Recent advances in numerical methods for compressible two-phase flow with heat & mass transfers

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Outline

Main theme: Compressible 2-phase (liquid-gas) solver for metastable fluids: application to cavitation & flashing flows

1. Motivation
2. Constitutive law for metastable fluid
3. Mathematical model with & without heat & mass transfer
4. Stiff relaxation solver

Outline

Main theme: Compressible 2-phase (liquid-gas) solver for metastable fluids: application to cavitation & flashing flows

1. Motivation
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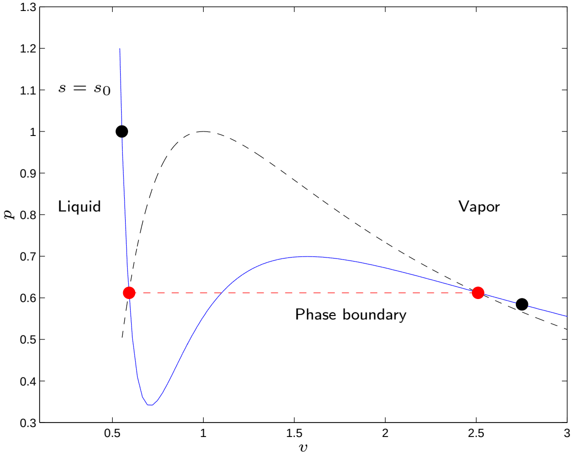
3. Mathematical model with & without heat & mass transfer
4. Stiff relaxation solver

- Flashing flow means a flow with dramatic evaporation of liquid due to pressure drop
- Solver preserves total energy conservation & employ convex pressure law

Phase transition with non-convex EOS

Sample wave path for phase transition problem with non-convex EOS (require phase boundary modelling)



Dodecane 2-phase Riemann problem

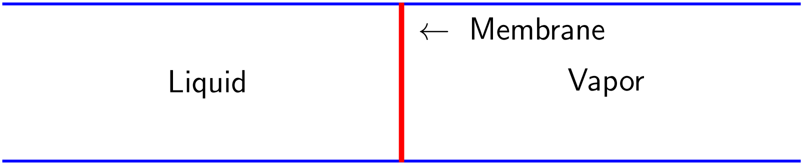
Saurel *et al.* (JFM 2008) & Zein *et al.* (JCP 2010):

- Liquid phase: Left-hand side ($0 \leq x \leq 0.75$m)

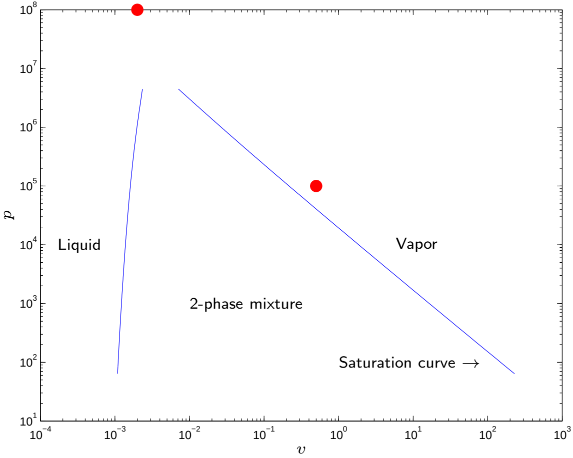
$$(\rho_v, \rho_l, u, p, \alpha_v)_L = \left(2\text{kg/m}^3,\ 500\text{kg/m}^3,\ 0,\ {\color{blue}10^8\text{Pa}},\ {\color{red}10^{-8}}\right)$$

- Vapor phase: Right-hand side ($0.75\text{m} < x \leq 1$m)

$$(\rho_v, \rho_l, u, p, \alpha_v)_R = \left(2\text{kg/m}^3,\ 500\text{kg/m}^3,\ 0,\ {\color{blue}10^5\text{Pa}},\ {\color{red}1 - 10^{-8}}\right),$$

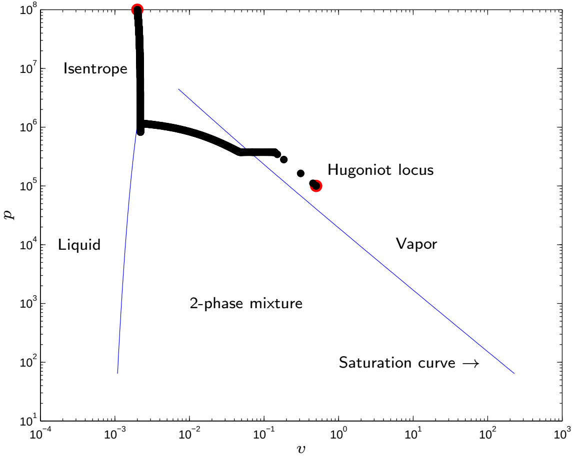


Dodecane 2-phase problem: Phase diagram

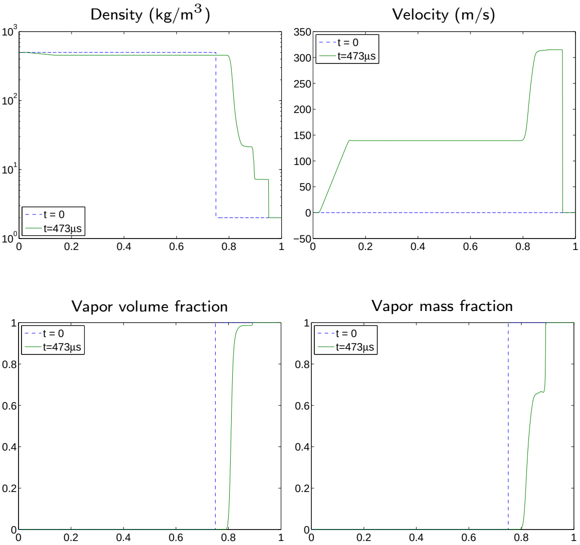


Dodecane 2-phase problem: Phase diagram

Wave path in p-v phase diagram



Dodecane 2-phase problem: Sample solution



4-wave

structure:

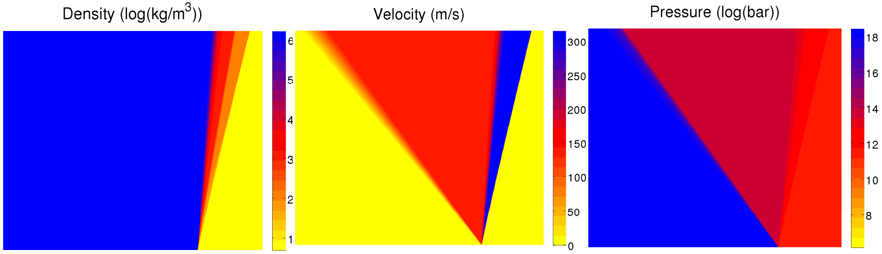
Rarefaction,

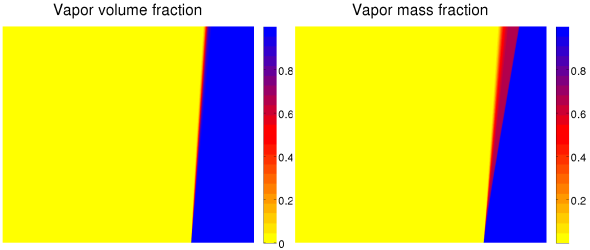
phase,

contact, &

shock

Dodecane 2-phase problem: Sample solution





All physical quantities are discontinuous across phase boundary

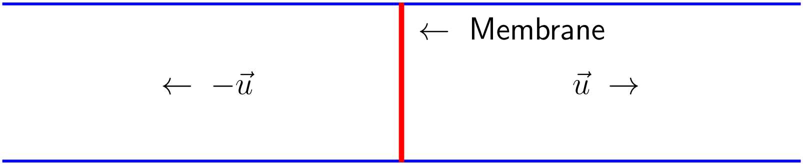
Expansion wave problem: Cavitation test

Saurel *et al.* (JFM 2008) & Zein *et al.* (JCP 2010):

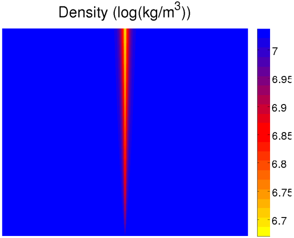
- Liquid-vapor mixture ($\alpha_{\text{vapor}} = 10^{-2}$) for water with

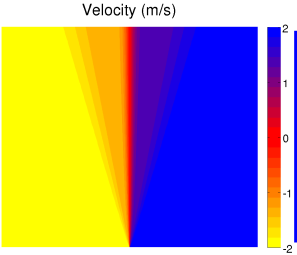
$$p_{\text{liquid}} = p_{\text{vapor}} = 1\text{bar}$$
$$T_{\text{liquid}} = T_{\text{vapor}} = 354.7284\text{K} < T^{\text{sat}}$$
$$\rho_{\text{vapor}} = 0.63\text{kg/m}^3 > \rho^{\text{sat}}_{\text{vapor}}, \quad \rho_{\text{liquid}} = 1150\text{kg/m}^3 > \rho^{\text{sat}}_{\text{liquid}}$$
$$g^{\text{sat}}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

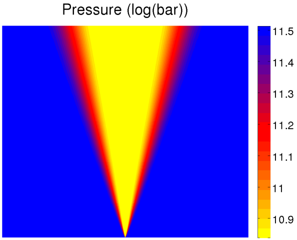
- Outgoing velocity $u = 2\text{m/s}$

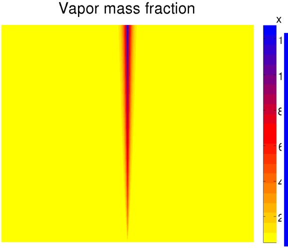


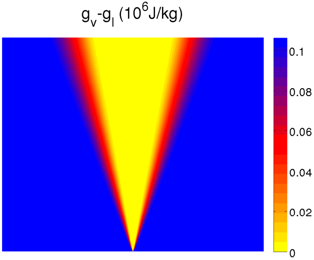
Expansion wave problem: Sample solution





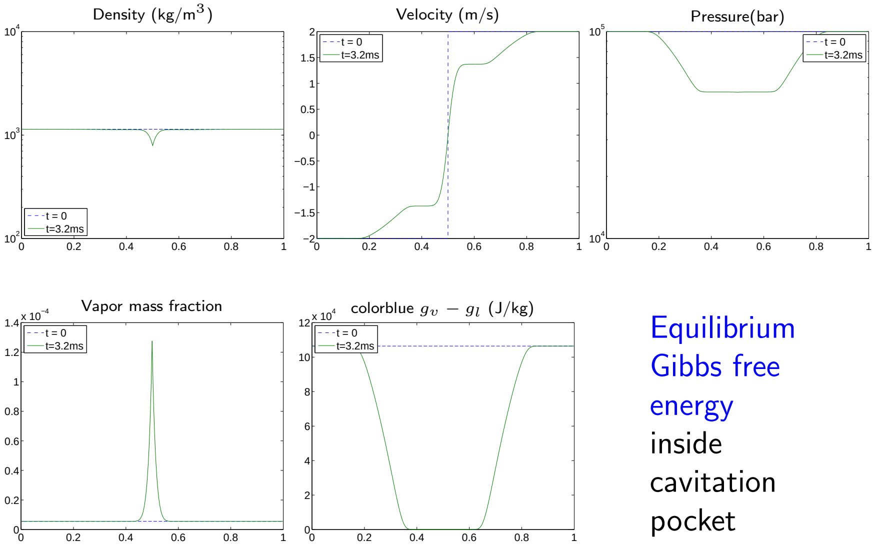






Cavitation pocket formation & mass transfer

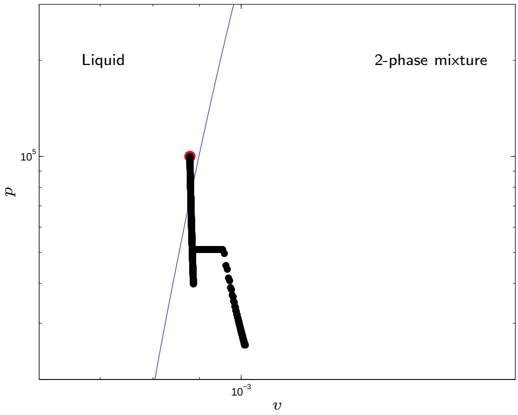
Expansion wave problem: Sample solution



Equilibrium Gibbs free energy inside cavitation pocket

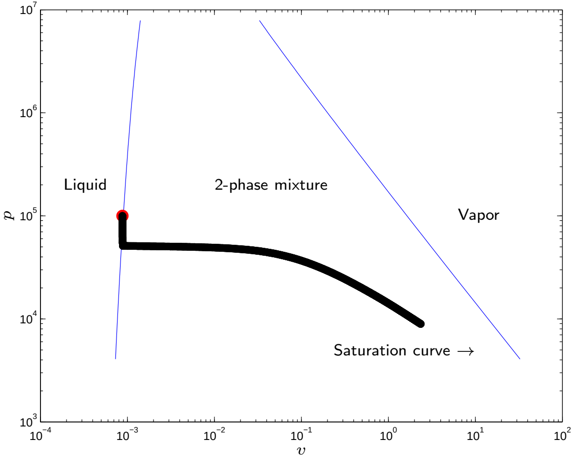
Expansion wave problem: Phase diagram

Solution remains in 2-phase mixture; phase separation has not reached

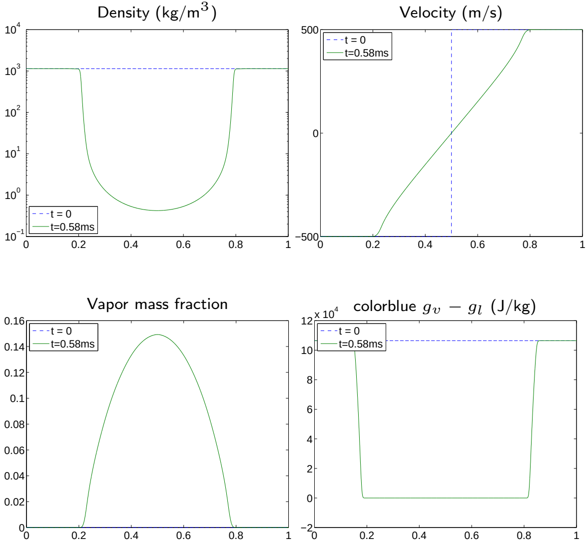


Expansion wave $\vec{u} = 500$m/s: Phase diagram

With faster $\vec{u} = 500$m/s, phase separation becomes more evident



Expansion wave $\vec{u} = 500\text{m/s}$: Sample solution



Equilibrium Gibbs free energy inside cavitation pocket

Constitutive law: Metastable fluid

Stiffened gas equation of state (SG EOS) with

- Pressure

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

- 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 $g_k = a_k + p_k v_k, \quad v_k = 1/\rho_k$

Metastable fluid: 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

Metastable fluid: Saturation curves

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

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

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

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

Metastable fluid: Saturation curves

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

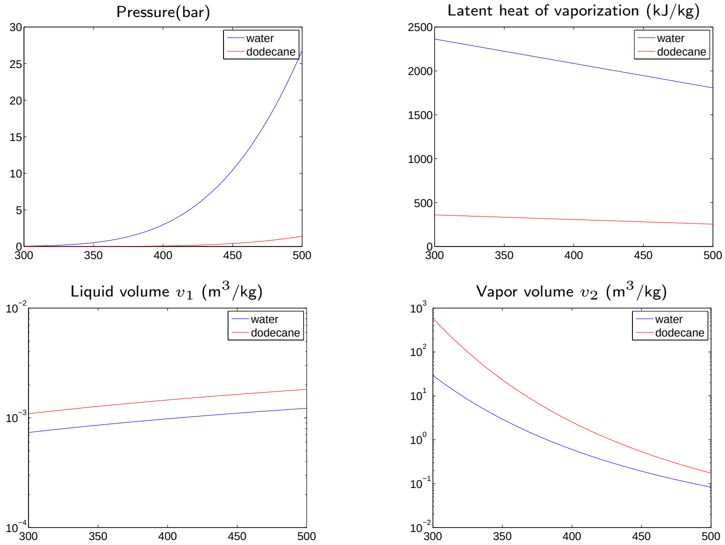
or, from $dg_1 = dg_2$, we get Clausius-Clapeyron equation

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

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

Metastable fluid: Saturation curves (Cont.)

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



Mathematical Models

Phase tranition models for compressible 2-phase flow include

1. 7-equation model (Baer-Nunziato type)
   - Zein, Hantke, Warnecke (JCP 2010)
2. Reduced 5-equation model (Kapila type)
   - Saurel, Petitpas, Berry (JFM 2008)
3. Homogeneous 6-equation model
   - Zein *et al.* , Saurel *et al.* , Pelanti & Shyue (JCP 2014)
4. Homogeneous equilibrium model
   - Dumbser, Iben, & Munz (CAF 2013), Hantke, Dreyer, & Warnecke (QAM 2013)
5. Navier-Stokes-Korteweg model
   - Prof. Kröner's talk tomorrow

7-equation model: Without phase transition

7-equation non-equilibrium model of Baer & Nunziato (1986)

$$\partial_t (\alpha\rho)_1 + \nabla\cdot(\alpha\rho\vec{u})_1 = 0$$

$$\partial_t (\alpha\rho)_2 + \nabla\cdot(\alpha\rho\vec{u})_2 = 0$$

$$\partial_t (\alpha\rho\vec{u})_1 + \nabla\cdot(\alpha\rho\vec{u}\otimes\vec{u})_1 + \nabla(\alpha p)_1 = p_I\nabla\alpha_1 + \lambda(\vec{u}_2 - \vec{u}_1)$$

$$\partial_t (\alpha\rho\vec{u})_2 + \nabla\cdot(\alpha\rho\vec{u}\otimes\vec{u})_2 + \nabla(\alpha p)_2 = -p_I\nabla\alpha_1 - \lambda(\vec{u}_2 - \vec{u}_1)$$

$$\partial_t (\alpha E)_1 + \nabla\cdot(\alpha E\vec{u} + \alpha p\vec{u})_1 = p_I\vec{u}_I\cdot\nabla\alpha_1 + \mu p_I(p_2 - p_1) + \lambda\vec{u}_I\cdot(\vec{u}_2 - \vec{u}_1)$$

$$\partial_t (\alpha E)_2 + \nabla\cdot(\alpha E\vec{u} + \alpha p\vec{u})_2 = -p_I\vec{u}_I\cdot\nabla\alpha_1 - \mu p_I(p_2 - p_1) - \lambda\vec{u}_I\cdot(\vec{u}_2 - \vec{u}_1)$$

$$\partial_t\alpha_1 + \vec{u}_I\cdot\nabla\alpha_1 = \mu(p_1 - p_2) \qquad (\alpha_1 + \alpha_2 = 1)$$

α_k: volume fraction, ρ_k: density, $\vec{u}_k$: velocity

$p_k(\rho_k, e_k)$: pressure, e_k: specific internal energy

$E_k = \rho_k e_k + \rho_k\vec{u}_k\cdot\vec{u}_k/2$: specific total energy, $k = 1, 2$

7-equation model: Closure relations

p_I & $\vec{u}_I$: interfacial pressure & velocity, *e.g.*,

- Baer & Nunziato (1986): $p_I = p_2, \quad \vec{u}_I = \vec{u}_1$
- Saurel & Abgrall (JCP 1999, JCP 2003)

$$p_I = \alpha_1 p_1 + \alpha_2 p_2, \quad \vec{u}_I = \frac{\alpha_1 \rho_1 \vec{u}_1 + \alpha_2 \rho_2 \vec{u}_2}{\alpha_1 \rho_1 + \alpha_2 \rho_2}$$

$$p_I = \frac{p_1/Z_1 + p_2/Z_2}{1/Z_1 + 1/Z_2}, \quad \vec{u}_I = \frac{\vec{u}_1 Z_1 + \vec{u}_2 Z_2}{Z_1 + Z_2}, \quad Z_k = \rho_k c_k$$

μ & λ: non-negative relaxation parameters that express rates pressure & velocity toward equilibrium, respectively

$$\mu = \frac{S_I}{Z_1 + Z_2}, \quad \lambda = \frac{S_I Z_1 Z_2}{Z_1 + Z_2}, \quad S_I(\text{Interfacial area})$$

7-equation model: With phase transition

7-equation model with heat & mass transfers (Zein *et al.*):

$$\partial_t (\alpha\rho)_1 + \nabla \cdot (\alpha\rho\vec{u})_1 = \dot{m}$$

$$\partial_t (\alpha\rho)_2 + \nabla \cdot (\alpha\rho\vec{u})_2 = -\dot{m}$$

$$\partial_t (\alpha\rho\vec{u})_1 + \nabla \cdot (\alpha\rho\vec{u} \otimes \vec{u})_1 + \nabla(\alpha p)_1 = p_I \nabla\alpha_1 + \lambda (\vec{u}_2 - \vec{u}_1) + \vec{u}_I \dot{m}$$

$$\partial_t (\alpha\rho\vec{u})_2 + \nabla \cdot (\alpha\rho\vec{u} \otimes \vec{u})_2 + \nabla(\alpha p)_2 = -p_I \nabla\alpha_1 - \lambda (\vec{u}_2 - \vec{u}_1) - \vec{u}_I \dot{m}$$

$$\partial_t (\alpha E)_1 + \nabla \cdot (\alpha E\vec{u} + \alpha p\vec{u})_1 = p_I \vec{u}_I \cdot \nabla\alpha_1 + \mu p_I (p_2 - p_1) + \lambda \vec{u}_I \cdot (\vec{u}_2 - \vec{u}_1) + \mathcal{Q} + (e_I + \vec{u}_I \cdot \vec{u}_I/2)\,\dot{m}$$

$$\partial_t (\alpha E)_2 + \nabla \cdot (\alpha E\vec{u} + \alpha p\vec{u})_2 = -p_I \vec{u}_I \cdot \nabla\alpha_1 - \mu p_I (p_2 - p_1) - \lambda \vec{u}_I \cdot (\vec{u}_2 - \vec{u}_1) - \mathcal{Q} - (e_I + \vec{u}_I \cdot \vec{u}_I/2)\,\dot{m}$$

$$\partial_t \alpha_1 + \vec{u}_I \cdot \nabla\alpha_1 = \mu (p_1 - p_2) + \frac{\mathcal{Q}}{q_I} + \frac{\dot{m}}{\rho_I}$$

Mass transfer modelling

Typical apporach to mass transfer modelling assumes

$$\dot{m} = \dot{m}^+ + \dot{m}^-$$

- Singhal *et al.* (1997) & Merkel *et al.* (1998)

$$\dot{m}^+ = \frac{C_{\mathrm{prod}}(1-\alpha_1)\max(p-p_v,0)}{t_\infty \rho_1 U_\infty^2/2}$$

$$\dot{m}^- = \frac{C_{\mathrm{liq}}\alpha_1\rho_1 \min(p-p_v,0)}{\rho_v t_\infty \rho_1 U_\infty^2/2}$$

- Kunz *et al.* (2000)

$$\dot{m}^+ = \frac{C_{\mathrm{prod}}\alpha_1^2(1-\alpha_1)}{\rho_1 t_\infty}, \quad \dot{m}^- = \frac{C_{\mathrm{liq}}\alpha_1\rho_v \min(p-p_v,0)}{\rho_1 t_\infty \rho_1 U_\infty^2/2}$$

Mass transfer modelling

- Singhal *et al.* (2002)

$$\dot{m}^+ = \frac{C_{\mathrm{prod}}\sqrt{\kappa}}{\sigma}\rho_1\rho_v\left[\frac{2}{3}\frac{\max(p-p_v,0)}{\rho_1}\right]^{1/2}$$

$$\dot{m}^- = \frac{C_{\mathrm{liq}}\sqrt{\kappa}}{\sigma}\rho_1\rho_v\left[\frac{2}{3}\frac{\min(p-p_v,0)}{\rho_1}\right]^{1/2}$$

- Senocak & Shyy (2004)

$$\dot{m}^+ = \frac{\max(p-p_v,0)}{(\rho_1-\rho_c)(V_{vn}-V_{1n})^2 t_\infty},\ \dot{m}^- = \frac{\rho_1\min(p-p_v,0)}{\rho_v(\rho_1-\rho_c)(V_{vn}-V_{1n})^2 t_\infty}$$

- Hosangadi & Ahuja (JFE 2005)

$$\dot{m}^+ = C_{\mathrm{prod}}\frac{\rho_v}{\rho_l}(1-\alpha_1)\frac{\min(p-p_v,0)}{\rho_\infty U_\infty^2/2}$$

$$\dot{m}^- = C_{\mathrm{liq}}\frac{\rho_v}{\rho_l}\alpha_1\frac{\max(p-p_v,0)}{\rho_\infty U_\infty^2/2}$$

Phase transition model: 7-equation

We assume

$$\mathcal{Q} = \theta\,(T_2 - T_1)$$

for heat transfer &

$$\dot{m} = \nu\,(g_2 - g_1)$$

for mass transfer

- $\theta \geq 0$ expresses rate towards thermal equilibrium $T_1 \to T_2$
- $\nu \geq 0$ expresses rate towards diffusive equilibrium $g_1 \to g_2$, & is nonzero only at 2-phase mixture & metastable state $T_{\text{liquid}} > T_{\text{sat}}$

7-equation model: Numerical approximation

Write 7-equation model in compact form

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

Solve by fractional-step method

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

   $$\partial_t q = \psi_\mu(q) + \psi_\lambda(q) + \psi_\theta(q) + \psi_\nu(q)$$

   in various flow regimes under relaxation limits

Reduced 5-equation model: With phase transition

Saurel *et al.* considered 7-equation model in asymptotic limits λ & $\mu \to \infty$, *i.e.*, flow towards mechanical equilibrium: $\vec{u}_1 = \vec{u}_2 = \vec{u}$ & $p_1 = p_2 = p$, *i.e.*, reduced 5-equation model

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

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

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

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

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

$$\bar{K}_s = \left(\frac{\alpha_1}{K_s^1} + \frac{\alpha_2}{K_s^2} \right)^{-1}, \quad q_I = \left(\frac{K_s^1}{\alpha_1} + \frac{K_s^2}{\alpha_2} \right) \Big/ \left(\frac{\Gamma_1}{\alpha_1} + \frac{\Gamma_2}{\alpha_2} \right)$$

$$\rho_I = \left(\frac{K_s^1}{\alpha_1} + \frac{K_s^2}{\alpha_2} \right) \Big/ \left(\frac{c_1^2}{\alpha_1} + \frac{c_2^2}{\alpha_2} \right), \quad K_s^\iota = \rho_\iota c_\iota^2$$

Phase transition model: 5-equation

- Mixture entropy $s = Y_1 s_1 + Y_2 s_2$ admits nonnegative variation

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

- Mixture pressure p determined from total internal energy

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

- Model is hyperbolic with non-monotonic sound speed c_p:

$$\frac{1}{\rho c_p^2} = \frac{\alpha_1}{\rho_1 c_1^2} + \frac{\alpha_2}{\rho_2 c_2^2}$$

- Limit interface model, *i.e.*, as θ & $\nu \to \infty$ (thermo-chemical relaxation), is homogeneous equilibrium model

Homogeneous equilibrium model

Homogeneous equilibrium model (HEM) 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

- System is closed by

$$p_1 = p_2 = p, \quad T_1 = T_2 = T, \quad \& \quad g_1 = g_2 = g$$

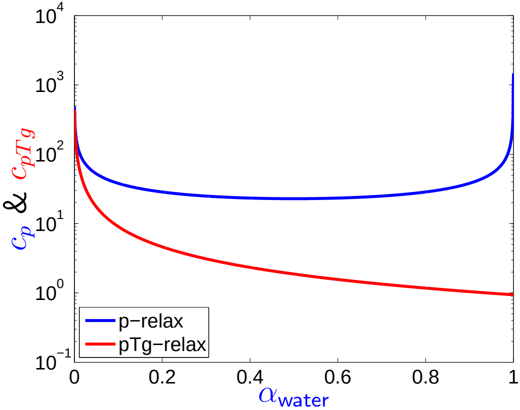
- Speed of sound c_{pTg} satisfies

$$\frac{1}{\rho c_{pTg}^2} = \frac{1}{\rho c_p^2} + T \left[\frac{\alpha_1 \rho_1}{C_{p1}} \left(\frac{ds_1}{dp} \right)^2 + \frac{\alpha_2 \rho_2}{C_{p2}} \left(\frac{ds_2}{dp} \right)^2 \right]$$

Equilibrium speed of sound: Comparison

- Sound speeds follow subcharacteristic condition $c_{pTg} \leq c_p$
- Sound speed limits follow

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



5-equation model: Numerical approximation

Write 5-equation model in compact form

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2. Stiff relaxation step
   Solve system of ordinary differential equations

   $$\partial_t q = \psi_\theta(q) + \psi_\nu(q)$$

   in various flow regimes under relaxation limits

HEM: Numerical approximation

Write HEM in compact form

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

Compute solution numerically, *e.g.*, Godunov-type method, requires Riemann solver for elementary waves to fulfil

1. Jump conditions across discontinuities
2. Kinetic condition
3. Entropy condition

Numerical approximation: summary

1. Solver based on 7-equation model is viable one for wide variety of problems, but is expensive to use

2. Solver based on reduced 5-equation model is robust one for sample problems, but is difficult to achieve admissible solutions under extreme flow conditions

3. Solver based on HEM is mathematically attracive one

Numerical approximation: summary

1. Solver based on 7-equation model is viable one for wide variety of problems, but is expensive to use

2. Solver based on reduced 5-equation model is robust one for sample problems, but is difficult to achieve admissible solutions under extreme flow conditions

3. Solver based on HEM is mathematically attracive one

Numerically advantageous to use 6-equation model as opposed to 5-equation model (Saurel *et al.* , Pelanti & Shyue)

6-equation model: With phase transition

6-equation single-velocity 2-phase model with stiff mechanical, thermal, & chemical relaxations reads

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

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

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

Phase transition model: 6-equation

$\mu, \theta, \nu \to \infty$: 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 $T_1 \to T_2$,
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 $T_{\text{liquid}} > T_{\text{sat}}$

Phase transition model: 6-equation

6-equation model in compact form

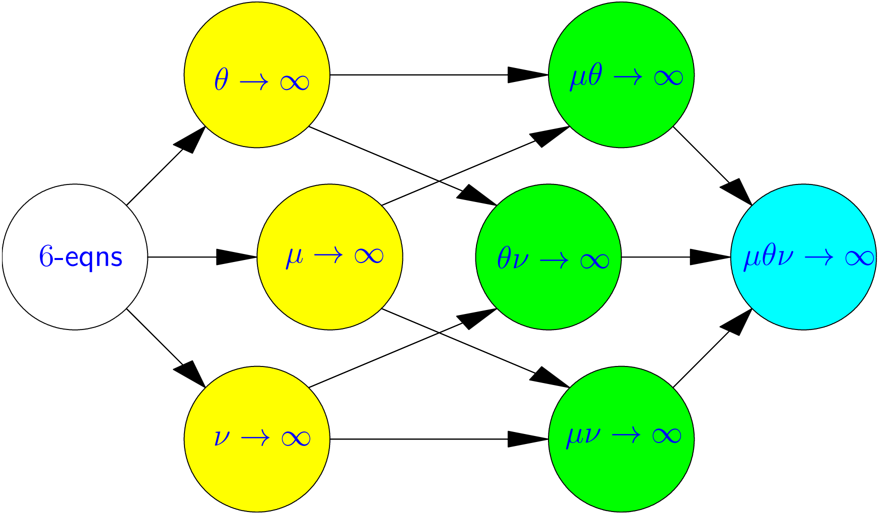
$$\partial_t q + \nabla \cdot f(q) + w\left(q, \nabla q\right) = \psi_\mu(q) + \psi_\theta(q) + \psi_\nu(q)$$

where

$$\begin{aligned}
q &= \left[\alpha_1\rho_1,\ \alpha_2\rho_2,\ \rho\vec{u},\ \alpha_1 E_1,\ \alpha_2 E_2,\ \alpha_1\right]^T \\
f &= \left[\alpha_1\rho_1\vec{u},\ \alpha_2\rho_2\vec{u},\ \rho\vec{u}\otimes\vec{u} + (\alpha_1 p_1 + \alpha_2 p_2) I_N,\right. \\
&\qquad \left.\alpha_1\left(E_1 + p_1\right)\vec{u},\ \alpha_2\left(E_2 + p_2\right)\vec{u},\ 0\right]^T \\
w &= \left[0,\ 0,\ 0,\ \mathcal{B}\left(q, \nabla q\right),\ -\mathcal{B}\left(q, \nabla q\right),\ \vec{u}\cdot\nabla\alpha_1\right]^T \\
\psi_\mu &= \left[0,\ 0,\ 0,\ \mu p_I\left(p_2 - p_1\right),\ \mu p_I\left(p_1 - p_2\right),\ \mu\left(p_1 - p_2\right)\right]^T \\
\psi_\theta &= \left[0,\ 0,\ 0,\ \mathcal{Q},\ -\mathcal{Q},\ \mathcal{Q}/q_I\right]^T \\
\psi_\nu &= \left[\dot{m},\ -\dot{m},\ 0,\ e_I\dot{m},\ -e_I\dot{m},\ \dot{m}/\rho_I\right]^T
\end{aligned}$$

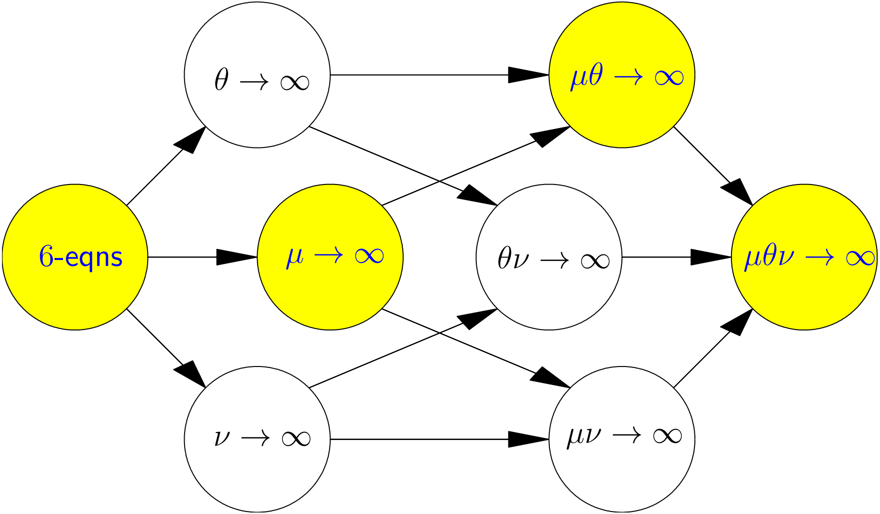
Phase transition model: 6-equation

Flow hierarchy in 6-equation model: H. Lund (SIAP 2012)



Phase transition model: 6-equation

Stiff limits as $\mu \to \infty$, $\mu\theta \to \infty$, & $\mu\theta\nu \to \infty$ sequentially



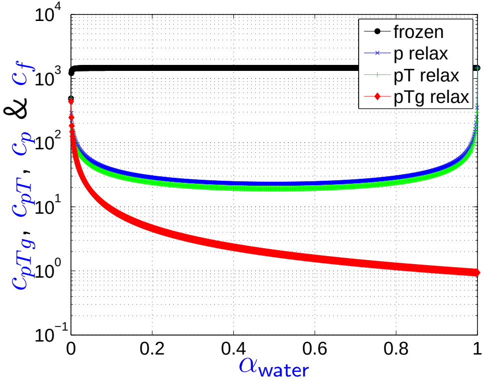
Equilibrium speed of sound: Comparison

- Sound speeds follow subcharacteristic condition

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

- Limit of sound speed

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



6-equation model: Numerical approximation

As before, we begin by solving non-stiff hyperbolic equations in step 1, & continue by applying 3 sub-steps as

2. Stiff mechanical relaxation step

   Solve system of ordinary differential equations ($\mu \to \infty$)

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

   with initial solution from step 1 as $\mu \to \infty$

3. Stiff thermal relaxation step ($\mu \ \& \ \theta \to \infty$)

   Solve system of ordinary differential equations

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

4. Stiff thermo-chemical relaxation step ($\mu, \ \theta, \ \& \ \nu \to \infty$)

   Solve system of ordinary differential equations

   $$\partial_t q = \psi_\mu(q) + \psi_\theta(q) + \psi_\nu(q)$$

Take solution from previous step as initial condition

6-equation model: Stiff relaxation solvers

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

Stiff mechanical relaxation step

Look for solution of ODEs in limit $\mu \to \infty$

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

with initial condition q^0 (solution after non-stiff hyperbolic step) & under mechanical equilibrium condition

$$p_1 = p_2 = p$$

Stiff mechanical relaxation step (Cont.)

We find easily

$$
\begin{aligned}
\partial_t\left(\alpha_1\rho_1\right) = 0 \quad &\Longrightarrow \quad \alpha_1\rho_1 = \alpha_1^0\rho_1^0 \\
\partial_t\left(\alpha_2\rho_2\right) = 0 \quad &\Longrightarrow \quad \alpha_2\rho_2 = \alpha_2^0\rho_2^0 \\
\partial_t\left(\rho\vec{u}\right) = 0 \quad &\Longrightarrow \quad \rho\vec{u} = \rho^0\vec{u}^0 \\
\partial_t\left(\alpha_1 E_1\right) = \mu p_I\left(p_2 - p_1\right) \quad &\Longrightarrow \quad \partial_t\left(\alpha\rho e\right)_1 = -p_I\partial_t\alpha_1 \\
\partial_t\left(\alpha_2 E_2\right) = \mu p_I\left(p_1 - p_2\right) \quad &\Longrightarrow \quad \partial_t\left(\alpha\rho e\right)_2 = -p_I\partial_t\alpha_2
\end{aligned}
$$

Integrating latter two equations with respect to time

$$
\int \partial_t\left(\alpha\rho e\right)_k \, dt = -\int p_I\partial_t\alpha_k \, dt
$$

$$
\Longrightarrow \qquad \alpha_k\rho_k e_k - \alpha_k^0\rho_k^0 e_k^0 = -\bar{p}_I\left(\alpha_k - \alpha_k^0\right) \qquad \text{or}
$$

$$
\Longrightarrow \qquad e_k - e_k^0 = -\bar{p}_I\left(1/\rho_k - 1/\rho_k^0\right) \qquad (\text{use } \alpha_k\rho_k = \alpha_k^0\rho_k^0)
$$

Take $\bar{p}_I = (p_I^0 + p)/2$ or p, for example

Stiff mechanical relaxation step (Cont.)

We find condition for ρ_k in p, $k = 1, 2$

Combining that with saturation condition for volume fraction

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

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

Stiff mechanical relaxation step (Cont.)

We find condition for ρ_k in p, $k = 1, 2$

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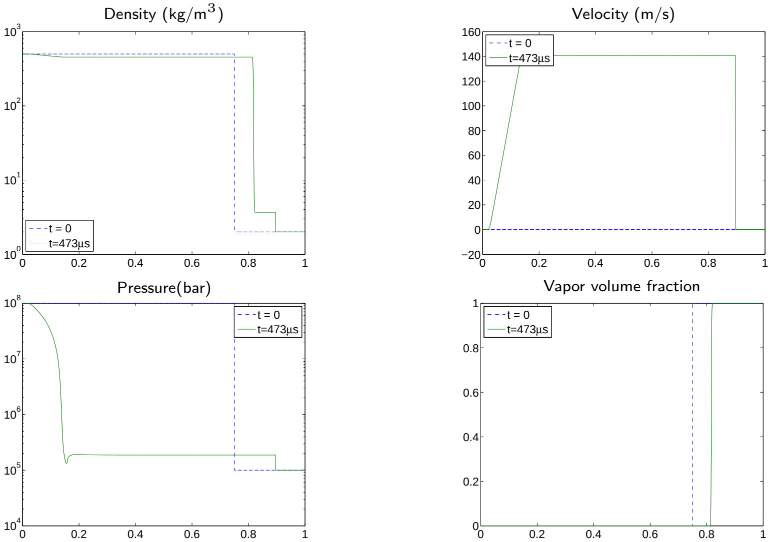
With that, ρ_k, α_k can be determined & state vector q is updated from current time to next

Relaxed solution depends strongly on initial condition from non-stiff hyperbolic step

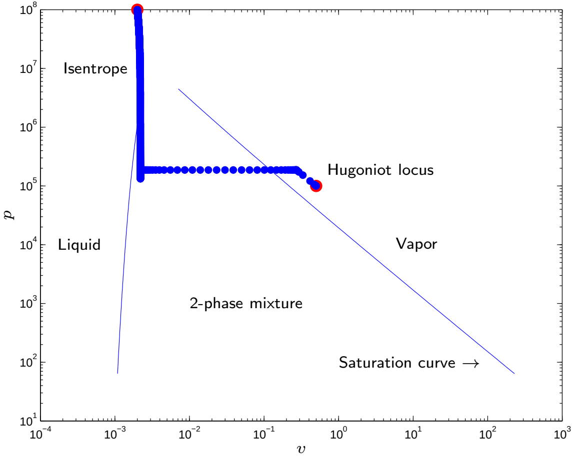
Dodecane 2-phase Riemann problem: p relaxation

Mechanical-equilibrium solution at $t = 473\mu s$



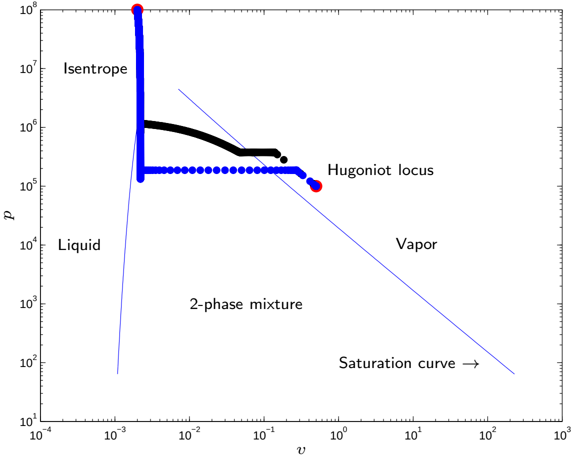
Dodecane 2-phase problem: Phase diagram

Wave path after p-relaxation in p-v phase diagram



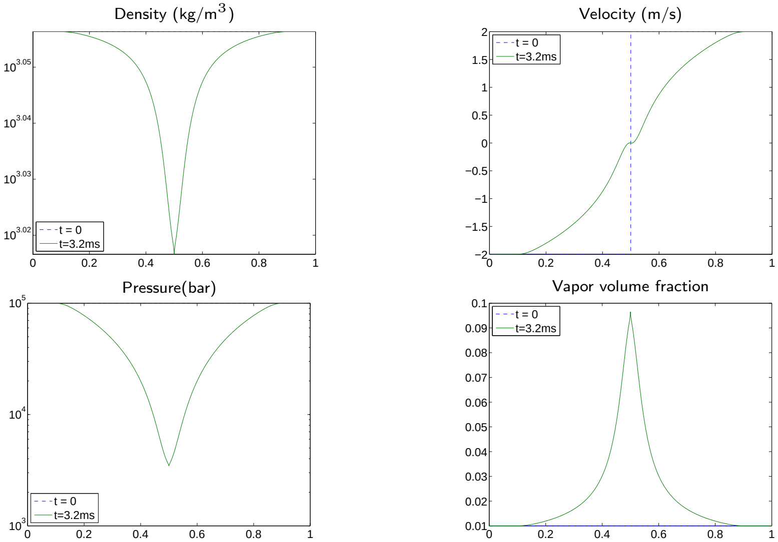
Dodecane 2-phase problem: Phase diagram

Wave path comparison between solutions after p- & pTg-relaxation in p-v phase diagram



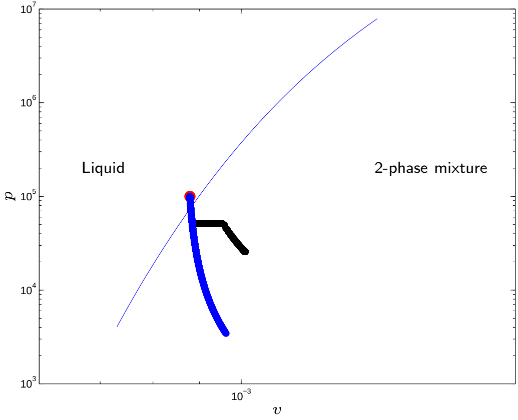
Expansion wave problem: p relaxation

Mechanical-equilibrium solution at $t = 3.2\text{ms}$



Expansion wave problem: Phase diagram

Wave path comparison between solutions after p- & pTg-relaxation in p-v phase diagram



Stiff thermal relaxation step

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

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

under mechanical-thermal equilibrium conditons

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

Stiff thermal relaxation step (Cont.)

We find easily

$$\partial_t (\alpha_1 \rho_1) = 0 \quad \Longrightarrow \quad \alpha_1 \rho_1 = \alpha_1^0 \rho_1^0$$

$$\partial_t (\alpha_2 \rho_2) = 0 \quad \Longrightarrow \quad \alpha_2 \rho_2 = \alpha_2^0 \rho_2^0$$

$$\partial_t (\rho \vec{u}) = 0 \quad \Longrightarrow \quad \rho \vec{u} = \rho^0 \vec{u}^0$$

$$\partial_t (\alpha_k E_k) = \frac{\theta}{q_I} (T_2 - T_1) \quad \Longrightarrow \quad \partial_t (\alpha \rho e)_k = q_I \partial_t \alpha_k$$

Integrating latter two equations with respect to time

$$\int \partial_t (\alpha \rho e)_k \; dt = \int q_I \partial_t \alpha_k \; dt$$

$$\Longrightarrow \quad \alpha_k \rho_k e_k - \alpha_k^0 \rho_k^0 e_k^0 = -\bar{q}_I \left(\alpha_k - \alpha_k^0 \right)$$

Take $\bar{q}_I = (q_I^0 + q_I)/2$ or q_I, for example, & find algebraic equation for α_1, by imposing

$$T_2 \left(e_2, \alpha_2^0 \rho_2^0 / (1 - \alpha_1) \right) - T_1 \left(e_1, \alpha_1^0 \rho_1^0 / \alpha_1 \right) = 0$$

Stiff thermal relaxation step: Algebraic approach

Impose mechanical-thermal equilibrium directly to

1. Saturation condition

$$\frac{Y1}{\rho_1(p,T)} + \frac{Y_2}{\rho_2(p,T)} = \frac{1}{\rho^0}$$

2. Equilibrium of internal energy

$$Y_1 \, e_1(p,T) + Y_2 \, e_2(p,T) = e^0$$

Give 2 algebraic equations for 2 unknowns p & T

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

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

Stiff thermo-chemical relaxation step

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

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

under mechanical-thermal-chemical equilibrium conditons

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

Stiff thermal-chemical relaxation step (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 $\alpha_k\rho_k \neq \alpha_k^0\rho_k^0$ & $Y_k \neq Y_k^0$, $k = 1, 2$

Impose mechanical-thermal-chemical equilibrium to

1. Saturation condition for temperature

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

2. Saturation condition for volume fraction

$$\frac{Y_1}{\rho_1(p, T)} + \frac{Y_2}{\rho_2(p, T)} = \frac{1}{\rho^0}$$

3. Equilibrium of internal energy

$$Y_1\, e_1(p, T) + Y_2\, e_2(p, T) = e^0$$

Stiff thermal-chemical relaxation step (Cont.)

From saturation condition for temperature

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

we get T in terms of p, while from

$$\frac{Y_1}{\rho_1(p, T)} + \frac{Y_2}{\rho_2(p, T)} = \frac{1}{\rho^0}$$

&

$$Y_1 \, e_1(p, T) + Y_2 \, e_2(p, T) = e^0$$

we obtain algebraic equation for p

$$Y_1 = \frac{1/\rho_2(p) - 1/\rho^0}{1/\rho_2(p) - 1/\rho_1(p)} = \frac{e^0 - e_2(p)}{e_1(p) - e_2(p)}$$

which is solved by iterative method

Stiff thermal-chemical relaxation step (Cont.)

- Having known Y_k & p, T can be solved from, *e.g.*,

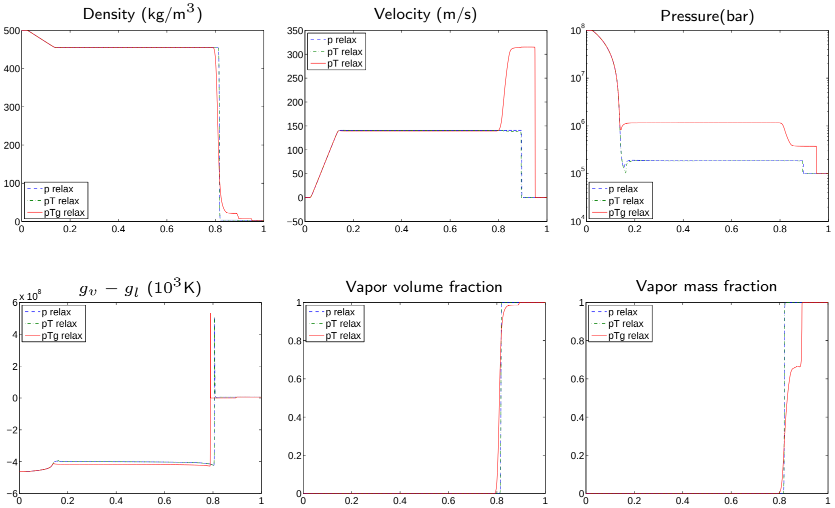
$$Y_1\, e_1(p, T) + Y_2\, e_2(p, T) = e^0$$

  yielding update ρ_k & α_k

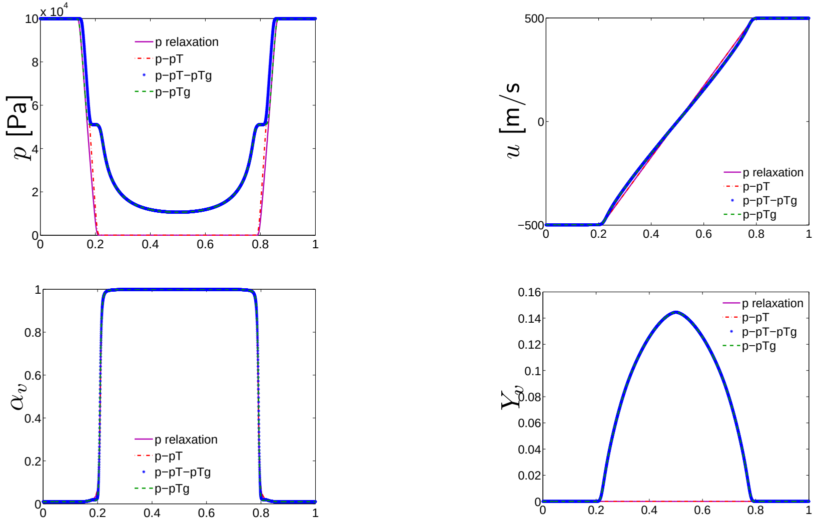
- Feasibility of solutions, *i.e.*, positivity of physical quantities ρ_k, α_k, p, & T, for example
  - Employ hybrid method *i.e.*, combination of above method with differential-based approach (not discuss here), when it becomes necessary

Dodecane 2-phase Riemann problem

Comparison p-,pT-& p-pTg-relaxation solution at $t = 473\mu s$



Expansion wave problem: $\vec{u} = 500\text{m/s}$



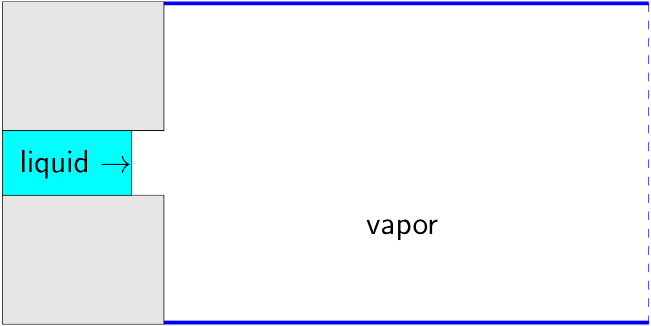
High-pressure fuel injector

Inject fluid: Liquid dodecane containing small amount α_{vapor}

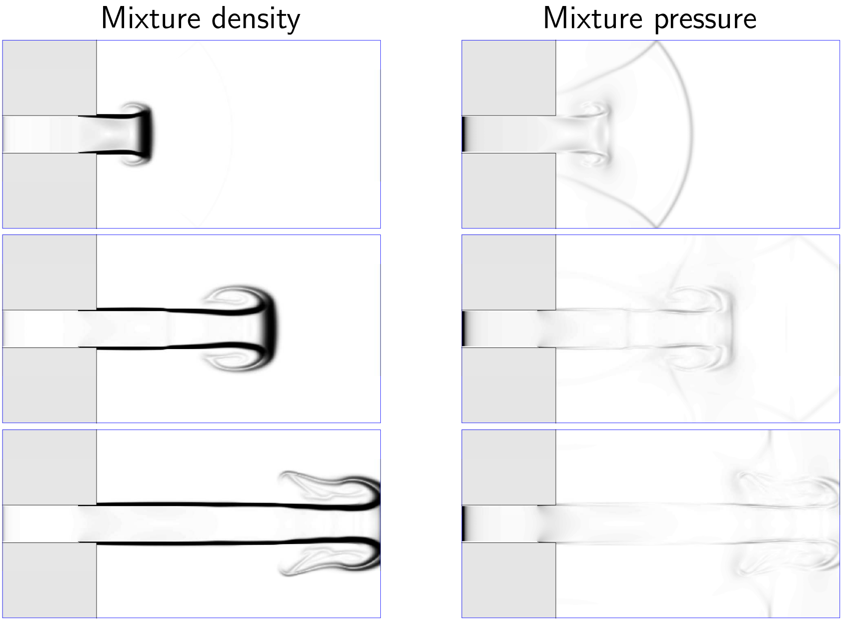
- Pressure & temperature are in equilibrium with $p = 10^8$ Pa & $T = 640K$

Ambient fluid: Vapor dodecane containing small amount α_{liquid}

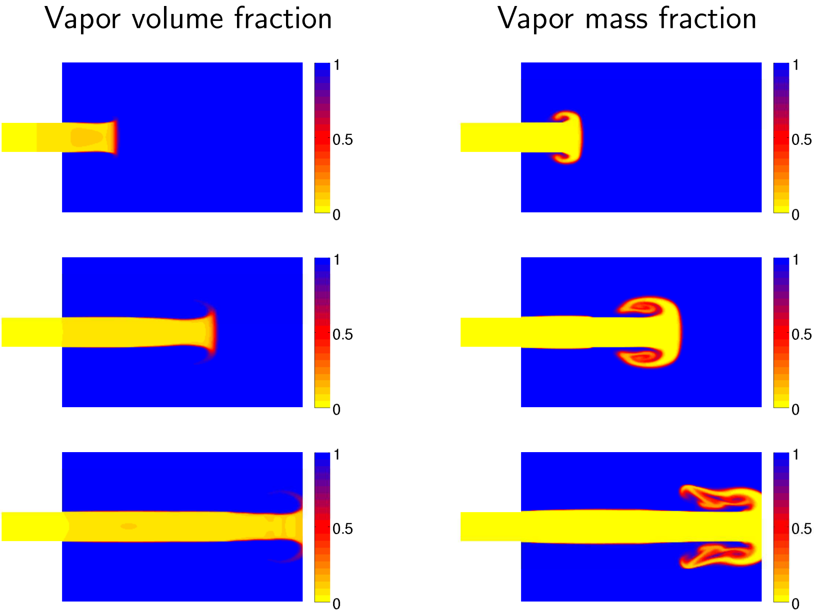
- Pressure & temperature are in equilibrium with $p = 10^5$ Pa & $T = 1022K$



High-pressure fuel injector ($\alpha_{v,l} = 10^{-4}$): p-relax

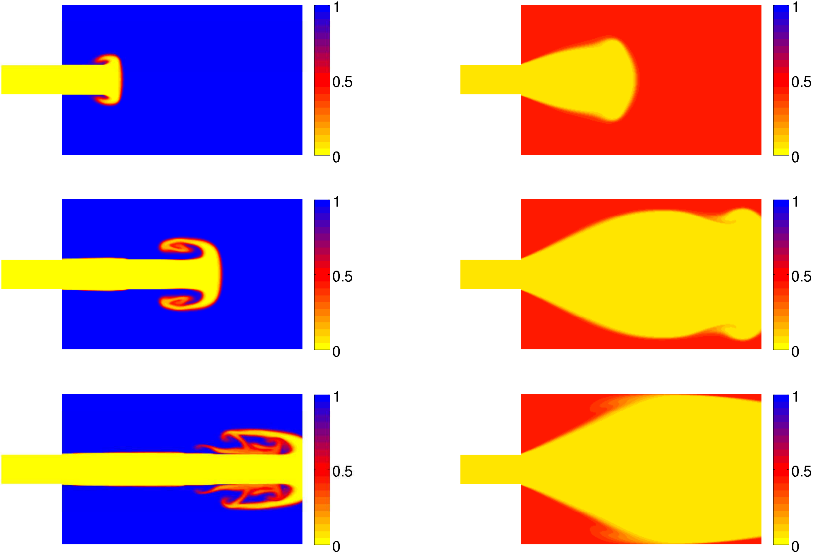


High-pressure fuel injector: p-relax



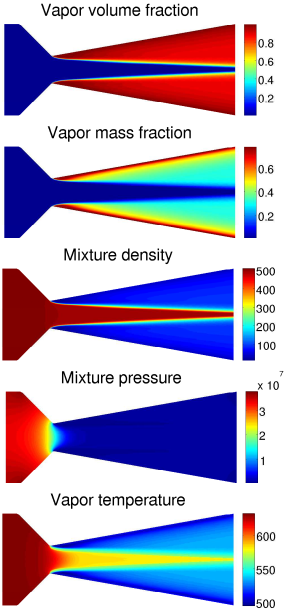
Fuel injector: p-pT-pTg relaxation

Vapor mass fraction: $\alpha_{v,l} = 10^{-4}$ (left) vs. 10^{-2} (right)

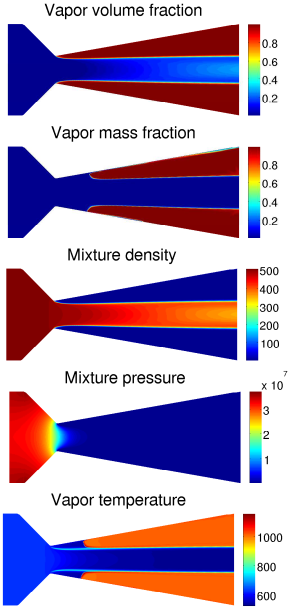


High-pressure fuel injector

With thermo-chemical relaxation

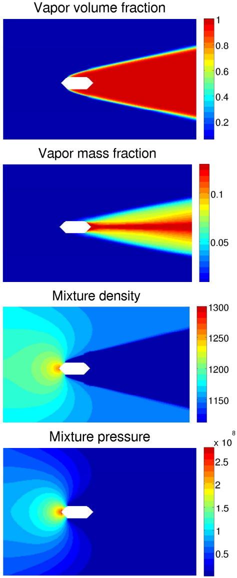


No thermo-chemical relaxation

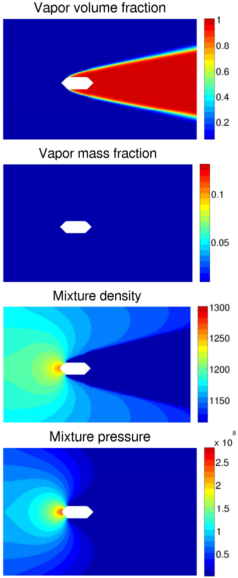


High-speed underwater projectile

With thermo-chemical relaxation



No thermo-chemical relaxation



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Thank you