Homogeneous relaxation models & methods for compressible two-phase flow

I: Reduced models

Keh-Ming Shyue

Institute of Applied Mathematical Sciences
National Taiwan University

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

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. Homogeneous relaxation model (HRM) for compressible 2-phase flow with & without heat & mass transfer
4. Reduced 5-, 4-, & 3-equation model of HRM

Flashing flow means a flow with dramatic evaporation of liquid due to pressure drop

Outline

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

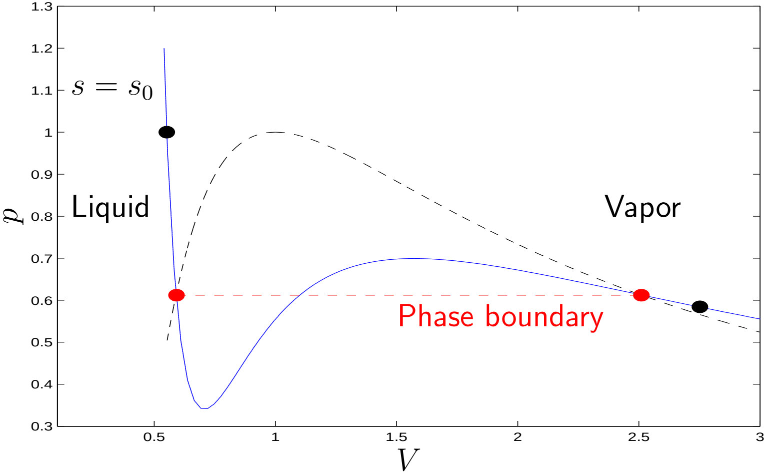
1. Motivation
2. Constitutive law for metastable fluid
3. Homogeneous relaxation model (HRM) for compressible 2-phase flow with & without heat & mass transfer
4. Reduced 5-, 4-, & 3-equation model of HRM

Flashing flow means a flow with dramatic evaporation of liquid due to pressure drop

Numerical solver of relaxation type will be discussed in next lecture

Phase transition: Thermodynamic path I

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



Phase transition: Thermodynamic path II

Figure extracted from Saurel *et al.* (JFM 2008)

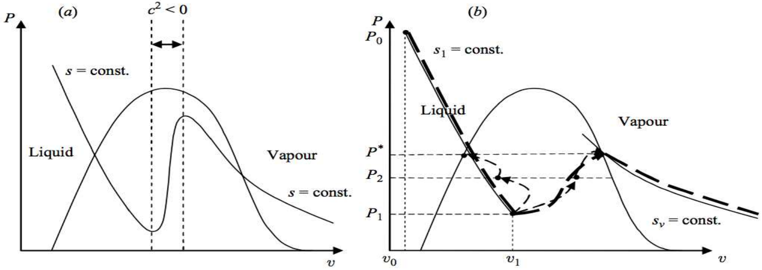


FIGURE 7. Schematic representation of the thermodynamic path using a cubic EOS compared to the kinetic process represented in dashed lines. *(a)* With the cubic EOS, hyperbolicity is lost in the spinodal zone. *(b)* The present model consists of using a kinetic transformation to connect the isentropes of liquid and vapour. As no thermodynamic path is involved, the mixture sound speed is always defined. In the kinetic approach, from a metastable liquid (end of liquid isentrope) non-equilibrium vapour and liquid are produced at constant specific volume for the mixture. Vapour production makes the pressure increase. During kinetic evolution the non-equilibrium points of liquid and vapour move in the direction of saturation curves. At each non-equilibrium state pressure equilibrium is assumed. When thermodynamic equilibrium is reached, liquid and vapour states are located on saturation curves. Then, if the specific volume is increased, the equilibrium concentration evolves and as limit case, the vapour expands along an isentrope starting from the saturation curve. Note that when the various non-equilibrium states are omitted, the global transformation path (the bold dashed line), composed of two thermodynamic paths and a kinetic one, gives a transformation very closed to that of van der Waals. The main difference is that ill-posedness issues have been removed.

Dodecane 2-phase Riemann problem

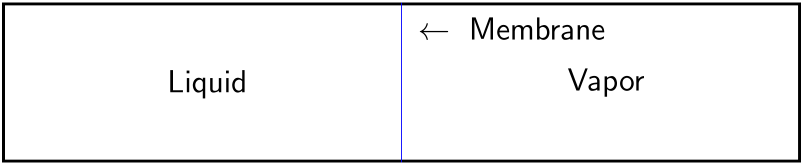
Saurel *et al.* (JFM 2008) & Zein *et al.* (JCP 2010):

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

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

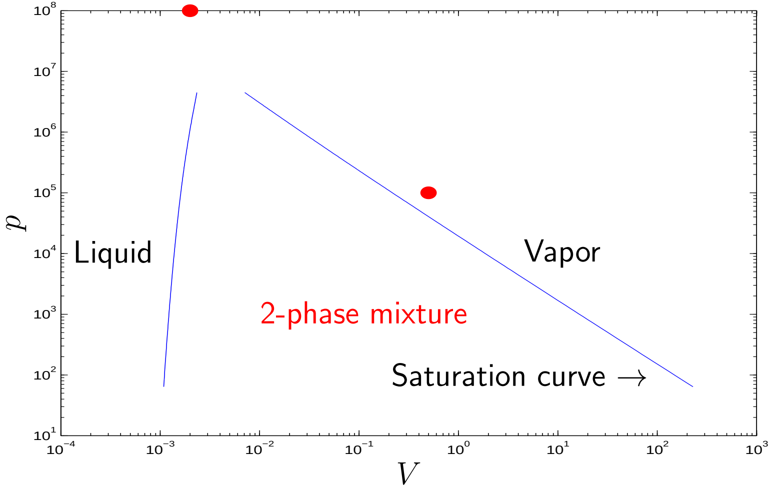
- Vapor phase: Right-hand side ($0.75\text{m} < x \leq 1$m)

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



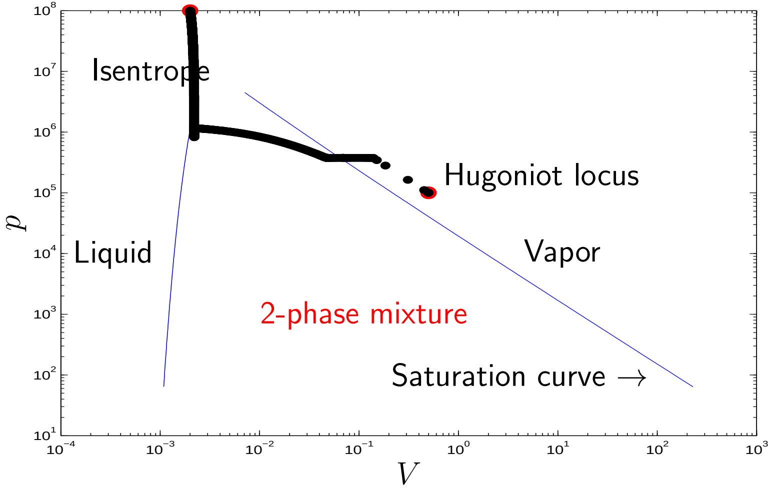
Dodecane 2-phase problem: Phase diagram

Initial condition in p-V phase diagram



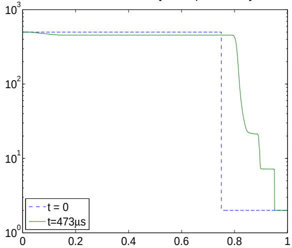
Dodecane 2-phase problem: Phase diagram

Thermodynamic path in p-V phase diagram

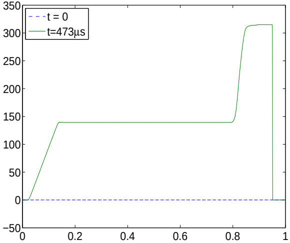


Dodecane 2-phase problem: Sample solution

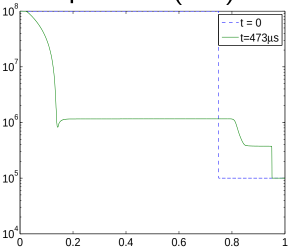
density (kg/m^3)



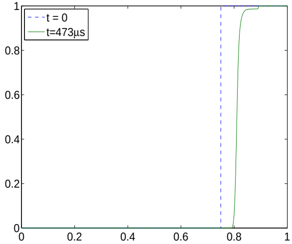
velocity (m/s)



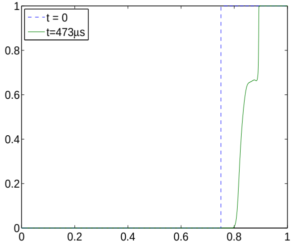
pressure(bar)



vapor volume fraction

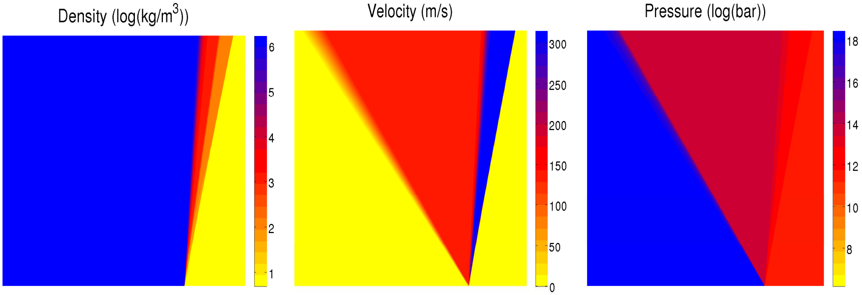


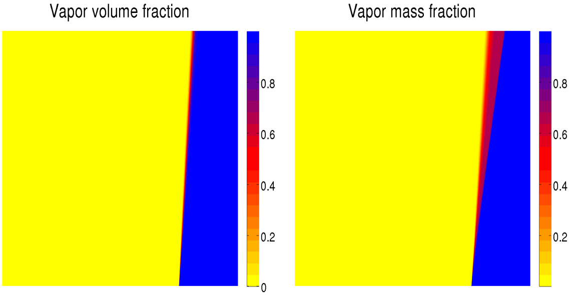
vapor mass fraction



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

Dodecane 2-phase problem: Sample solution





All physical quantities are discon- tinuous across phase boundary

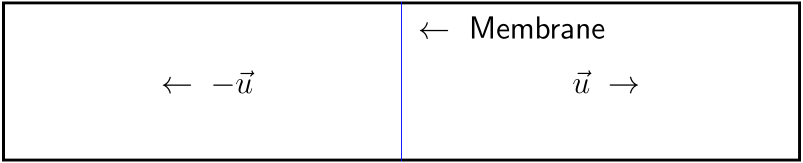
Expansion wave problem: Cavitation test

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

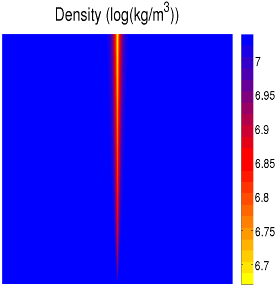
- Liquid-vapor mixture ($\alpha_{\text{vapor}} = 10^{-2}$) for water with

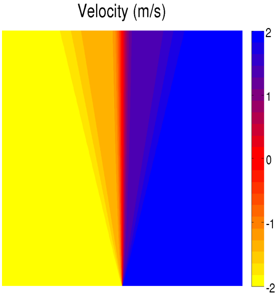
$$p_{\text{liquid}} = p_{\text{vapor}} = 1\text{bar}$$
$$T_{\text{liquid}} = T_{\text{vapor}} = 354.7284\text{K} < T^{\text{sat}}$$
$$\rho_{\text{vapor}} = 0.63\text{kg/m}^3 > \rho^{\text{sat}}_{\text{vapor}}, \quad \rho_{\text{liquid}} = 1150\text{kg/m}^3 > \rho^{\text{sat}}_{\text{liquid}}$$
$$g^{\text{sat}}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

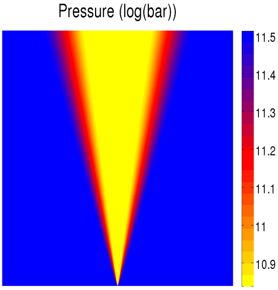
- Outgoing velocity $u = 2\text{m/s}$

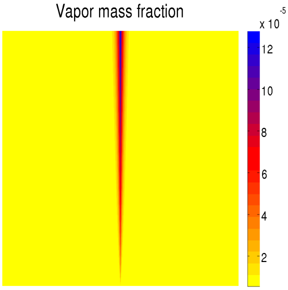


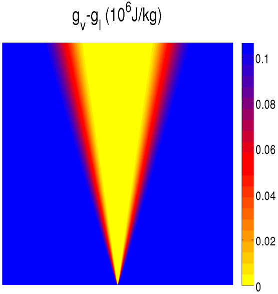
Expansion wave problem: Sample solution







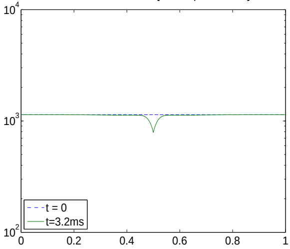




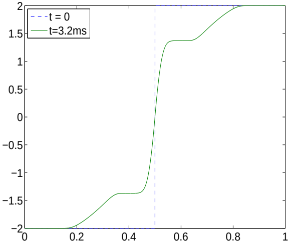
Cavitation pocket formation & mass transfer

Expansion wave problem: Sample solution

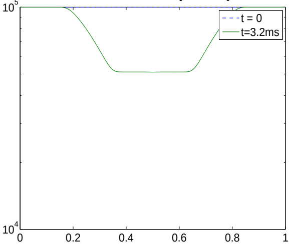
density $(\mathrm{kg/m^3})$



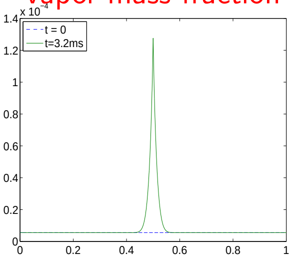
velocity $(\mathrm{m/s})$



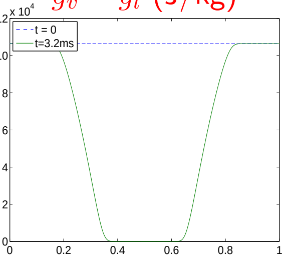
pressure(bar)



vapor mass fraction



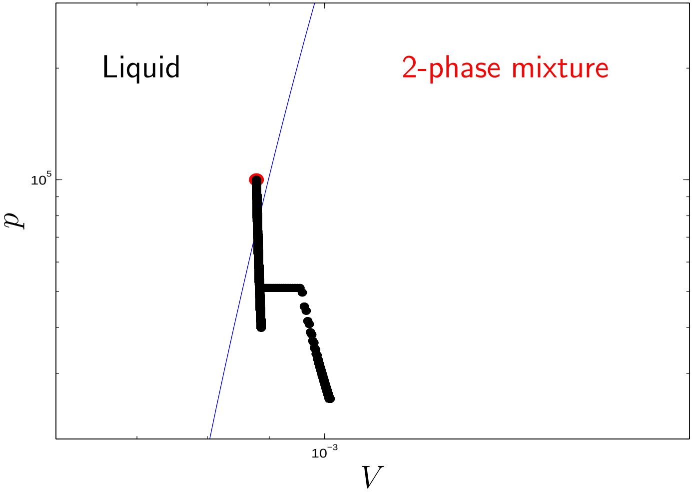
$g_v - g_l$ (J/kg)



Equilibrium Gibbs free energy inside cavitation pocket

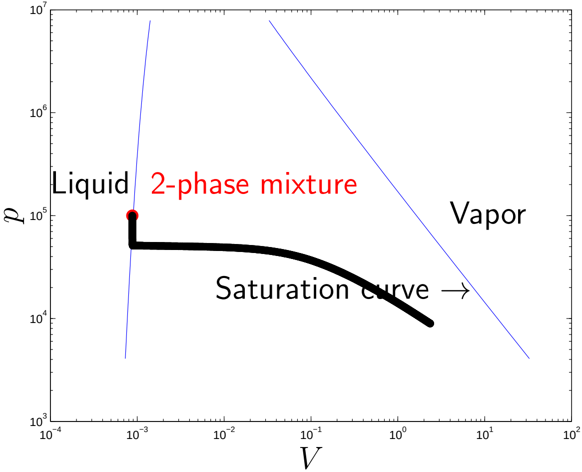
Expansion wave problem: Phase diagram

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



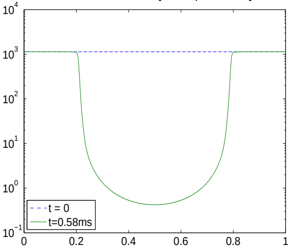
Expansion wave $\vec{u} = 500\mathrm{m/s}$: Phase diagram

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

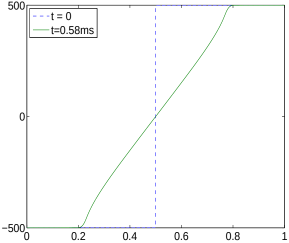


Expansion wave $\vec{u} = 500\mathrm{m/s}$: Sample solution

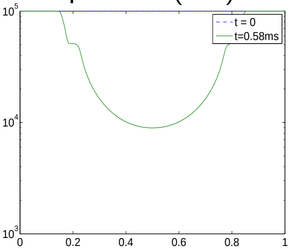
density $(\mathrm{kg/m^3})$



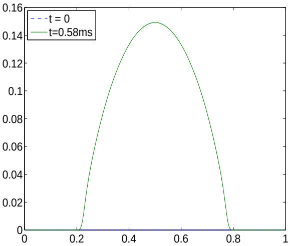
velocity $(\mathrm{m/s})$



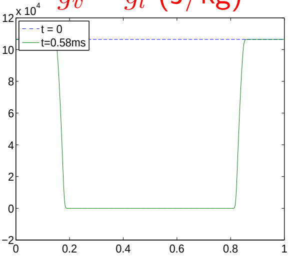
pressure(bar)



vapor mass fraction



$g_v - g_l$ (J/kg)



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 $g_k = a_k + p_k V_k$

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 · K))	0	-23.4×10^3
C_v (J/(kg · 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 · K))	0	-24.4×10^3
C_v (J/(kg · K))	1077.7	1956.45

Metastable fluid: Saturation curve

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

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

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

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

Metastable fluid: Saturation curve

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

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

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

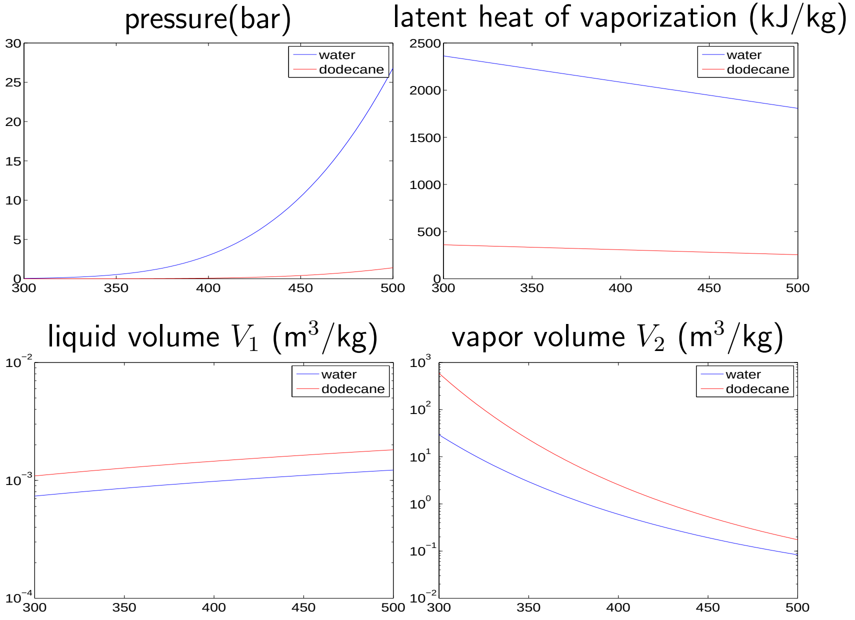
$$C = \frac{C_{p2} - C_{p1}}{C_{p2} - C_{v2}}, \qquad D = \frac{C_{p1} - C_{v1}}{C_{p2} - C_{v2}}$$

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

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



Homogeneous relaxation model: 2-phase case

Consider 1-velocity homogeneous relaxation model (HRM) for compressible 2-phase flow of form

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

$\Sigma(w,\nabla w)$ is non-conservative product (w: state vector)

$$
\Sigma = \vec{u}\cdot\left[Y_1\nabla(\alpha_2 p_2) - Y_2\nabla(\alpha_1 p_1)\right], \quad Y_k = \frac{\alpha_k\rho_k}{\rho}
$$

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

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)

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

- 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)

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

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

HRM model in compact form

$$\partial_t w + \nabla \cdot f(w) + \mathcal{B}\left(w, \nabla w\right) = \psi_\mu(w) + \psi_\theta(w) + \psi_\nu(w)$$

where

$$w = \left[\alpha_1,\ \alpha_1\rho_1,\ \alpha_2\rho_2,\ \rho\vec{u},\ \alpha_1\rho_1 E_1,\ \alpha_2\rho_1 E_2,\ \alpha_1\right]^T$$

$$f = \Big[\alpha_1\rho_1\vec{u},\ \alpha_2\rho_2\vec{u},\ \rho\vec{u}\otimes\vec{u} + (\alpha_1 p_1 + \alpha_2 p_2)\overline{\overline{I}},$$
$$\alpha_1\left(\rho_1 E_1 + p_1\right)\vec{u},\ \alpha_2\left(\rho_2 E_2 + p_2\right)\vec{u},\ 0\Big]^T$$

$$\mathcal{B} = \left[0,\ 0,\ 0,\ \Sigma\left(w, \nabla w\right),\ -\Sigma\left(w, \nabla w\right),\ \vec{u}\cdot\nabla\alpha_1\right]^T$$

$$\psi_\mu = \left[0,\ 0,\ 0,\ \mu p_I\left(p_2 - p_1\right),\ \mu p_I\left(p_1 - p_2\right),\ \mu\left(p_1 - p_2\right)\right]^T$$

$$\psi_\theta = \left[0,\ 0,\ 0,\ \theta T_I\left(T_2 - T_1\right),\ \theta T_I\left(T_1 - T_2\right),\ 0\right]^T$$

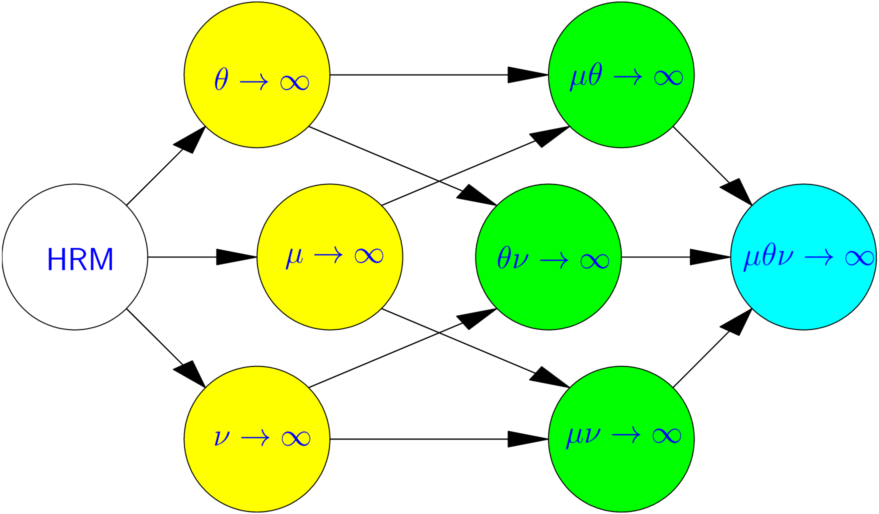
$$\psi_\nu = \Big[\nu\left(g_2 - g_1\right),\ \nu\left(g_1 - g_2\right),\ 0,\ \nu g_I\left(g_2 - g_1\right),$$
$$\nu g_I\left(g_1 - g_2\right),\ \nu v_I\left(g_1 - g_2\right)\Big]^T$$

HRM: Mathematical structure

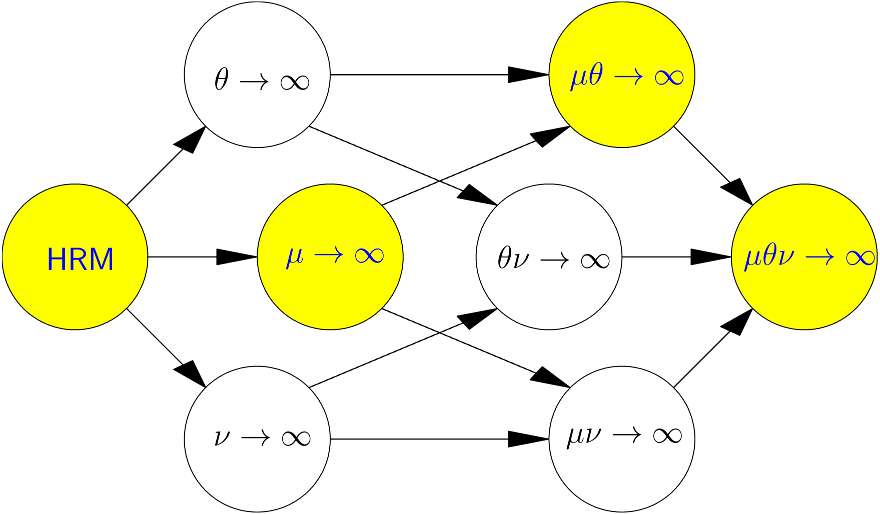
- Balance Laws with non-conservative products
  - Classical Rankine-Hugoniot conditions for discontinuous solutions need to be modified
- Stiff relaxation terms
- Model is hyperbolic when physical states lie in region of thermodynamic stability
- Reduced model when $\mu \to 0$, $\theta \to 0$, $\nu \to 0$, or $\mu \to \infty$, $\theta \to \infty$, $\nu \to \infty$ is popular in practice

Homogeneous relaxation model: Hierarchy

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



Sequence of HRM limits we considered are $\mu \to \infty$, $\mu\theta \to \infty$, & $\mu\theta\nu \to \infty$



HRM: with pressure relaxation only

Assumes frozen thermal & chemical relaxation, *i.e.*, $\theta = 0$ & $\nu = 0$, HRM becomes 2-pressure volume-transfer model with pressure relaxation

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

That is, model written in compact form

$$
\partial_t w + \nabla \cdot f(w) + \mathcal{B}(w, \nabla w) = \psi_\mu(w)
$$

Reduced 5-equation model: HRM with pressure relaxation $\mu \to \infty$, $\theta = 0$ & $\nu = 0$

Assume $\mu = 1/\varepsilon$ & apply formal asymptotic analysis to HRM with stiff pressure relaxation term, Murrone & Guillard (JCP 2005) proved as $\varepsilon \to 0$ leading order approximation is

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

Mixture pressure $p = p(\rho e, \rho_1, \rho_2, \alpha_1)$ determined from

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

Reduced 5-equation model: Entropy transport

1. It can be shown entropy of each phase s_k now satisfies

$$\frac{Ds_k}{Dt} = \partial_t s_k + \vec{u} \cdot \nabla s_k = 0, \quad \text{for} \quad k = 1, 2$$

2. Since product $\alpha_1 \alpha_2$ is expected to be small, Shyue (JCP 1998), Allaire, Clerc, & Kokh (JCP 2002) proposed to use

$$\partial_t \alpha_1 + \vec{u} \cdot \nabla \alpha_1 = 0$$

yielding so-called 5-equation transport model

In this case phase entropies follow

$$\left(\frac{\partial p_1}{\partial s_1}\right)_{\rho_1} \frac{Ds_1}{Dt} - \left(\frac{\partial p_2}{\partial s_2}\right)_{\rho_2} \frac{Ds_2}{Dt} = \left(\rho_1 c_1^2 - \rho_2 c_2^2\right) \nabla \cdot \vec{u}$$

Reduced 5-equation model: Mixture EOS convexity

Define specific volume of mixture V as

$$V = Y_1 V_1 + Y_2 V_2$$

Y_k remains constant across compression waves & each phase follows its own isentropic curves $Ds_k/Dt = 0$ for $k = 1, 2$

From second thermodynamic law $de_k = T ds_k - p dV_k$, we have

$$de_k(p, V_k) + p dV_k = 0 \quad \Longrightarrow \quad V_k(p)$$

Derivatives of specific volume with respect to pressure are

$$\frac{dV(p)}{dp} = Y_1 \frac{dV_1(p)}{dp} + Y_2 \frac{dV_2(p)}{dp} < 0 \quad \text{if} \quad \frac{dV_k(p)}{dp} = \frac{-1}{\rho_k c_k^2} < 0$$

$$\frac{d^2V(p)}{dp^2} = Y_1 \frac{d^2V_1(p)}{dp^2} + Y_2 \frac{d^2V_2(p)}{dp^2} > 0 \quad \text{if} \quad \frac{d^2V_k(p)}{dp^2} > 0$$

Mixture compression waves have same qualitative bahavior as single phase compressible flow

Reduced 5-equation model: Volume fraction

Volume-fraction equation can be viewed as differential form of pressure equilibrium condition

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

Reduced 5-equation model: Volume fraction

Volume-fraction equation can be viewed as differential form of pressure equilibrium condition

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

That is, result from differentiating above along fluid trajectory

$$\left(\frac{\partial p_1}{\partial \rho_1}\right)_{s_1} \frac{D\rho_1}{Dt} + \left(\frac{\partial p_1}{\partial s_1}\right)_{\rho_1} \frac{Ds_1}{Dt} = \left(\frac{\partial p_2}{\partial \rho_2}\right)_{s_2} \frac{D\rho_2}{Dt} + \left(\frac{\partial p_2}{\partial s_2}\right)_{\rho_2} \frac{Ds_2}{Dt}$$

Using (i) phase sound speed $c_k^2 = \partial_{\rho_k} p_k$, (ii) phase mass equations

$$\frac{D\rho_k}{Dt} = -\frac{\rho_k}{\alpha_k}\frac{D\alpha_k}{Dt} - \rho_k \nabla \cdot \vec{u}$$

& (iii) isentropic assumption along $Ds_k/Dt = 0$, we get

$$-\frac{\rho_1 c_1^2}{\alpha_1}\frac{D\alpha_1}{Dt} - \rho_1 c_1^2 \nabla \cdot \vec{u} = -\frac{\rho_2 c_2^2}{\alpha_2}\frac{D\alpha_2}{Dt} - \rho_2 c_2^2 \nabla \cdot \vec{u}$$

Rearranging terms & using $\alpha_1 + \alpha_2 = 1$, we find

$$\begin{aligned}\frac{D\alpha_1}{Dt} &= \left(\frac{\rho_2 c_2^2 - \rho_1 c_1^2}{\rho_1 c_1^2/\alpha_1 + \rho_2 c_2^2/\alpha_2}\right) \nabla \cdot \vec{u} \\ &= K \; \nabla \cdot \vec{u}, \qquad \frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{u} \cdot \nabla\end{aligned}$$

Rearranging terms & using $\alpha_1 + \alpha_2 = 1$, we find

$$\begin{aligned} \frac{D\alpha_1}{Dt} &= \left(\frac{\rho_2 c_2^2 - \rho_1 c_1^2}{\rho_1 c_1^2/\alpha_1 + \rho_2 c_2^2/\alpha_2} \right) \nabla \cdot \vec{u} \\ &= K \; \nabla \cdot \vec{u}, \qquad \frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{u} \cdot \nabla \end{aligned}$$

Assume $K < 0$, *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)

Reduced 5-equation model: Subcharacteristic

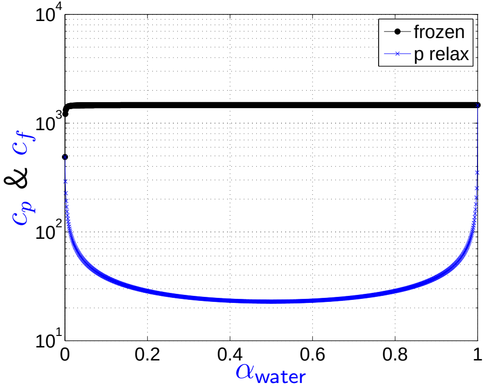
Mechanical equilibrium sound speed $c_p \leq c_f$ (frozen speed)

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

Reduced 5-equation model: Subcharacteristic

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

Reduced 5-equation model: Derivation

Take formal asymptotic expansion ansatz

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

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

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

We get

$$\frac{D}{Dt}\left(p_1^0 + \varepsilon p_1^1 + \cdots\right) + \rho_1 c_1^2 \nabla \cdot \vec{u} = \frac{\rho_1 c_{I1}^2}{\alpha_1}\frac{1}{\varepsilon}\left[\left(p_2^0 - p_1^0\right) + \varepsilon\left(p_2^1 - p_1^1\right) + \cdots\right]$$

$$\frac{D}{Dt}\left(p_2^0 + \varepsilon p_2^1 + \cdots\right) + \rho_2 c_2^2 \nabla \cdot \vec{u} = \frac{\rho_2 c_{I2}^2}{\alpha_2}\frac{1}{\varepsilon}\left[\left(p_1^0 - p_2^0\right) + \varepsilon\left(p_1^1 - p_2^1\right) + \cdots\right]$$

$$\frac{D}{Dt}\left(\alpha_1^0 + \varepsilon\alpha_1^1 + \cdots\right) = \frac{1}{\varepsilon}\left[\left(p_1^0 - p_2^0\right) + \varepsilon\left(p_1^1 - p_2^1\right) + \cdots\right]$$

Collecting equal power of ε, we have

- $O(1/\varepsilon)$

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

- $O(1)$

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

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 4-equation model

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)

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

Model closure: isobaric-isothermal,*i.e.*, p & T equilibrium

Mechanical-thermal equilibrium speed of sound satisfies

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

Model closure: pT equilibrium solution

With stiffened gas EOS, it follows from

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

that we have

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

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

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

Reduced 3-equation model

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

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

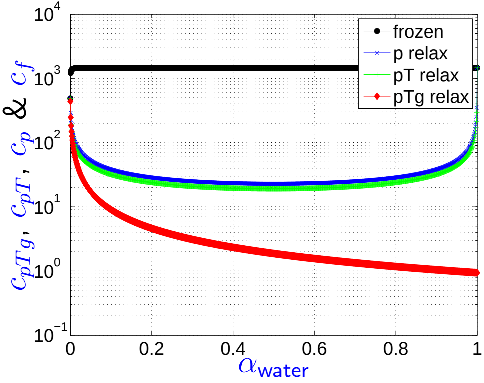
Equilibrium speed of sound: Comparison

- 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

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

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

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

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

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

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

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

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

Reduced model: Remarks

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

Reduced model: Remarks

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

2. 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

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

To ensure conservation of mixture total energy include

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

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.*,

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

Phase tranition models: Summary

1. 7-equation model (Baer-Nunziato type)
   - Zein, Hantke, Warnecke (JCP 2010)
2. Reduced 5-equation model (Kapila *et al.* type)
   - Saurel, Petitpas, Berry (JFM 2008)
3. Homogeneous 4- or 6-equation relaxation 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