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

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Outline

Compressible 2-phase solver for matastable fluids: application to cavitation & flashing flows

1. Motivation
2. Constitutive law for metastable fluid
3. 6-equation single-velocity 2-phase flow model
    - Model with & without heat & mass transfer
4. Stiff relaxation solver

- Mixture-energy-consistent method means total energy conservation & pressure consistency
- Flashing flow means a flow with dramatic evaporation of liquid due to pressure drop

Motivation: Dodecane 2-phase Riemann problem

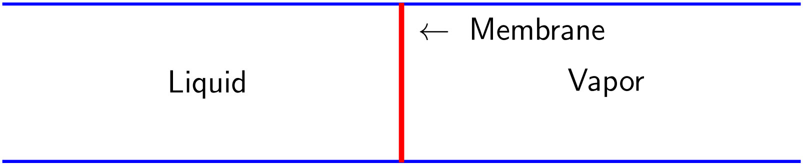
Riemann data for metastable dodecane modelled by SG EOS

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

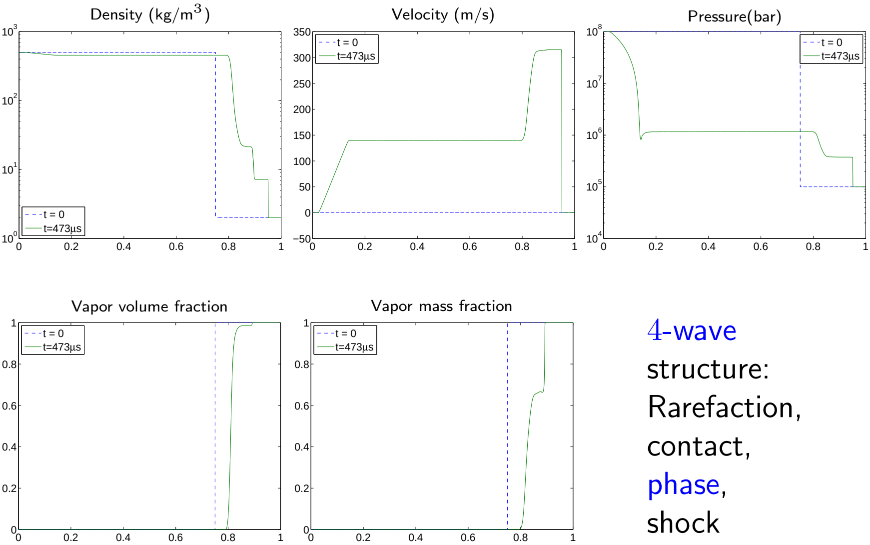
$$(\rho_v, \rho_l, u, p, \alpha_v)_L = \left(2\text{kg/m}^3,\ 500\text{kg/m}^3,\ 0,\ 10^8\text{Pa},\ 10^{-8}\right)$$

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

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

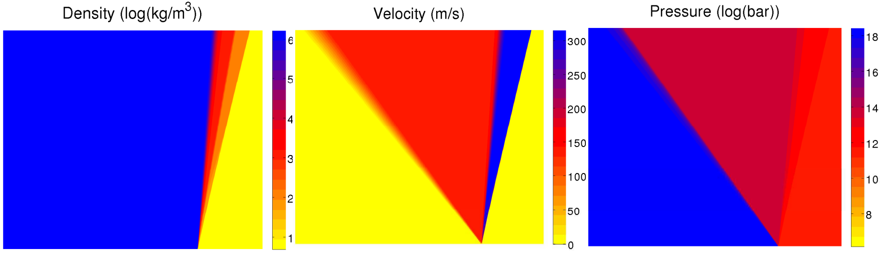


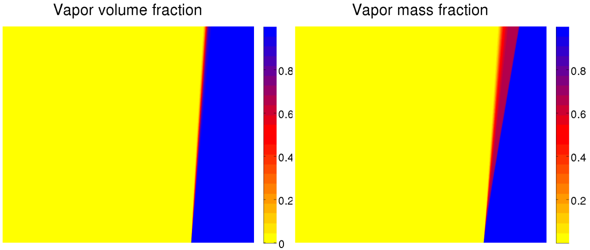
Dodecane 2-phase problem: Sample solution



4-wave structure: Rarefaction, contact, phase, shock

Dodecane 2-phase problem: Sample solution





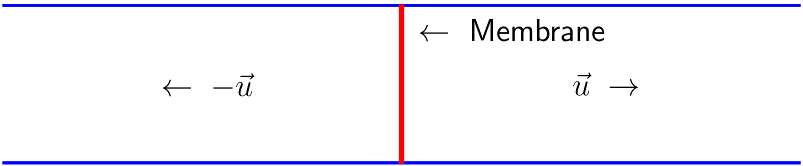
All physical quantities are discon-tinuous across phase boundary

Expansion wave problem: Cavitation test

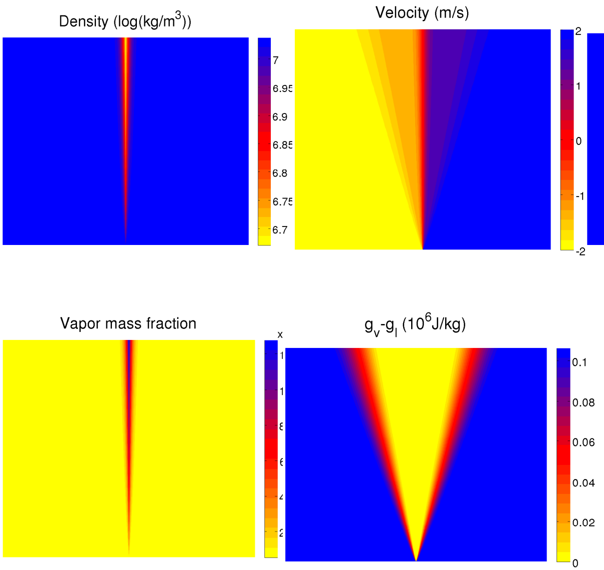
- Liquid-vapor mixture ($\alpha_{\text{vapor}} = 10^{-2}$) for water with

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

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

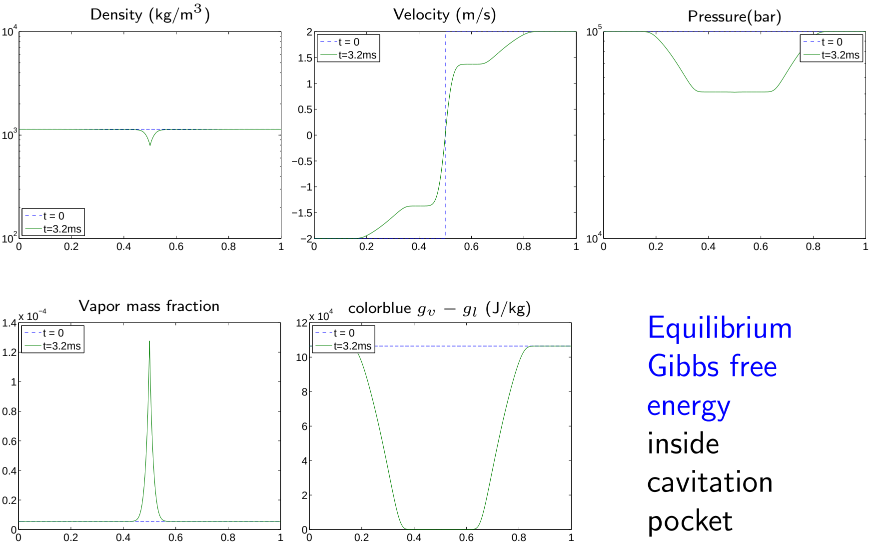


Expansion wave problem: Sample solution



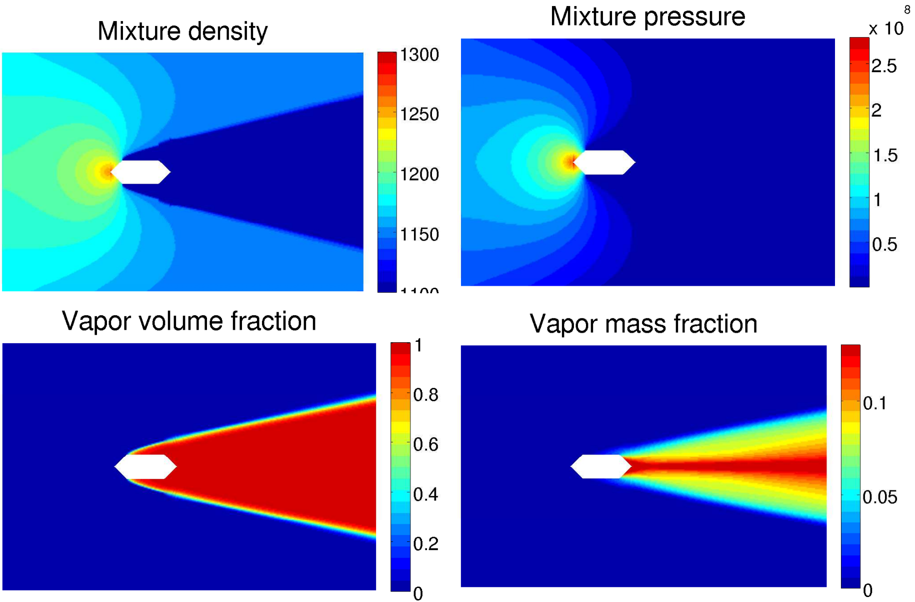
Cavitation pocket formation & mass transfer

Expansion wave problem: Sample solution



Equilibrium Gibbs free energy inside cavitation pocket

High-speed underwater projectile



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

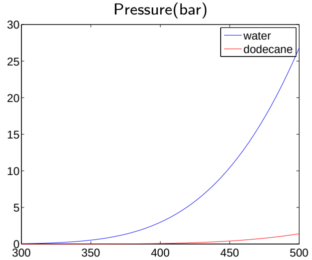
or, from $dg_1 = dg_2$, we get Clausius-Clapeyron equation

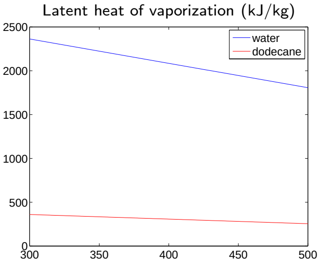
$$\frac{dp(T)}{dT} = \frac{L_h}{T(v_2 - v_1)}$$

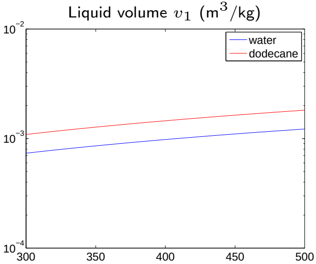
$L_h = T(s_2 - s_1)$: latent heat of vaporization

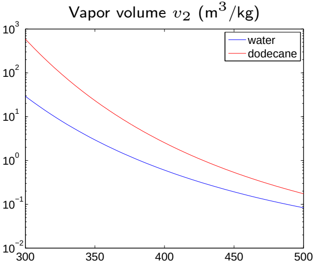
Metastable fluid: Saturation curves (Cont.)

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









Compressible 2-phase flow: 6-equation model

6-equation single-velocity 2-phase model with stiff mechanical relaxation of Saurel *et al.* (JCP 2009) reads

$$
\begin{aligned}
&\partial_t\left(\alpha_1\rho_1\right)+\nabla\cdot\left(\alpha_1\rho_1\vec{u}\right)=0\\
&\partial_t\left(\alpha_2\rho_2\right)+\nabla\cdot\left(\alpha_2\rho_2\vec{u}\right)=0\\
&\partial_t(\rho\vec{u})+\nabla\cdot\left(\rho\vec{u}\otimes\vec{u}\right)+\nabla\left(\alpha_1p_1+\alpha_2p_2\right)=0\\
&\partial_t\left(\alpha_1\rho_1e_1\right)+\nabla\cdot\left(\alpha_1\rho_1e_1\vec{u}\right)+\alpha_1p_1\nabla\cdot\vec{u}=\mu p_I\left(p_2-p_1\right)\\
&\partial_t\left(\alpha_2\rho_2e_2\right)+\nabla\cdot\left(\alpha_2\rho_2e_2\vec{u}\right)+\alpha_2p_2\nabla\cdot\vec{u}=\mu p_I\left(p_1-p_2\right)\\
&\partial_t\alpha_1+\vec{u}\cdot\nabla\alpha_1=\mu\left(p_1-p_2\right)
\end{aligned}
$$

- μ: relaxation parameter for volume-transfer rate as $p_1\to p_2$; assume stiff $\mu\to\infty$ limit
- p_I: interfacial pressure,

$$p_I=\frac{p_1/Z_1+p_2/Z_2}{1/Z_1+1/Z_2},\quad Z_i=\rho_ic_i$$

6-equation model (Cont.)

- Include conservation of mixture total energy also

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

for purpose of maintaining numerical conservation of total energy

- Phasic entropy equations for s_k are

$$\alpha_k \rho_k T_k \frac{ds_k}{dt} = \mu \left(p_1 - p_2\right)^2 \frac{Z_k}{Z_1 + Z_2} \geq 0 \qquad \text{for } k = 1, 2,$$

yielding nonnegative variation of mixture entropy $s = Y_1 s_1 + Y_2 s_2$

- Model is hyperbolic with monotone speed of sound c_f as

$$c_f^2 = Y_1 c_1^2 + Y_2 c_2^2, \qquad Y_k = \frac{\alpha_k \rho_k}{\rho}$$

6-equation model: Reduced model

6-equation model approaches to reduced 5-equation model asymptotically as $\mu \to \infty$

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

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-monotone sound speed c_p:

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

6-equation model: Reduced model (Cont.)

- Volume-fraction equation is differential form of pressure equilibrium condition

$$p_1\left(\rho_1, s_1\right) = p_2\left(\rho_2, s_2\right)$$

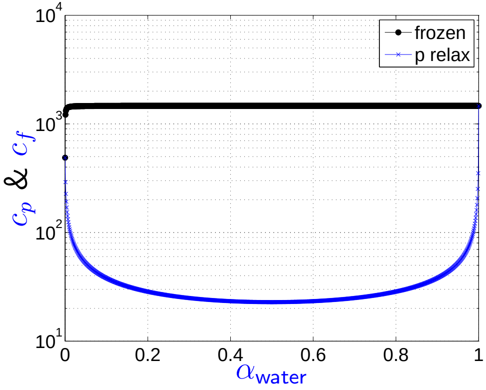
Assume $K = \left(\rho_2 c_2^2 - \rho_1 c_1^2\right) / \left(\rho_1 c_1^2/\alpha_1 + \rho_2 c_2^2/\alpha_2\right) < 0$, *i.e.*, $\rho_2 c_2^2 < \rho_1 c_1^2$ (phase 1 less compressible)

- Compaction effect $(K\ \nabla \cdot \vec{u} > 0)$
  α_1 increases when $\nabla \cdot \vec{u} < 0$ (compression or shock waves)
- Relaxation effect $(K\ \nabla \cdot \vec{u} < 0)$
  α_1 decreases when $\nabla \cdot \vec{u} > 0$ (expansion waves)
- No effect
  α_1 remains unchanged when $\nabla \cdot \vec{u} = 0$ (contacts)

p relaxation: Subcharacteristic condition

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

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



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

6-equation model: Phasic-total-energy-based

Alternative 6-equation model based on phasic total energy is

$$
\begin{aligned}
&\partial_t\left(\alpha_1\rho_1\right)+\nabla\cdot\left(\alpha_1\rho_1\vec{u}\right)=0\\
&\partial_t\left(\alpha_2\rho_2\right)+\nabla\cdot\left(\alpha_2\rho_2\vec{u}\right)=0\\
&\partial_t\left(\rho\vec{u}\right)+\nabla\cdot\left(\rho\vec{u}\otimes\vec{u}\right)+\nabla\left(\alpha_1p_1+\alpha_2p_2\right)=0\\
&\partial_t\left(\alpha_1E_1\right)+\nabla\cdot\left(\alpha_1E_1\vec{u}+\alpha_1p_1\vec{u}\right)+\mathcal{B}\left(q,\nabla q\right)=\mu p_I\left(p_2-p_1\right)\\
&\partial_t\left(\alpha_2E_2\right)+\nabla\cdot\left(\alpha_2E_2\vec{u}+\alpha_2p_2\vec{u}\right)-\mathcal{B}\left(q,\nabla q\right)=\mu p_I\left(p_1-p_2\right)\\
&\partial_t\alpha_1+\vec{u}\cdot\nabla\alpha_1=\mu\left(p_1-p_2\right)
\end{aligned}
$$

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

$$\mathcal{B}=\vec{u}\cdot\left[Y_1\nabla\left(\alpha_2p_2\right)-Y_2\nabla\left(\alpha_1p_1\right)\right]$$

Model is hyperbolic with monotonic speed of sound c_f as well & is basis for mixture-energy-consistent method

6-equation model (Cont.)

6-equation model in compact form

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

where

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

Relaxation scheme

Fractional-step method is employed to solve 6-equation model

That is,

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 mechanical relaxation step
   Solve system of ordinary differential equations

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

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

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

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

Integrating latter two equations with respect to time

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

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

$$\Longrightarrow \quad e_k - e_k^0 = -\bar{p}_I\left(1/\rho_k - 1/\rho_k^0\right)$$ (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, $k = 1, 2$

Combining that with saturation condition for volume fraction

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

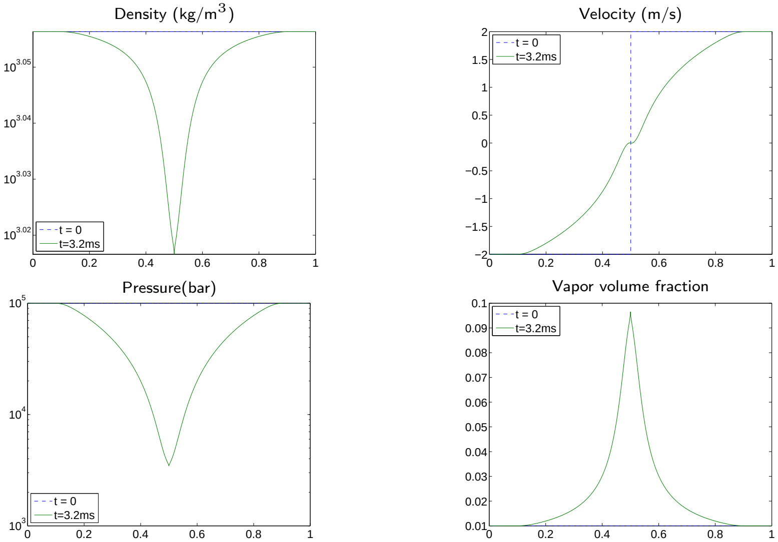
leads to algebraic equation (quadratic one with SG EOS) for relaxed pressure p

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

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

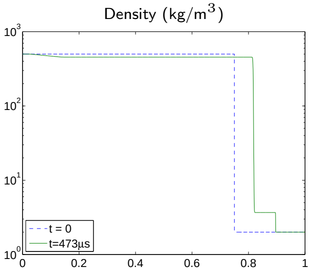
Expansion wave problem: p relaxation

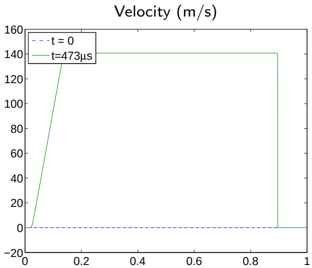
Mechanical-equilibrium solution at $t = 3.2$ms

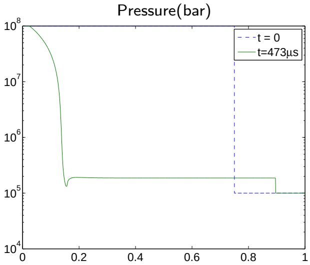


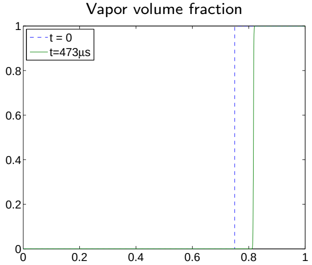
Dodecane 2-phase Riemann problem: p relaxation

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









6-equation model: With heat & mass transfer

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

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

Assume $Q = \theta \left(T_2 - T_1\right)$, $\qquad \dot{m} = \nu \left(g_2 - g_1\right)$

6-equation with heat & mass transfer (Cont.)

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

1. Volume transfer via pressure relaxation: $\mu\left(p_1 - p_2\right)$
   - 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: $\theta\left(T_2 - T_1\right)$
   - θ expresses rate towards thermal equilibrium $T_1 \to T_2$,
3. Mass transfer via thermo-chemical relaxation: $\nu\left(g_2 - g_1\right)$
   - ν expresses rate towards diffusive equilibrium $g_1 \to g_2$, & is nonzero only at 2-phase mixture & metastable state $T_{\text{liquid}} > T_{\text{sat}}$

6-equation with heat & mass transfer (Cont.)

Modified 6-equation model in compact form

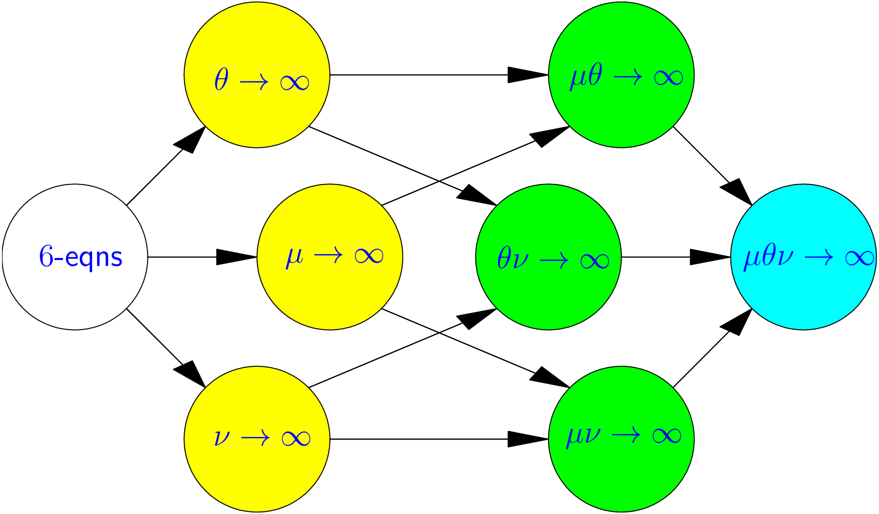
$$\partial_t q + \nabla \cdot f(q) + w\left(q, \nabla q\right) = \psi_\mu(q) + \psi_\theta(q) + \psi_\nu(q)$$

where

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

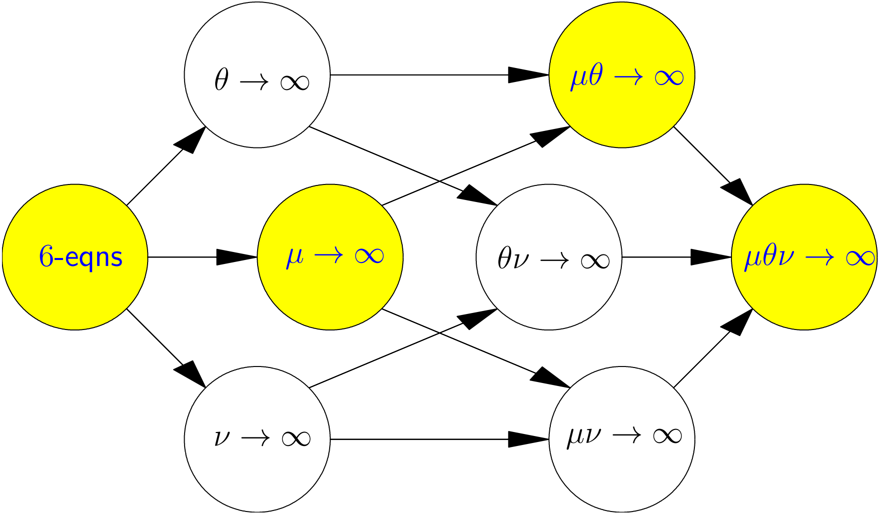
6-equation with heat & mass transfer (Cont.)

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



6-equation with heat & mass transfer (Cont.)

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



Relaxation scheme: With heat & mass transfer

Continue from previous algorithm for 6-equation model with stiff mechanical relaxation, 2 sub-steps are included

3. Stiff thermal relaxation step
   Solve system of ordinary differential equations

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

4. Stiff thermo-chemical relaxation step
   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

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)

Stiff thermal relaxation step

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

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

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

$$\begin{aligned}
\partial_t\left(\alpha_1\rho_1\right) &= 0 &\Longrightarrow\quad& \alpha_1\rho_1 = \alpha_1^0\rho_1^0\\
\partial_t\left(\alpha_2\rho_2\right) &= 0 &\Longrightarrow\quad& \alpha_2\rho_2 = \alpha_2^0\rho_2^0\\
\partial_t\left(\rho\vec{u}\right) &= 0 &\Longrightarrow\quad& \rho\vec{u} = \rho^0\vec{u}^0\\
\partial_t\left(\alpha_k E_k\right) &= \frac{\theta}{q_I}\left(T_2 - T_1\right) &\Longrightarrow\quad& \partial_t\left(\alpha\rho e\right)_k = q_I\partial_t\alpha_k
\end{aligned}$$

Integrating latter two equations with respect to time

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

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

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:

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

Reduced model: Thermal relaxation step

Reduced model after thermal relaxation step is (Saurel *et al.* 2008, Flåtten *et al.* 2010)

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

- Mixture entropy ρs satisfy

$$\partial_t (\rho s) + \nabla \cdot (\rho s \vec{u}) = \theta \left(1 + \frac{p_{eq}}{q_I}\right) \frac{(T_2 - T_1)^2}{T_1 T_2} \geq 0$$

- Mechanical-thermal equilibrium sound speed c_{pT} satisfies

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

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

Reduced model: Thermo-chemical relaxation step

Reduced model after thermo-chemical relaxation 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

- Mixture entropy ρs satisfies

$$\partial_t (\rho s) + \nabla \cdot (\rho s \vec{u}) = \nu \frac{(g_2 - g_1)^2}{T_{eq}} \geq 0$$

- Speed of sound c_{pTg} satisfies

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

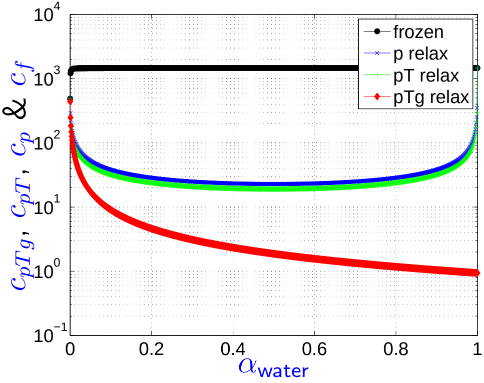
Equilibrium speed of sound: Comparison

- Sound speeds follow subcharacteristic condition

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

- 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

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

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

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

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

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

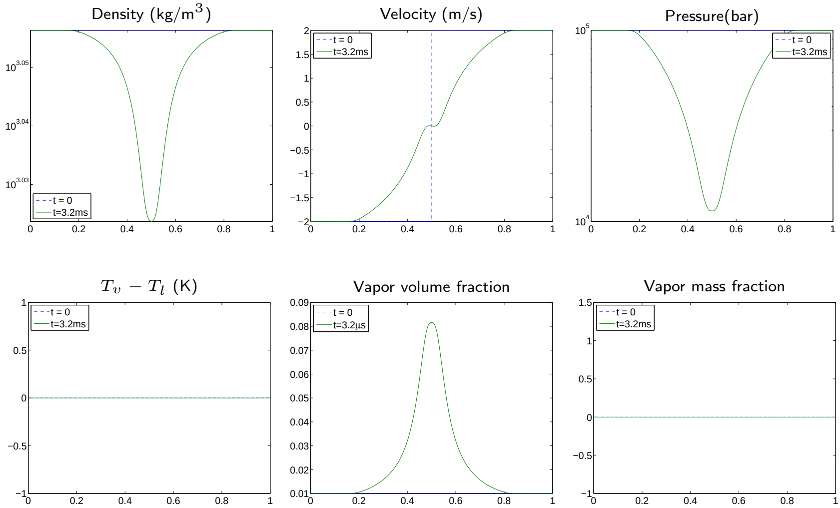
$$\bar{K}_s = \left(\frac{\alpha_1}{K_s^1} + \frac{\alpha_2}{K_s^2}\right)^{-1}, \quad K_s^\iota = \rho_\iota c_\iota^2$$

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

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

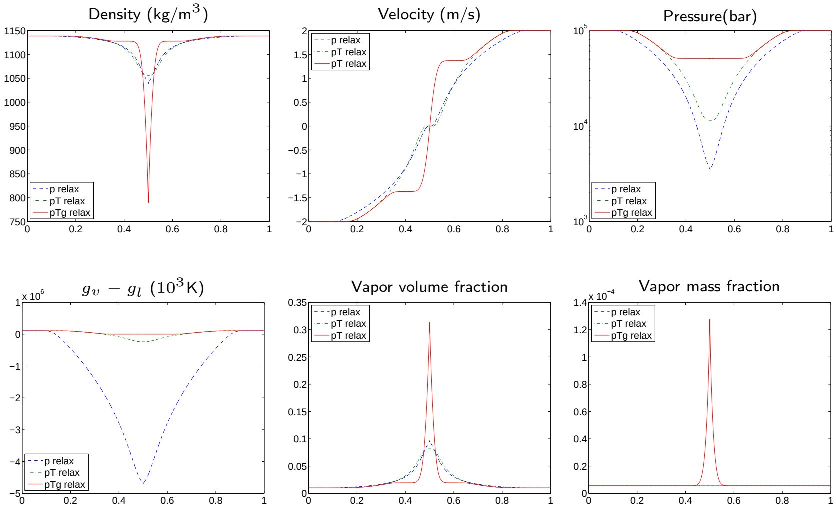
Expansion wave problem: p-pT relaxation

Mechanical-thermal-equilibrium solution at $t = 3.2$ms

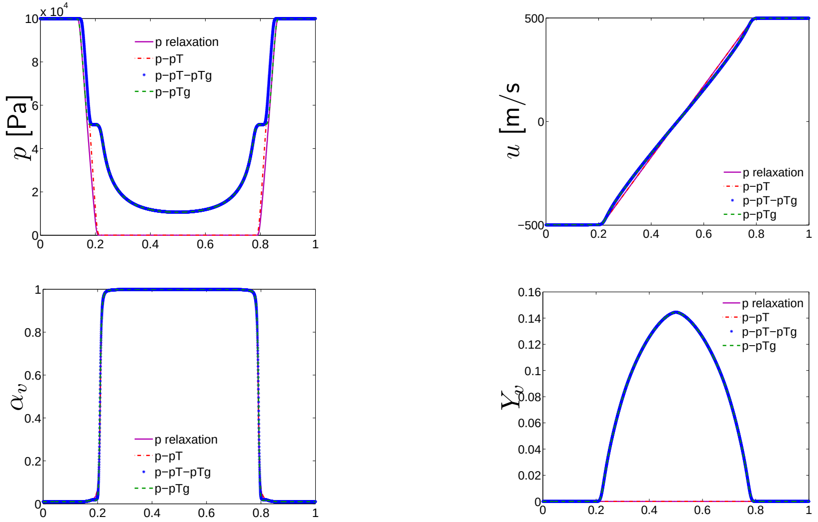


Expansion wave problem (Cont.)

Comparison p-, pT- & p-pTg-relaxation solution at $t = 3.2$ms

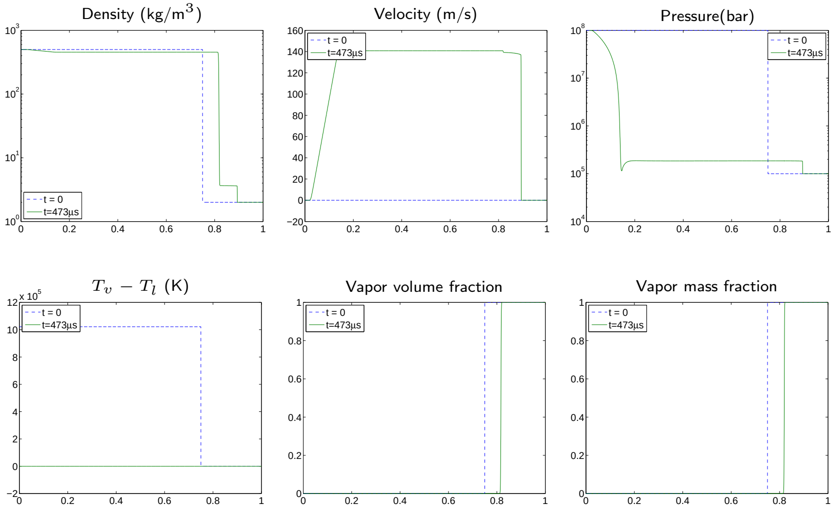


Expansion wave problem: $\vec{u} = 500\mathrm{m/s}$



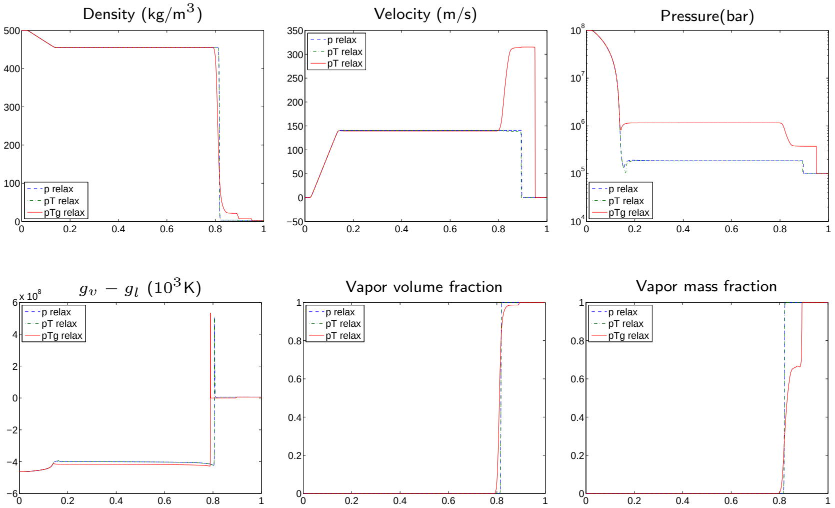
Dodecane 2-phase problem: p-pT relaxation

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



Dodecane 2-phase Riemann problem (Cont.)

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



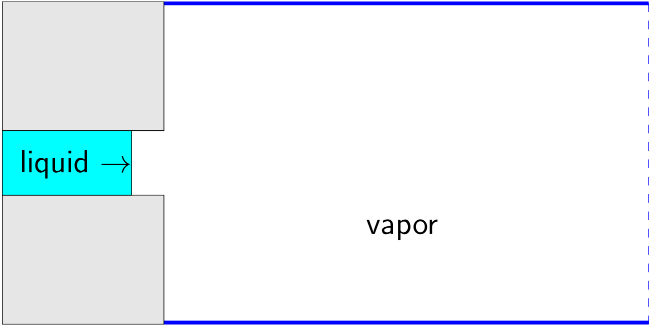
High-pressure fuel injector

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

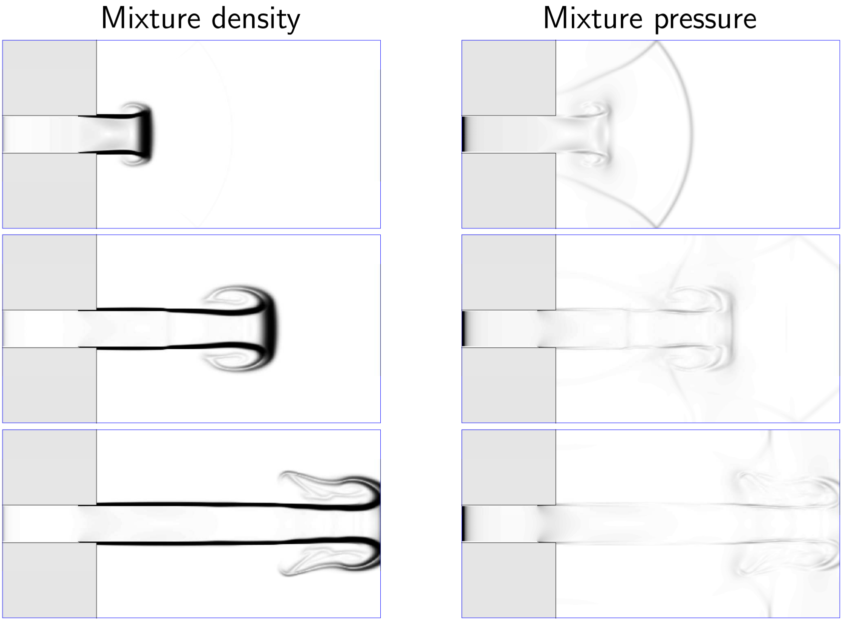
- Pressure & temperature are in equilibrium with
  $p = 10^8$ Pa & $T = 640K$

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

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

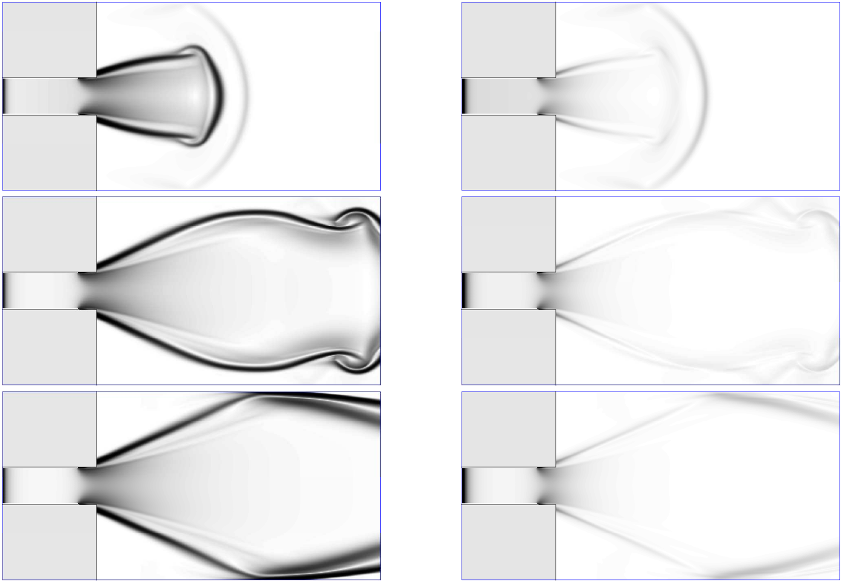


High-pressure fuel injector: $\alpha_{v,l} = 10^{-4}$



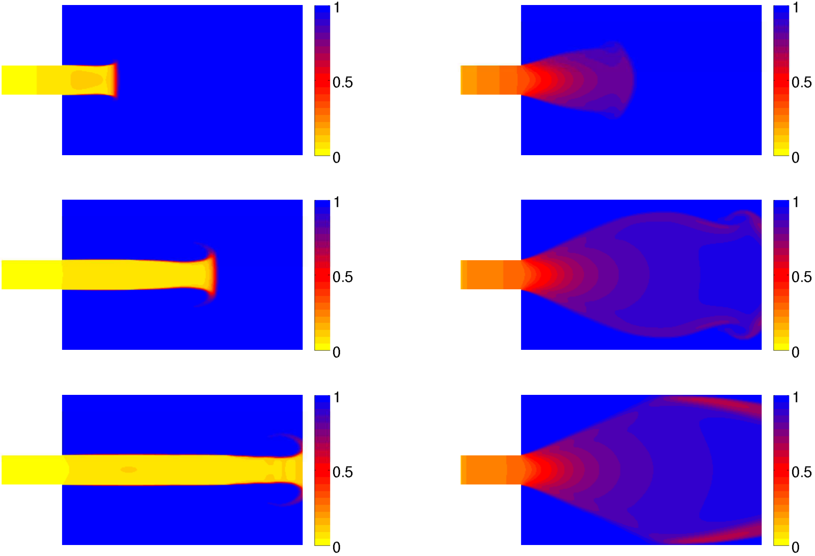
High-pressure fuel injector: $\alpha_{v,l} = 10^{-2}$

Mixture density | Mixture pressure



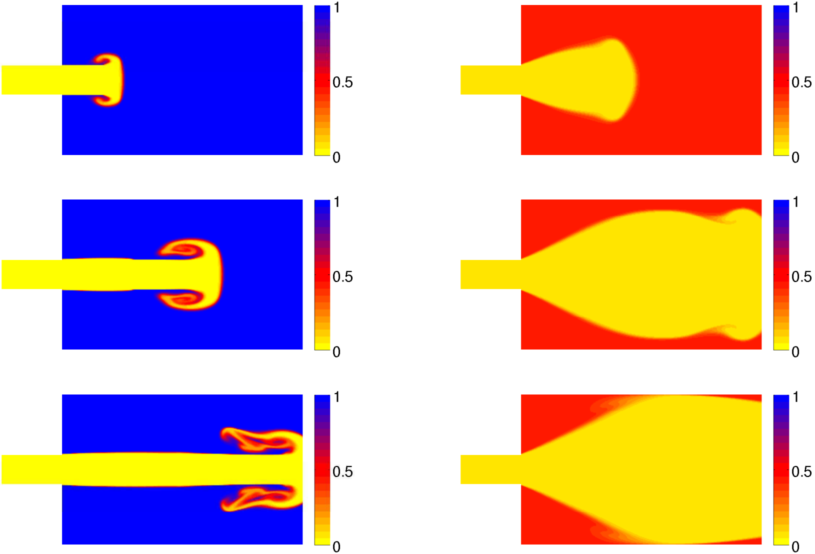
High-pressure fuel injector (Cont.)

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



High-pressure fuel injector (Cont.)

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



High-pressure fuel injector: Remark

Numerical solver (to be discussed) uses

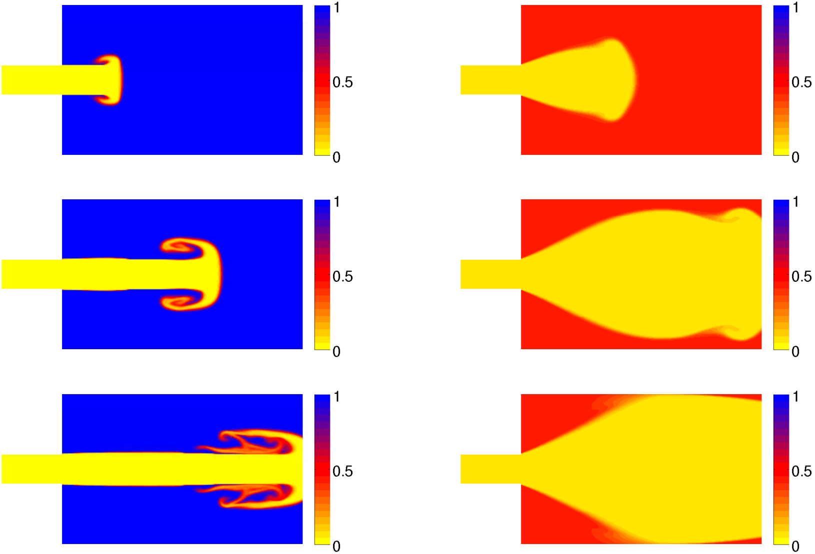
- 400×200 uniform Cartesian grid
- 6-equation single-velocity two-phase model with stiff mechanical relaxation
- Consitutive law is stiffened gas equation of state
- Model is solved in stiff limit towards equilibrium pressure $p_{\text{liquid}} = p_{\text{vapor}}$, while admitting different temperatures $T_{\text{liquid}} \neq T_{\text{vapor}}$ & entropies $s_{\text{liquid}} \neq s_{\text{vapor}}$

Observation:

- Higher $\alpha_{v,l}$ in fluid mixture, higer volume transfer expansion (Is this correct statement ? If so, to what extent)

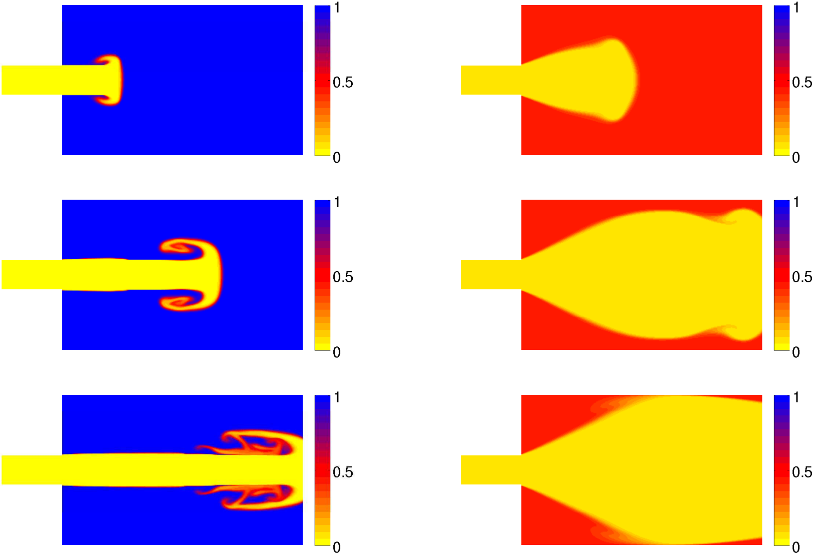
Fuel injector: p-pT relaxation

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



Fuel injector: p-pT-pTg relaxation

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



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Thank you