$\frac{Y_1}{\rho_1(p,T)} + \frac{Y_2}{\rho_2(p,T)} = \frac{1}{\rho}$$

&

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

we obtain algebraic equation for p

$$Y_1 = \frac{1/\rho_2(p) - 1/\rho}{1/\rho_2(p) - 1/\rho_1(p)} = \frac{e - e_2(p)}{e_1(p) - e_2(p)}$$

which is solved by iterative method

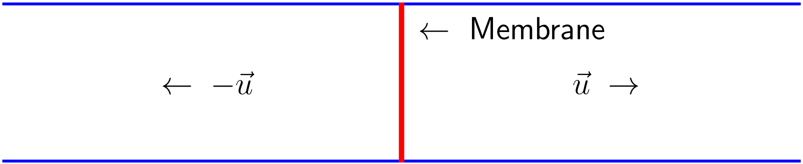
pTg relaxation (Cont.)

With that, T can be solved from either condition for volume fraction or equilibrium of internal energy (quadratic equation for SG EOS), yielding ρ_k & α_k update

Expansion wave problem: Cavitation test

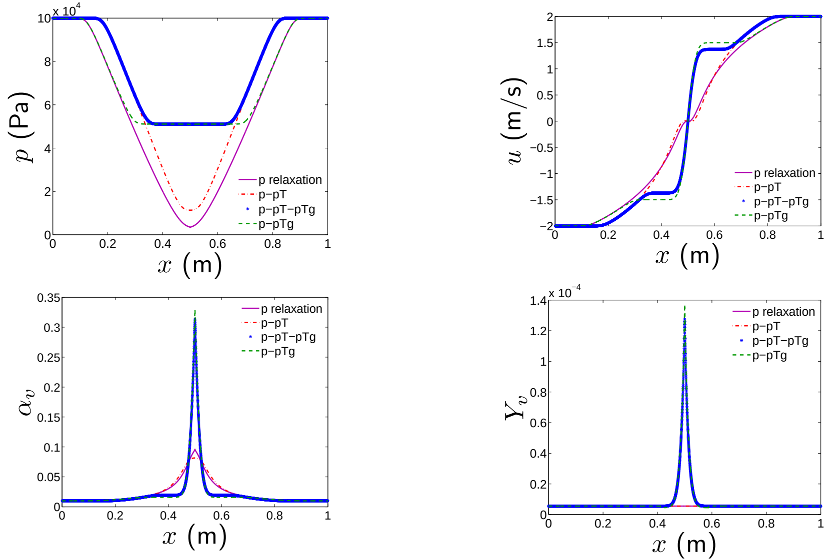
Liquid-vapor mixture ($\alpha_{\text{vapor}} = 1/5$) with initial states

$$p_{\text{liquid}} = p_{\text{vapor}} = 1\text{bar}$$
$$T_{\text{liquid}} = T_{\text{vapor}} = 354.7284\text{K} < T^{\text{sat}}$$
$$\rho_{\text{vapor}} = 0.63\text{kg/m}^3 > \rho^{\text{sat}}_{\text{vapor}}, \quad \rho_{\text{liquid}} = 1150\text{kg/m}^3 > \rho^{\text{sat}}_{\text{liquid}}$$
$$g^{\text{sat}} > g_{\text{vapor}} > g_{\text{liquid}}$$



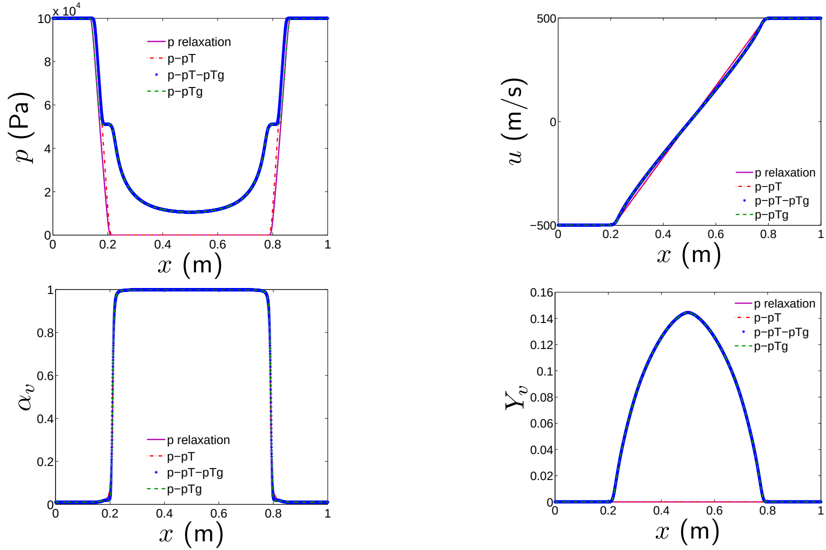
Cavitation test: $\vec{u} = 2\mathrm{m/s}$

Snap shot of computed solution at time $t = 3.2\mathrm{ms}$



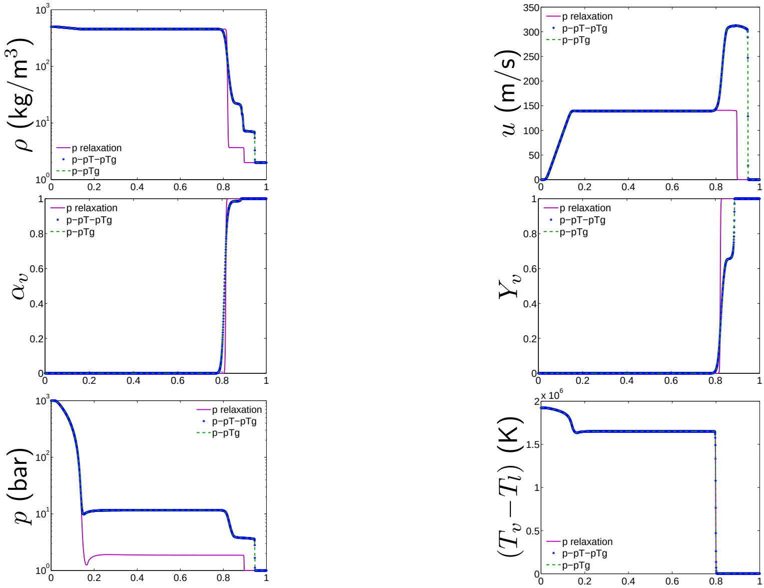
Cavitation test: $\vec{u} = 500\text{m/s}$

Snap shot of computed solution at time $t = 0.58$ms



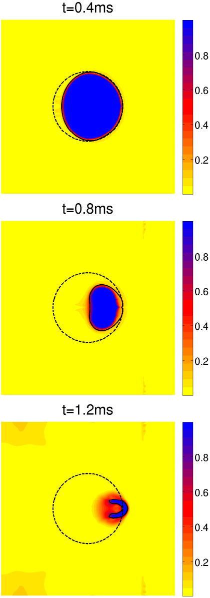
Dodecane liquid-vapor shock tube problem

Snap shot of computed solution at time $t = 473\mu$s

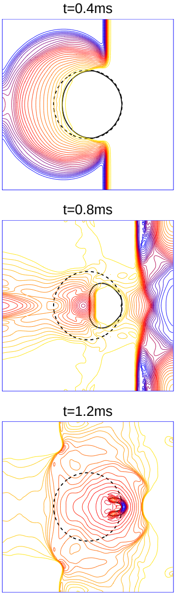


Vapor-bubble compression: pTg relaxation results

Vapor mass fraction



Mixture pressure



Future perspective

- Low Mach solver for weakly compressible flow
- Model with granular pressure for gas-liquid-soild flow
- Robust & stable stiff solver for real materials

Thank you