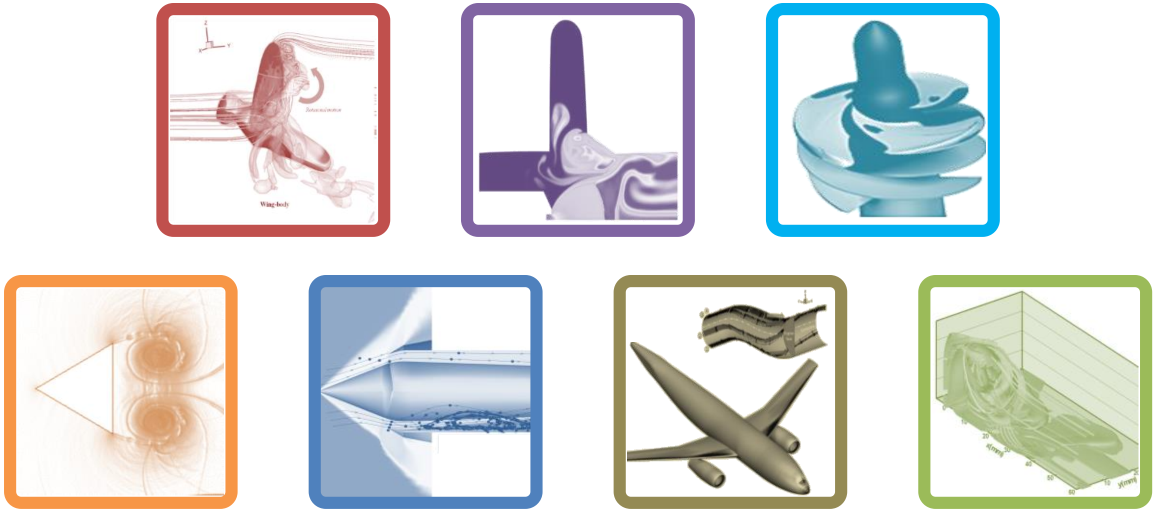
Multiphase model study



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  - **SIM (Sharp Interface Method)**
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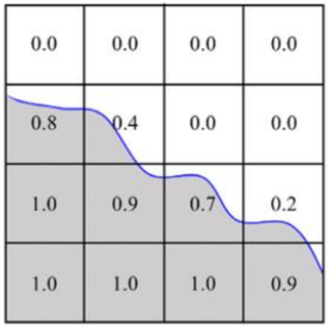
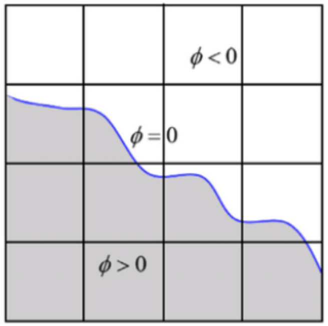
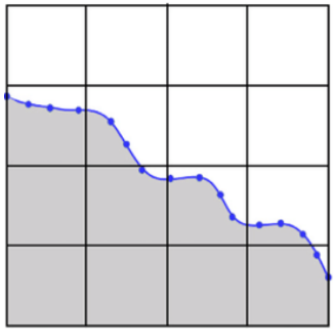
- **Phase change phenomenon**
- **7 equation model (non-relaxation model)**
- **6 equation model (μ relaxation model)**
- **5 equation model (μ, p relaxation model)**

Multiphase model study

- **Interface method**
  - **Sharp interface method (SIM)**
    - Interface is considered as a sharp discontinuity.
    - Lagrangian type
      - When fluid flows, Unbounded deformation and mesh distortions → Unpractical
    - Eulerian type
      - A fixed mesh with an additional equation for tracking and reconstructing the interface
      - Volume of fluid (VOF) – **it is different from homogenous mixture model.**
        - the cells are occupied by each volume fraction (α), transport with the flow.
      - Level-set equation
        - At the interface the number is set as zero, and far from the interface the numbers are positive or negative.
        - With large pressure and density ratios, the interface can be not obvious.
        - Mixture momentum and energy are not conserved.
      - Front tracking method
        - Interfaces is explicitly tracked.
    - Limitations
      - It can't create interface that are not present initially as gas pockets in cavitating flows.
      - It can't solve interfaces separating pure fluids and mixture.

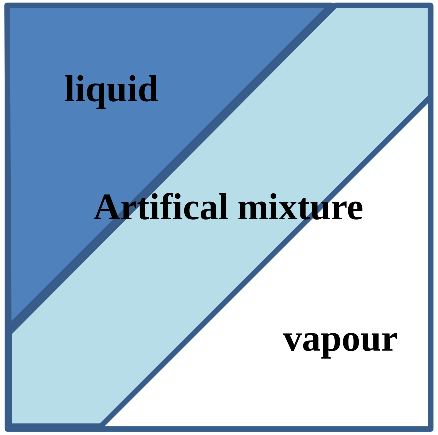






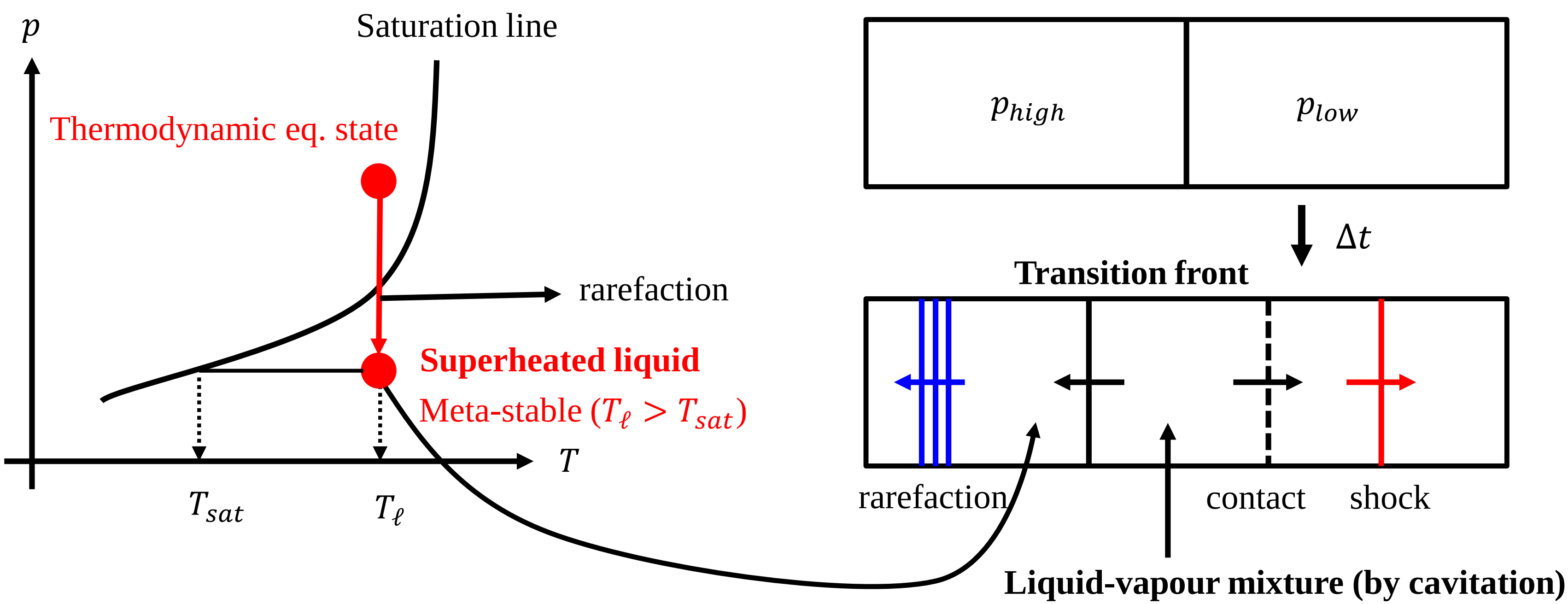
Multiphase model study

- **Interface method**
  - **Diffuse interface method (DIM) – Our Framework**
    - Interfaces is considered as artificial mixture s created by numerical diffusion.
    - Challenge
      - Physically, mathematically and numerically consistent thermodynamic laws for the artificial mixture
    - Advantages
      - The same algorithm in both pure fluids and mixture
      - it can create interfaces that are not present initially in contrast to SIM.
      - It can deal with interfaces separating pure fluids and mixtures as condensed explosive.
    - Hyperbolic multiphase flow models such as total non-eq. model or mechanical eq. model.



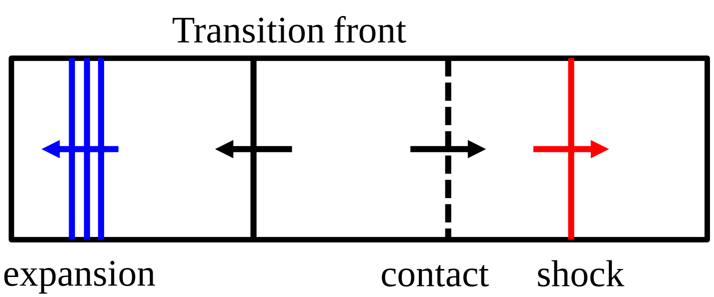
Multiphase model study

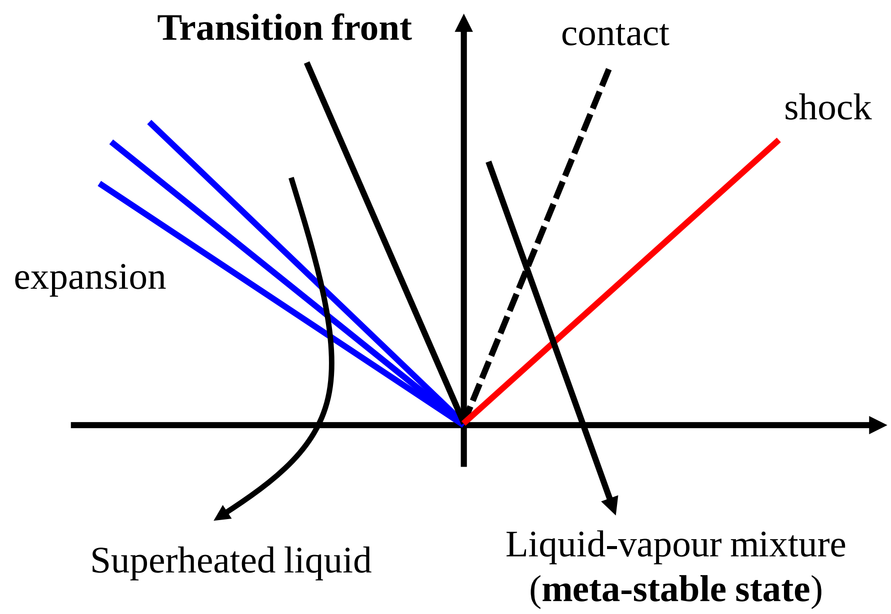
- **Phase change phenomenon**
  - **Cavitation**
    - **Superheated liquid** in metastable releases internal energy (metastable energy)
      - Producing pure vapour or vapour-liquid mixture (if retrograde); **cavitation ➔ Strong disturbance**
    - Associated experiment (Simoes-Moreira & Shepherd, 1999)
      - It have to be considered that liquid and vapour are compressible. (∵ **wave propagation - rarefaction, shock, etc.**)
      - In real situation, rarefaction can be occur due to geometrical effect (ex. Nozzle, etc.)



Multiphase model study

- **Multiphase model**
  - **Have to ability to deal with**
    - Interfaces of simple contact (non-condensable gas – water interface, **no mass transfer**)
    - Evaporating interfaces (vapour – water interface, **mass transfer that occur under $T_\ell > T_{sat}$**)





Multiphase model study

- **Multiphase model**
  - **Relaxation time scales**
    - Dependent on many parameter of the fluids
    - Pressure relaxation time ($\propto 1/\mu$)
      - Compressibility of the fluids
      - Two phase mixture topology
    - Velocity relaxation time ($\propto 1/\lambda$)
      - Fluid viscosity
      - Pressure relaxation process
    - Temperature relaxation time ($\propto 1/H$)
      - Thermal conductivity of the fluids (arise from the collisions of the molecules of the fluids)

      → For temperature equilibrium, a large number of collisions is required.
    - Gibbs free energy relaxation time ($\propto 1/\nu$)
      - Local chemical relaxation
  - **Order of relaxation time**
    - **Pressure ($1/\mu$) $\leq$ velocity ($1/\lambda$) $\ll$ temperature ($1/H$) $\ll$ Gibbs free energy ($1/\nu$)**

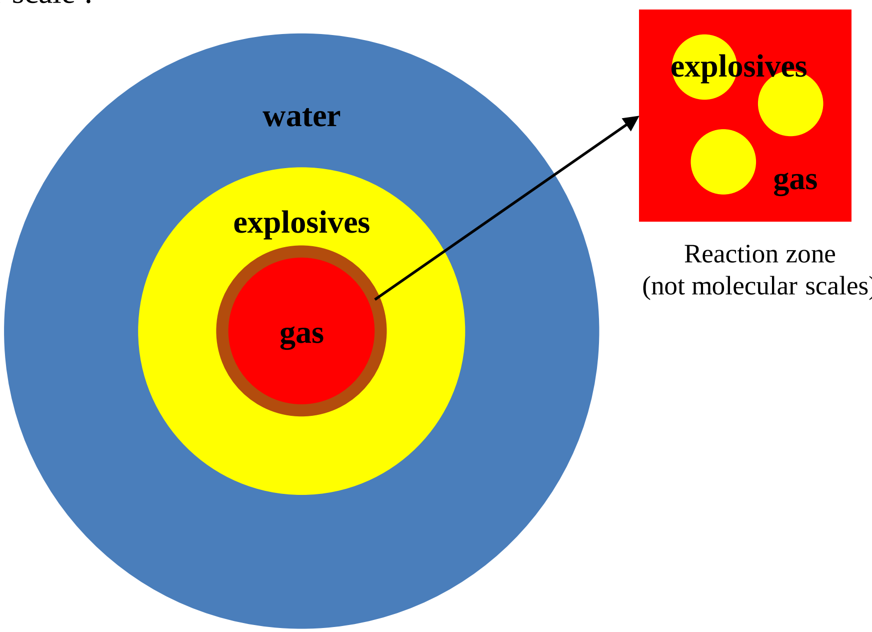
    ➔ In many physical situations, pressure and velocity relax instantaneously. ($p, \boldsymbol{v}$ equilibrium)

Multiphase model study

- **Multiphase model**
  - **Order of relaxation time**
    - Validity of temperature equilibrium
      - In gaseous detonation model, molecular collisions are so intense. → temperature equilibrium.
      - For detonations in heterogeneous explosives, molecular collisions aren’t sufficient (mixing is at not molecular scale) → temperature non-equilibrium.

➔ “Spark generated UNDEX” that is our goal can be considered as “gaseous detonation model” because mixture zone with cavitation occurring at interfaces is at molecular scale .

[Gaseous detonation model]



[Heterogeneous Explosive model]

Multiphase model study

- **Multiphase model**
  - **P-T equilibrium model**
    - Mixture Euler eq. with a cubic EOS (ex. Vdw EOS, etc.)
      - A cubic EOS cause a loss of hyperbolicity in the spinodal region.

      ➔ **The squared sound speed may become negative and wave propagation has no physical meaning.**
    - Mixture Euler eq. with a tabular EOS or a combination of pure phase EOSs ($p - T - \mu$ relaxation) – 3 eq.
      - No loss of hyperbolicity (∵ not use cubic EOS)
      - No metastable states
      - Unable to deal with interfaces between a liquid and non-condensable gas
    - Mixture Euler eq. + mass fraction eq. with a relaxation term ($\dot{m}$) – 4 eq.
      - Unable to deal with interfaces between a liquid and non-condensable gas

      (∵ not isothermal state at interface between a liquid and ncgas ($T_g \neq T_\ell$))
  - **T non-equilibrium model**
    - Five equation model ($p - \boldsymbol{v}$ relaxation)
      - Unconditionally hyperbolic
      - Two mass eq. + one mixture momentum eq. + one mixture energy eq. + advection eq. for volume fraction
    - Six equation models (p relaxation)
      - Advection eq. for volume fraction + two mass eq. + two energy eq. + one mixture momentum eq.
    - Seven equation models (non-equilibrium)
      - Unconditionally hyperbolic
      - Balance eq. of mass, momentum and energy of each fluid + advection eq. for volume fraction

Multiphase model study

- **7 equation model (non-equilibrium model) of Baer-Nunziato**
  - **Volume fraction eq.**

$$\frac{\partial \alpha_1}{\partial t} + \boldsymbol{u_I} \cdot \nabla \alpha_1 = \mu(p_1 - p_2)$$

  - **Each phase's balance eq. (k = 1,2)**

$$\frac{\partial \alpha_1 \rho_1}{\partial t} + \mathrm{div}(\alpha_1 \rho_1 \boldsymbol{u_1}) = 0$$

$$\frac{\partial \alpha_1 \rho_1 \boldsymbol{u_1}}{\partial t} + \mathrm{div}(\alpha_1 \rho_k \boldsymbol{u_k} \times \boldsymbol{u_k}) + \nabla(\alpha_1 p_1) = p_I \nabla \alpha_1 + \lambda(\boldsymbol{u_2} - \boldsymbol{u_1}) = 0$$

$$\frac{\partial \alpha_1 \rho_1 E_1}{\partial t} + \mathrm{div}(\alpha_1(\rho_1 E_1 + p_1)\boldsymbol{u_1}) = p_I \boldsymbol{u_I} \cdot \nabla \alpha_1 + \lambda \boldsymbol{u_I} \cdot (\boldsymbol{u_2} - \boldsymbol{u_1}) + p_I \mu(p_2 - p_1) + H(T_2 - T_1)$$

$$\frac{\partial \alpha_2 \rho_2}{\partial t} + \mathrm{div}(\alpha_2 \rho_2 \boldsymbol{u_2}) = 0$$

$$\frac{\partial \alpha_2 \rho_2 \boldsymbol{u_2}}{\partial t} + \mathrm{div}(\alpha_2 \rho_k \boldsymbol{u_k} \times \boldsymbol{u_k}) + \nabla(\alpha_2 p_2) = p_I \nabla \alpha_2 + \lambda(\boldsymbol{u_1} - \boldsymbol{u_2}) = 0$$

$$\frac{\partial \alpha_2 \rho_2 E_2}{\partial t} + \mathrm{div}(\alpha_2(\rho_2 E_2 + p_2)\boldsymbol{u_2}) = p_I \boldsymbol{u_I} \cdot \nabla \alpha_2 + \lambda \boldsymbol{u_I} \cdot (\boldsymbol{u_1} - \boldsymbol{u_2}) + p_I \mu(p_1 - p_2) + H(T_1 - T_2)$$

Multiphase model study

- **7 equation model (non-equilibrium model)**
  - **Unconditionally hyperbolic**
    - Characteristic wave speeds; $\boldsymbol{u_k},\ \boldsymbol{u_k}+\boldsymbol{c_k},\ \boldsymbol{u_k}-\boldsymbol{c_k},\ \boldsymbol{u_I}$
  - **Symmetric closure relations (Saurel *et al*. 2003)**
    - Relaxation coefficients($\mu,\ \lambda$) can be determined.
    - Under the continuous limit of the discrete two-phase flow

$$\mu = \frac{S_I}{Z_1 + Z_2}, \qquad \lambda = Z_1 Z_2 \mu$$

      - Z: acoustic impedance ($Z = \rho c$)
  - **Interface variables**
    - Saurel *et al*. (2003)

$$p_I = \frac{Z_1 p_2 + Z_2 p_1}{Z_1 + Z_2} + \text{sign}\left(\frac{\partial \alpha_1}{\partial x}\right)\frac{(u_2 - u_1) Z_1 Z_2}{Z_1 + Z_2}, \qquad u_I = \frac{Z_1 u_1 + Z_2 u_2}{Z_1 + Z_2} + \text{sign}\left(\frac{\partial \alpha_1}{\partial x}\right)\frac{p_2 - p_1}{Z_1 + Z_2}$$

    - Baer & Nunziato (1986)

$$p_I = p_1, \qquad u_I = u_2$$

    - Under stiff mechanical relaxation ($\mu, \lambda \to \infty$), both interface variables can be inter-changeable.

Multiphase model study

- **7 equation model (non-equilibrium model)**
  - **Primitive variables**
    - Volume fraction eq.

$$\frac{\partial \alpha_1}{\partial t} = -\boldsymbol{u_I} \cdot \nabla \alpha_1 + \mu (p_1 - p_2)$$

    - Each phase's balance eq.

$$\frac{\partial \alpha_1 \rho_1}{\partial t} = -\mathrm{div}(\alpha_1 \rho_1 \boldsymbol{u_1})$$

$$\frac{\partial \boldsymbol{u_1}}{\partial t} = -\boldsymbol{u_1} \cdot \boldsymbol{\nabla u_1} - \frac{1}{\rho_1} \nabla p_1 + \frac{p_I - p_1}{\alpha_1 \rho_1} \nabla \alpha_1 + \frac{\lambda}{\alpha_1 \rho_1} (\boldsymbol{u_2} - \boldsymbol{u_1})$$

$$\frac{\partial p_1}{\partial t} = -\rho_1 c_1^2 \mathrm{div}(\boldsymbol{u_1}) + \frac{\Gamma_1}{\alpha_1} \left[p_I - \rho_1^2 \left(\frac{\partial e_1}{\partial \rho_1} \right)_{p_1} \right] (\boldsymbol{u_I} - \boldsymbol{u_1}) \cdot \nabla \alpha_1 + \mu \frac{\Gamma_1}{\alpha_1} \left[p_I - \rho_1^2 \left(\frac{\partial e_1}{\partial \rho_1} \right)_{p_1} \right] (p_2 - p_1) + \lambda \frac{\Gamma_1}{\alpha_1} (\boldsymbol{u_I} - \boldsymbol{u_1})(\boldsymbol{u_2} - \boldsymbol{u_1}) + \frac{\Gamma_1}{\alpha_1} H(T_2 - T_1)$$

$$\frac{\partial \alpha_2 \rho_2}{\partial t} = -\mathrm{div}(\alpha_2 \rho_2 \boldsymbol{u_2})$$

$$\frac{\partial \boldsymbol{u_2}}{\partial t} = -\boldsymbol{u_2} \cdot \boldsymbol{\nabla u_2} - \frac{1}{\rho_2} \nabla p_2 + \frac{p_I - p_2}{\alpha_2 \rho_2} \nabla \alpha_2 + \frac{\lambda}{\alpha_1 \rho_1} (\boldsymbol{u_1} - \boldsymbol{u_2})$$

$$\frac{\partial p_2}{\partial t} = -\rho_2 c_2^2 \mathrm{div}(\boldsymbol{u_2}) + \frac{\Gamma_2}{\alpha_2} \left[p_I - \rho_2^2 \left(\frac{\partial e_2}{\partial \rho_2} \right)_{p_2} \right] (\boldsymbol{u_I} - \boldsymbol{u_2}) \cdot \nabla \alpha_2 + \mu \frac{\Gamma_2}{\alpha_2} \left[p_I - \rho_2^2 \left(\frac{\partial e_2}{\partial \rho_2} \right)_{p_2} \right] (p_1 - p_2) + \lambda \frac{\Gamma_2}{\alpha_2} (\boldsymbol{u_I} - \boldsymbol{u_2})(\boldsymbol{u_1} - \boldsymbol{u_2}) + \frac{\Gamma_2}{\alpha_2} H(T_1 - T_2)$$

      - Γ_K: Gruneisen coefficient of phase k

$$\Gamma_k = \frac{1}{\rho_k} \left(\frac{\partial p_k}{\partial e_k} \right)_{\rho_k}$$

Multiphase model study

- **5 equation model (pressure-velocity relaxation model)**
  - **From the asymptotic limit of non-equilibrium multiphase model (7 eq.)**
    - Asymptotic limit: the least effect term(or no meaning term) is removed.
  - **In the limit of stiff mechanical relaxation $\mu, \lambda(1/\epsilon) \rightarrow \infty$**
    - Velocity and pressure reach equilibrium state ($p_1 = p_2 = p_{eq}, \quad \boldsymbol{u_1} = \boldsymbol{u_2} = \boldsymbol{u_{eq}}$)

$$\frac{\partial \alpha_1}{\partial t} + \boldsymbol{u} \cdot \nabla \alpha_1 = \frac{\alpha_1 \alpha_2 (\rho_2 c_2^2 - \rho_1 c_1^2)}{\alpha_2 \rho_1 c_1^2 + \alpha_1 \rho_2 c_2^2} \mathrm{div}(\boldsymbol{u}) + \frac{\alpha_1 \alpha_2}{\alpha_2 \rho_1 c_1^2 + \alpha_1 \rho_2 c_2^2} \left(\frac{\Gamma_1}{\alpha_1} + \frac{\Gamma_2}{\alpha_2} \right) H(T_2 - T_1)$$

$$\frac{\partial \alpha_1 \rho_1}{\partial t} + \mathrm{div}(\alpha_1 \rho_1 \boldsymbol{u}) = 0, \qquad \frac{\partial \alpha_2 \rho_2}{\partial t} + \mathrm{div}(\alpha_2 \rho_2 \boldsymbol{u}) = 0$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \mathrm{div}(\rho \boldsymbol{u} \times \boldsymbol{u}) + \nabla p = 0$$

$$\frac{\partial \rho E}{\partial t} + \mathrm{div}\big(\boldsymbol{u}(\rho E + p)\big) = 0$$

      - Mixture density: $\rho = \alpha_1 \rho_1 + \alpha_2 \rho_2$
      - Mixture total energy:

$$E = \frac{\alpha_1 \rho_1}{\rho} E_1 + \frac{\alpha_2 \rho_2}{\rho} E_2$$

  - **Unconditionally hyperbolic**
    - Characteristic wave speeds; $\boldsymbol{u}, \quad \boldsymbol{u} + \boldsymbol{c_w}, \ \boldsymbol{u} - \boldsymbol{c_w}$

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

      - c_w(Wood speed of sound) has non-monotonic behavior versus volume fraction (α)

Multiphase model study

- **5 equation model (pressure-velocity relaxation model)**
  - **Effect of mass transfer**
    - A finite rate of mass transfer

$$\frac{\partial \alpha_1}{\partial t} + \boldsymbol{u} \cdot \nabla \alpha_1 = \frac{\alpha_1 \alpha_2 (\rho_2 c_2^2 - \rho_1 c_1^2)}{\alpha_2 \rho_1 c_1^2 + \alpha_1 \rho_2 c_2^2} \mathrm{div}(\boldsymbol{u}) + \frac{\alpha_1 \alpha_2}{\alpha_2 \rho_1 c_1^2 + \alpha_1 \rho_2 c_2^2} \left(\frac{\Gamma_1}{\alpha_1} + \frac{\Gamma_2}{\alpha_2} \right) H(T_2 - T_1) + \frac{\rho \dot{\boldsymbol{Y}}}{\boldsymbol{\rho_I}}$$

$$\frac{\partial \alpha_1 \rho_1}{\partial t} + \mathrm{div}(\alpha_1 \rho_1 \boldsymbol{u}) = \rho \dot{Y}$$

$$\frac{\partial \alpha_2 \rho_2}{\partial t} + \mathrm{div}(\alpha_2 \rho_2 \boldsymbol{u}) = -\rho \dot{Y}$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \mathrm{div}(\rho \boldsymbol{u} \times \boldsymbol{u}) + \nabla p = 0$$

$$\frac{\partial \rho E}{\partial t} + \mathrm{div}\big(\boldsymbol{u}(\rho E + p)\big) = 0$$

  - **Determination for mass transfer ($\dot{Y}$), interface density ($\boldsymbol{\rho_I}$)**
    - Entropy production eq.

by mass transfer

$$\dot{Y}_k \frac{d s_k}{dt} = \pm \frac{H(T_2 - T_1)}{\rho T_k} \pm \frac{\dot{Y}_k (h_2 - h_1)}{\frac{\Gamma_k T_k}{\alpha_k} \left(\frac{\alpha_1}{\Gamma_1} + \frac{\alpha_2}{\Gamma_2} \right)} + \frac{\dot{Y}_k}{T_k \left(\frac{\Gamma_1}{\alpha_1} + \frac{\Gamma_1}{\alpha_1} \right)} \left(\frac{\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}}{\boldsymbol{\rho_I}} - \left(\frac{c_1^2}{\alpha_1} + \frac{c_2^2}{\alpha_2} \right) \right)$$

by heat exchange

by pressure relaxation process caused by mass transfer

5 equation model (pressure-velocity relaxation model)

Determination for mass transfer ($\dot{Y}$), interface density (ρ_I)

- Entropy production eq.

$$\dot{Y}_k \frac{ds_k}{dt} = \pm \frac{H(T_2 - T_1)}{\rho T_k} \pm \frac{\dot{Y}_k (h_2 - h_1)}{\frac{\Gamma_k T_k}{\alpha_k}\left(\frac{\alpha_1}{\Gamma_1} + \frac{\alpha_2}{\Gamma_2}\right)} + \boxed{\frac{\dot{Y}_k}{T_k\left(\frac{\Gamma_1}{\alpha_1} + \frac{\Gamma_1}{\alpha_1}\right)}\left(\frac{\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}}{\boldsymbol{\rho_I}} - \left(\frac{c_1^2}{\alpha_1} + \frac{c_2^2}{\alpha_2}\right)\right)}$$

by pressure relaxation process caused by mass transfer

During mass transfer, pressure perturbations occurs. ($\dot{\boldsymbol{m}} \leftrightarrow \Delta \boldsymbol{p}$)

→ wave propagation by pressure perturbations makes vapour phase (evaporation)

→ evaporation is a continuous phenomenon

→ waves that cause evaporation are necessarily weak (**isentropic**)

$$\frac{\dot{Y}_k}{T_k\left(\frac{\Gamma_1}{\alpha_1} + \frac{\Gamma_1}{\alpha_1}\right)}\left(\frac{\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}}{\boldsymbol{\rho_I}} - \left(\frac{c_1^2}{\alpha_1} + \frac{c_2^2}{\alpha_2}\right)\right) = 0$$

$$\boldsymbol{\rho_I} = \frac{\frac{\boldsymbol{\rho_1 c_1^2}}{\boldsymbol{\alpha_1}} + \frac{\boldsymbol{\rho_2 c_2^2}}{\boldsymbol{\alpha_2}}}{\frac{\boldsymbol{c_1^2}}{\boldsymbol{\alpha_1}} + \frac{\boldsymbol{c_2^2}}{\boldsymbol{\alpha_2}}}$$

Multiphase model study

- **5 equation model (pressure-velocity relaxation model)**
  - **Determination for mass transfer ($\dot{Y}$), interface density (ρ_I)**
    - Thermodynamics 2nd law

$$\frac{H(T_2 - T_1)^2}{\rho} + (\bar{g}_2 - \bar{g}_1)T_I\dot{Y} \geq 0$$

- T_I: interface temperature

$$T_I = \frac{\left(\frac{\Gamma_1 T_1}{\alpha_1} + \frac{\Gamma_2 T_2}{\alpha_2}\right)}{\left(\frac{\Gamma_1}{\alpha_1} + \frac{\Gamma_2}{\alpha_2}\right)} \ (\geq 0)$$

- $\bar{g}_k$: gibbs free energy

$$\bar{g}_k = h_k - \frac{T_1 T_2}{T_I} s_k$$

➔ To satisfy thermodynamics 2nd law, $\dot{Y}$ have to be $\dot{Y} = \nu(\bar{g}_2 - \bar{g}_1)$ where ν is a positive relaxation parameter that controls the rate at which the mixture relaxes to thermodynamic equilibrium.

Multiphase model study

- **5 equation model (pressure-velocity relaxation model)**
  - **Final form**

$$\frac{\partial \alpha_1}{\partial t} + \boldsymbol{u}\cdot\nabla\alpha_1 = \frac{\alpha_1\alpha_2(\rho_2 c_2^2 - \rho_1 c_1^2)}{\alpha_2\rho_1 c_1^2 + \alpha_1\rho_2 c_2^2}\operatorname{div}(\boldsymbol{u}) + \frac{\alpha_1\alpha_2}{\alpha_2\rho_1 c_1^2 + \alpha_1\rho_2 c_2^2}\left(\frac{\Gamma_1}{\alpha_1} + \frac{\Gamma_2}{\alpha_2}\right)H(T_2 - T_1) + \rho\nu(\bar{g}_2 - \bar{g}_1)\frac{\frac{c_1^2}{\alpha_1} + \frac{c_2^2}{\alpha_2}}{\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}}$$

$$\frac{\partial \alpha_1\rho_1}{\partial t} + \operatorname{div}(\alpha_1\rho_1\boldsymbol{u}) = \rho\nu(\bar{g}_2 - \bar{g}_1)$$

$$\frac{\partial \alpha_2\rho_2}{\partial t} + \operatorname{div}(\alpha_2\rho_2\boldsymbol{u}) = \rho\nu(\bar{g}_1 - \bar{g}_2)$$

$$\frac{\partial \rho\boldsymbol{u}}{\partial t} + \operatorname{div}(\rho\boldsymbol{u}\times\boldsymbol{u}) + \nabla p = 0$$

$$\frac{\partial \rho E}{\partial t} + \operatorname{div}\big(\boldsymbol{u}(\rho E + p)\big) = 0$$

  - **Solution procedure**
    - Hyperbolic solver $(H,\ \nu = 0)$
      - For locations far from the interfaces
    - Stiff thermo-chemical solver $(H,\ \nu \to \infty)$
      - Near the interfaces $(\epsilon \le \alpha_1 \le 1 - \epsilon)$, relaxation can be assumed as a considerable rate.
      - If interface is simple contact (water – non condensable gas), $H,\ \nu = 0$

Multiplphase model study

- **5 equation model (pressure-velocity relaxation model)**
  - **Solution procedure**
    - Hyperbolic solver ($H,\ \nu = 0$) with heat and mass transfer

$$\frac{\partial \alpha_1}{\partial t} + \boldsymbol{u} \cdot \nabla \alpha_1 = \frac{\alpha_1 \alpha_2 (\rho_2 c_2^2 - \rho_1 c_1^2)}{\alpha_2 \rho_1 c_1^2 + \alpha_1 \rho_2 c_2^2} \operatorname{div}(\boldsymbol{u})$$

Non-conservative term

$$\frac{\partial \alpha_1 \rho_1}{\partial t} + \operatorname{div}(\alpha_1 \rho_1 \boldsymbol{u}) = 0$$

$$\frac{\partial \alpha_2 \rho_2}{\partial t} + \operatorname{div}(\alpha_2 \rho_2 \boldsymbol{u}) = 0$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \operatorname{div}(\rho \boldsymbol{u} \times \boldsymbol{u}) + \nabla p = 0$$

$$\frac{\partial \rho E}{\partial t} + \operatorname{div}\big(\boldsymbol{u}(\rho E + p)\big) = 0$$

➔ At each time step, non-equilibrium flow field's variables can be obtained.

- Volume fraction equations is non-conservation form.
  - The Riemann problem can't be solved because conventional shock relations aren't be used. So, The conventional Godunov-type schemes are not suitable.
  - The average of the volume fraction variable within a computational cell has no physical meaning.

(cf. Petitpas *et al.*, 2007, Saurel *et al.*, 2007)

Multiphase model study

- 5 equation model (pressure-velocity relaxation model)
  - Solution procedure
    - Stiff thermo-chemical solver ($H,\ \nu \rightarrow \infty$), ODEs

$$\frac{\partial \alpha_1}{\partial t} = \frac{\alpha_1 \alpha_2}{\alpha_2 \rho_1 c_1^2 + \alpha_1 \rho_2 c_2^2}\left(\frac{\Gamma_1}{\alpha_1} + \frac{\Gamma_2}{\alpha_2}\right) Q + \rho \dot{Y} \frac{\frac{c_1^2}{\alpha_1} + \frac{c_2^2}{\alpha_2}}{\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}} = \boldsymbol{S}_{\boldsymbol{\alpha_1}}$$

$$\frac{\partial \alpha_1 \rho_1}{\partial t} = \rho \dot{Y} = \boldsymbol{S}_{\boldsymbol{Y}}, \qquad \frac{\partial \alpha_2 \rho_2}{\partial t} = -\rho \dot{Y}$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} = 0, \qquad \frac{\partial \rho E}{\partial t} = 0$$

➔ It solved at **the interfaces** between water and vapour only.

- Closure relations for $Q(= f(H, T))$ and $\dot{Y}(= h(\nu, g))$ regarding relaxation parameter H and ν.

$$\frac{\partial \Delta T}{\partial t} = AQ + B\dot{Y}, \qquad \frac{\partial \Delta g}{\partial t} = A'Q + B'\dot{Y}$$

Where A, B, A', B' are functions of all flow variables and that dependent to specific EOS. (ex. SG EOS, etc)

$$\frac{(\Delta T)^{n+1} - (\Delta T)^n}{\Delta t} = A^n Q^n + B^n \dot{Y}^n, \qquad \frac{(\Delta g)^{n+1} - (\Delta g)^n}{\Delta t} = A'^n Q^n + B'^n \dot{Y}^n$$

Multiphase model study

- **5 equation model (pressure-velocity relaxation model)**
  - **Solution procedure**
    - Closure relations for $Q(= f(H,T))$ and $\dot{Y}(= h(\nu,g))$ regarding relaxation parameter H and ν.
      - The variables at time t^n is obtained by the non-conservation hyperbolic solver.
      - Infinite relaxation → the equilibrium has to be reached at the end of each time step (Δt) which imposed by CFL condition (explicit time scheme).
        → $(\Delta T)^{n+1} = 0,\ (\Delta g)^{n+1} = 0$

$$Q = -\frac{B'}{AB' - A'B}\frac{(\Delta T)^n}{\Delta t} - \frac{B}{AB' - A'B}\frac{(\Delta g)^n}{\Delta t}, \qquad \dot{Y} = \frac{A'}{AB' - A'B}\frac{(\Delta T)^n}{\Delta t} - \frac{A}{AB' - A'B}\frac{(\Delta g)^n}{\Delta t}$$

      - For preventing solution(α, Y) from stiff thermo-chemical solver to be negative,

$$S_{max,\alpha_1} = \begin{cases} \dfrac{1-\alpha_1}{\Delta t}, & \text{if } S_{\alpha_1} > 0 \\ \dfrac{-\alpha_1}{\Delta t}, & \text{otherwise} \end{cases} \qquad S_{max,Y} = \begin{cases} \dfrac{1-Y}{\Delta t}, & \text{if } S_Y > 0 \\ \dfrac{-Y}{\Delta t}, & \text{otherwise} \end{cases}$$

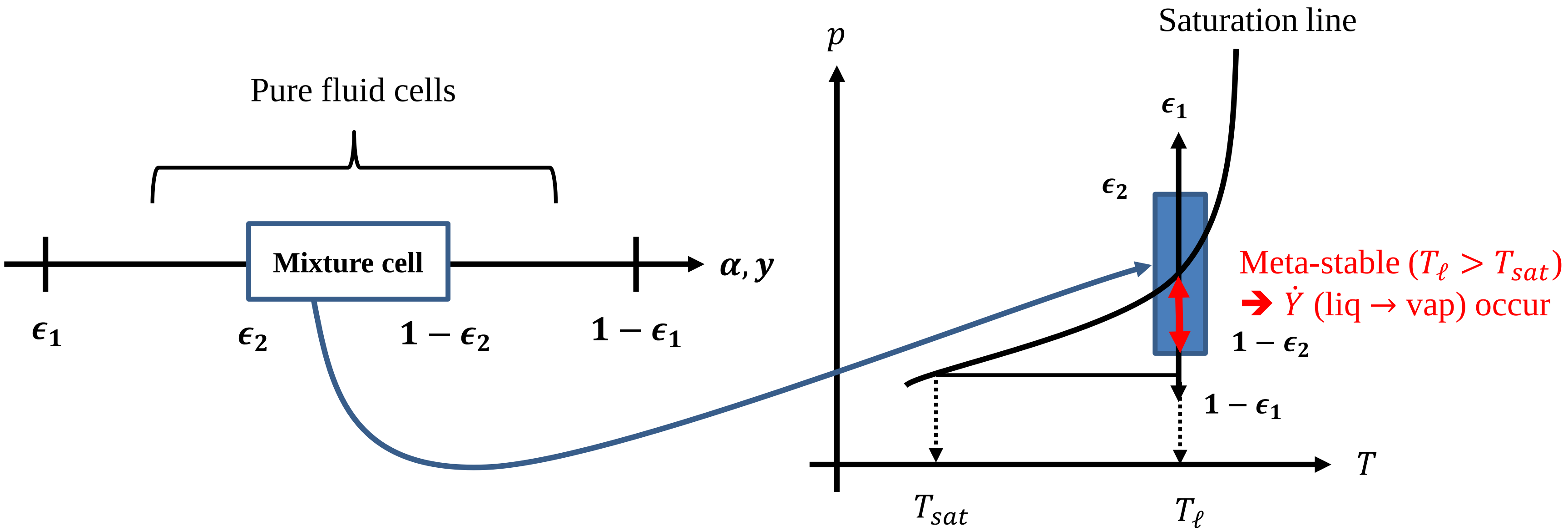
If it not satisfy $|S_{max,\alpha_1}| > |S_{\alpha_1}|$ and $|S_{max,Y}| > |S_{Y_1}|$, equation are stiff and time step has to be reduced.

      - Cf. stiff thermo-chemical solver is integrated over a fraction of the time step

$$\Delta t = \frac{S_{max,\alpha_1}}{S_{\alpha_1}}\frac{\Delta t}{2}$$

Multiphase model study

- **5 equation model (pressure-velocity relaxation model)**
  - **Solution procedure**
    - Location of interfaces
      - volume(α) and mass(Y) fractions → 1 ($1-\epsilon_1,\ \epsilon_1 = 10^{-8}$) → pure fluid cells
      - $\epsilon_2 \le \alpha, y \le 1-\epsilon_2,\ \epsilon_2 = 10^{-6}$ → mixture cells; **interfaces**
        - If ϵ_2 is taken too close to ϵ_1, evaporation may occur too early and not only in the interfacial zone (can occur during expansion waves).
      - If one of the fluids in the mixture cell is metastable ($T_k > T_{sat}(p)$), **mass transfer($\dot{Y}$) is occured.**

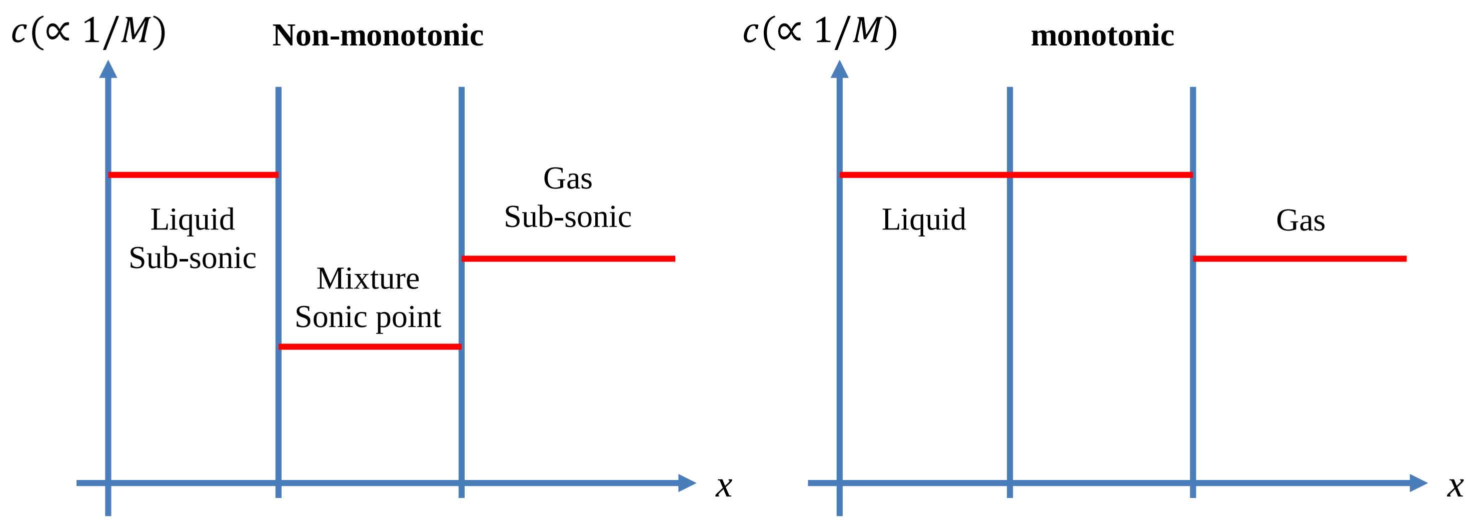


Multiphase model study

- **6 equation model (velocity relaxation model, finally $p - v$ relxation)**
  - **Strength (vs 5 equation model)**
    - The existence of non-conservative contribution in the volume fraction eq. of 5 equation model
      - Because of the variation of the volume fraction across the acoustic wave, the approximate Riemann solvers are not suitable.
      - When shocks and strong rarefaction wave are involved, volume fraction may be negative.

$$\frac{\partial \alpha_1}{\partial t} + \boldsymbol{u} \cdot \nabla \alpha_1 = \frac{\alpha_1 \alpha_2 (\rho_2 c_2^2 - \rho_1 c_1^2)}{\alpha_2 \rho_1 c_1^2 + \alpha_1 \rho_2 c_2^2} \mathrm{div}(\boldsymbol{u})$$ **Non-conservative term**

    - The non-monotonic behavior of 5 equation model
      - In the numerical diffusion of an interface, non-monotonic speed of sound can make two sonic points. (even when the flow is subsonic in both pure fluids) → affect the propagation of acoustic waves interacting with the interfacial zone.



Multiphase model study

- **6 equation model (velocity relaxation model, finally $p - v$ relxation)**
  - **Volume fraction eq.**

$$\frac{\partial \alpha_1}{\partial t} + \boldsymbol{u} \cdot \nabla \alpha_1 = \mu(p_1 - p_2)$$

  - **Each phase's balance eq. (k = 1,2)**
    - Energy eq. are based on internal energy ($\rho_k \varepsilon_k$).

$$\frac{\partial \alpha_1 \rho_1}{\partial t} + \mathrm{div}(\alpha_1 \rho_1 \boldsymbol{u}) = 0$$

$$\frac{\partial \alpha_1 \rho_1 \varepsilon_1}{\partial t} + \mathrm{div}(\alpha_1 \rho_1 \varepsilon_1 \boldsymbol{u}) + \alpha_1 p_1 \nabla \cdot \boldsymbol{u} = \mu p_I (p_2 - p_1)$$

$$\frac{\partial \alpha_2 \rho_2}{\partial t} + \mathrm{div}(\alpha_2 \rho_2 \boldsymbol{u}) = 0$$

$$\frac{\partial \alpha_2 \rho_2 \varepsilon_2}{\partial t} + \mathrm{div}(\alpha_2 \rho_2 \varepsilon_2 \boldsymbol{u}) + \alpha_2 p_2 \nabla \cdot \boldsymbol{u} = \mu p_I (p_1 - p_2)$$

→ Where interface pressure is determined similar to 7 eq model's way. $p_I = (Z_1 p_1 + Z_2 p_2)/(Z_1 + Z_2)$

  - **Mixture momentum eq.**

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \mathrm{div}(\rho \boldsymbol{u} \times \boldsymbol{u}) + \nabla(\alpha_1 p_1 + \alpha_2 p_2) = 0$$

➔ **With only pressure relaxation term**, not temperature relaxation term.

Multiphase model study

- **6 equation model (velocity relaxation model, finally $p - v$ relxation)**
  - **Energy eq. are based on total energy (E_k).**

$$\frac{\partial \alpha_1 E_1}{\partial t} + \mathrm{div}(\alpha_1 E_1 \boldsymbol{u} + \alpha_1 p_1 \boldsymbol{u}) + \Sigma(q, \nabla q) = \mu p_I (p_2 - p_1)$$

$$\frac{\partial \alpha_2 E_2}{\partial t} + \mathrm{div}(\alpha_2 E_2 \boldsymbol{u} + \alpha_2 p_2 \boldsymbol{u}) - \Sigma(q, \nabla q) = \mu p_I (p_1 - p_2)$$

    - Non-conservation term

$$\Sigma(q, \nabla q) = -\boldsymbol{u} \cdot \left(Y_2 \nabla(\alpha_1 p_1) - Y_1 \nabla(\alpha_2 p_2)\right) = -\boldsymbol{u} \cdot \left((Y_2 p_1 + Y_1 p_2)\nabla \alpha_1 + \alpha_1 Y_2 \nabla p_1 - \alpha_2 Y_1 \nabla p_2\right)$$

    - Although phasic total energy eq. are non-conservative form, mixture total energy is conservative.

$$\boldsymbol{\frac{\partial E}{\partial t} + \nabla \cdot (E u + \alpha_1 p_1 u + \alpha_2 p_2 u) = 0}$$

➔ Beneficial to satisfy **"Mixture energy consistent discretization"**

Multiphase model study

- **6 equation model (velocity relaxation model, finally $\boldsymbol{p-v}$ relxation)**
  - **With heat and mass transfer**

$$\frac{\partial \alpha_1}{\partial t} + \boldsymbol{u} \cdot \nabla \alpha_1 = \mu(p_1 - p_2) + \frac{\dot{\boldsymbol{m}}}{\boldsymbol{\rho_I}}$$

$$\frac{\partial \alpha_1 \rho_1}{\partial t} + \mathrm{div}(\alpha_1 \rho_1 \boldsymbol{u}) = \dot{\boldsymbol{m}}$$

$$\frac{\partial \alpha_2 \rho_2}{\partial t} + \mathrm{div}(\alpha_2 \rho_2 \boldsymbol{u}) = -\dot{\boldsymbol{m}}$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \mathrm{div}(\rho \boldsymbol{u} \times \boldsymbol{u}) + \nabla(\alpha_1 p_1 + \alpha_2 p_2) = 0$$

$$\frac{\partial \alpha_1 E_1}{\partial t} + \mathrm{div}(\alpha_1 E_1 \boldsymbol{u} + \alpha_1 p_1 \boldsymbol{u}) + \Sigma(q, \nabla q) = \mu p_I (p_2 - p_1) + \boldsymbol{Q} + \boldsymbol{e_I} \dot{\boldsymbol{m}}$$

$$\frac{\partial \alpha_2 E_2}{\partial t} + \mathrm{div}(\alpha_2 E_2 \boldsymbol{u} + \alpha_2 p_2 \boldsymbol{u}) - \Sigma(q, \nabla q) = \mu p_I (p_1 - p_2) - \boldsymbol{Q} - \boldsymbol{e_I} \dot{\boldsymbol{m}}$$

Where,

$$\Sigma(q, \nabla q) = -\boldsymbol{u} \cdot \big(Y_2 \nabla(\alpha_1 p_1) - Y_1 \nabla(\alpha_2 p_2)\big) = -\boldsymbol{u} \cdot \big((Y_2 p_1 + Y_1 p_2)\nabla \alpha_1 + \alpha_1 Y_2 \nabla p_1 - \alpha_2 Y_1 \nabla p_2\big)$$

$$\boldsymbol{Q} = \boldsymbol{H}(\boldsymbol{T_2} - \boldsymbol{T_1}), \qquad H = \begin{cases} \infty, & \text{if } 10^4 \le \alpha_1 \le 1 - \epsilon_1 \\ 0, & \text{otherwise} \end{cases}$$

$$\dot{\boldsymbol{m}} = \boldsymbol{\nu}(\boldsymbol{g_2} - \boldsymbol{g_1}), \qquad \nu = \begin{cases} \infty, & \text{if } \epsilon_1 \le \alpha_1 \le 1 - \epsilon_1 \text{ and } T_{liq} > T_{sat} \\ 0, & \text{otherwise} \end{cases}$$

Multiphase model study

- **6 equation model (velocity relaxation model, finally $p - v$ relxation)**
  - **Compact form**

$$\boldsymbol{\partial_t q + \nabla \cdot f(q) + \sigma(q, \nabla q) = \psi_\mu(q) + \psi_H(q) + \psi_\nu(q)}$$

$\nabla \cdot f(q)$: conservative term
$\sigma(q, \nabla q)$: non-conservative term
ψ_μ: mechanical relaxation term
ψ_H: thermal relaxation term
ψ_ν: chemical relaxation term

  - **Solution with only mechanical relaxation term**
    - Homogenous hyperbolic solver (step 1) – represented superscript 0

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

    - Stiff mechanical relaxation solver (ODEs) (step 2) – represented superscript *
      - the limit $\mu \to \infty$, $p_\ell = p_v = p$, ***not only at liquid-vapour interfaces***

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

      - The partial densities $(\alpha_k \rho_k)$, mixture momentum $(\rho \boldsymbol{u})$, mixture total energy (E), mixture internal energy (ε) remain constant because these aren't related to mechanical relaxation term (μ).

→ $(\alpha_k \rho_k)^0 = (\alpha_k \rho_k)^*,\ (\rho \boldsymbol{u})^0 = (\rho \boldsymbol{u})^*,\ E^0 = E^*,\ \varepsilon^0 = \varepsilon^*$

      - The volume fraction (α_1), mixture pressure (p), phasic internal energies $(\alpha_k \varepsilon_k)$ are updated by "**stiff mechanical solver**"

→ $\alpha_1^0 \neq \alpha_1^*,\ p^0 \neq p^*,\ (\alpha_k \varepsilon_k)^0 \neq (\alpha_k \varepsilon_k)^*$

Multiphase model study

- **6 equation model (velocity relaxation model, finally $p - v$ relxation)**
  - **Mixture energy consistent discretization**
    - For numerical solutions of multiphase, the quantities (partial density $\alpha_k \rho_k$, mixture density ρ, mixture momentum $\rho \boldsymbol{u}$, mixture energy E) have to be conserved.
      - numerical approximation of non-conservative term cause the inaccurate solutions in the shock.

    ➔ Godunov-type schemes can easily preserve conservation at the discrete level of quantities.
    - 6 eq model does not contain the total energy conservation eq., but two phasic energy eq.

    ➔ To be conservation of total energy at the discrete level and be consistent with the correct thermodynamics state, the phasic energy eq. have to be discretized.
    - Postulations of Mixture energy consistent
      - Mixture total energy conservation consistency

$$E^0 = \Sigma(\alpha_k E_k)^0 = E^{0,C}$$

$E^{0,C}$: discrete values of the mixture total energy by numerical approximation of total energy eq.

$(\partial_t E + \nabla \cdot (Eu + \alpha_1 p_1 u + \alpha_2 p_2 u) = 0)$

➔ the sum of the discrete values of the phasic total energies by step 1 must be equal discrete values of the mixture total energy.

- Relaxed pressure consistency

Mixture energy using mixture EOS derived under pressure equilibrium (mixture energy is constant)

$$\boxed{\varepsilon^{0,C}} = E^{0,C} - \frac{(\rho \boldsymbol{u})^0 \cdot (\rho \boldsymbol{u})^0}{2\rho^0} = \underline{\Sigma \alpha_k^* \varepsilon_k \left(p^*, \frac{(\alpha_k \rho_k)^0}{\alpha_k^*} \right)}$$

Sum of partial energy after pressure relaxation (partial energy vary)

➔ p^*(equilibrium) solved by step 2 must be equal the pressure computed by the mixture equation of state

(∵ To derive mixture equation of state, it assumed that pressure equilibrium is reached.)

Multiphase model study

- **6 equation model (velocity relaxation model, finally $p - v$ relxation)**
  - **Mixture energy consistent discretization**
    - Postulations of Mixture energy consistent
      - For **phasic total energy eq.**, a standard conservative schemes are used to conservative term

$$\partial_t(\alpha_k E_k) + \nabla \cdot (\alpha_k E_k \boldsymbol{u} + \alpha_k p_k \boldsymbol{u})$$

      - Symmetrically discretized non-conservative term $\Sigma(q, \nabla q)$ result in conservative discrete form of the mixture energy eq. (∵ cancellation of non-conservative discrete contributions)
      - Mixture total energy conservation consistency → Relaxed pressure consistency

    ➔ This process ensure to satisfy the postulations of mixture energy consistent and guarantee thermodynamically correct value of the equilibrium pressure p^* (**mixture total energy consistent**)

    - The difficulty with phasic internal energy eq.
      - Discretized phasic internal energies eq. ↛ a conservative discrete form of mixture total energy eq.

      → The additional mixture total energy eq. is required to correct the thermodynamic state predicted by the non-conservative internal energy eq.
      - It is not guarantee the relaxed pressure consistency

      (cf. Suerl *et al.*, 2009)

Multiphase model study

- **6 equation model (velocity relaxation model, finally $p - v$ relxation)**
  - **Mixture energy consistent discretization**
    - Stiff mechanical relaxation solver (ODEs)

$$\partial_t \alpha_1 = \mu(p_1 - p_2), \qquad \partial_t(\alpha_1 E_1) = \mu p_I(p_2 - p_1), \qquad \partial_t(\alpha_2 E_2) = \mu p_I(p_1 - p_2)$$

$$\partial_t(\alpha_k \rho_k) = 0, \qquad \partial_t(\rho \boldsymbol{u}) = 0$$

- The partial densities ($\alpha_k \rho_k$), mixture momentum ($\rho \boldsymbol{u}$) remain constant because the equations doesn't contain mechanical relaxation term (μ).

$$(\alpha_k \rho_k)^0 = (\alpha_k \rho_k)^*, \qquad (\rho \boldsymbol{u})^0 = (\rho \boldsymbol{u})^* \rightarrow \rho_0 = \rho^*, \qquad \boldsymbol{u}^{\mathbf{0}} = \boldsymbol{u}^*$$

Combining upper equations

$$\partial_t(\alpha_1 E_1) = \partial_t(\alpha_1 \rho_1 \varepsilon_1) = -p_I \partial_t \alpha_1, \qquad \partial_t(\alpha_2 E_2) = \partial_t(\alpha_2 \rho_2 \varepsilon_2) = p_I \partial_t \alpha_1$$

the sum of the phasic equations is zero.

$$\partial_t E = \partial_t(\rho\varepsilon) = 0 \rightarrow E^0 = E^*, \qquad (\rho\varepsilon)^0 = (\rho\varepsilon)^*$$

➔ Mixture total and internal energy are constant as the phasic pressure (p_k) reach equilibrium pressure (p^*) (under step 2)

- Interface pressure (p_I) assuming a linear variation with α_1

$$p_I = p_I^0 \frac{p_I^* - p_0^*}{\alpha_1^* - \alpha_1^0}(\alpha_1 - \alpha_1^0)$$

Multiphase model study

- **6 equation model (velocity relaxation model, finally $p - v$ relxation)**
  - **Mixture energy consistent discretization**
    - Stiff mechanical relaxation solver (ODEs)

$$\int_{\text{step1}(0)}^{\text{step2}(*)} \partial_t(\alpha_1 E_1) = \int_{\text{step1}(0)}^{\text{step2}(*)} \partial_t(\alpha_1\rho_1\varepsilon_1) = \int_{\text{step1}(0)}^{\text{step2}(*)} -p_I^0 \frac{p_I^* - p_0^*}{\alpha_1^* - \alpha_1^0}(\alpha_1 - \alpha_1^0)\partial_t\alpha_1$$

$$\int_{\text{step1}(0)}^{\text{step2}(*)} \partial_t(\alpha_2 E_2) = \int_{\text{step1}(0)}^{\text{step2}(*)} \partial_t(\alpha_2\rho_2\varepsilon_2) = \int_{\text{step1}(0)}^{\text{step2}(*)} p_I^0 \frac{p_I^* - p_0^*}{\alpha_1^* - \alpha_1^0}(\alpha_1 - \alpha_1^0)\partial_t\alpha_1$$

$$(\alpha_1 E_1)^* - (\alpha_1 E_1)^0 = (\alpha_1\varepsilon_1)^* - (\alpha_1\varepsilon_1)^0 = -\frac{p_I^0 + p_I^*}{2}(\alpha_1^* - \alpha_1^0)$$

$$(\alpha_2 E_2)^* - (\alpha_2 E_2)^0 = (\alpha_2\varepsilon_2)^* - (\alpha_2\varepsilon_2)^0 = \frac{p_I^0 + p_I^*}{2}(\alpha_1^* - \alpha_1^0)$$

- In the limit $\mu \to \infty$, $p_1^* = p_2^* = p_I^* = p$ and internal energy at final time $(\rho_k\varepsilon_k)^* = \mathrm{f}(p^*, (\alpha_k\rho_k)^0/\alpha_k^*)$ with together specific EOS (ex. SGEOS, etc.) → $\boldsymbol{p}^*, \boldsymbol{\alpha}_1^*$
- Using p^*, α_1^*, the relaxed pressure consistency can be verified (through mixture pressure law).

$$p^* = p\left(\varepsilon^0, \alpha_1^*, \frac{(\alpha_k\rho_k)^0}{\alpha_k^*}\right)$$

Where $(\rho\varepsilon)^0 = (\rho\varepsilon)^*$, $(\alpha_k\rho_k)^0 = (\alpha_k\rho_k)^*$

: Conservation-consistent discrete values of the mixture total energy, $E^0 = \Sigma(\alpha_k E_k)^0 = E^{0,C}$

→ Relaxed pressure consistency, $\varepsilon^0 = E^0 - \frac{(\rho\boldsymbol{u})^0 \cdot (\rho\boldsymbol{u})^0}{2\rho^0} = \alpha_1^*\,\varepsilon_1\left(\boldsymbol{p}^*, \frac{(\alpha_1\rho_1)^0}{\alpha_1^*}\right) + \alpha_2^*\varepsilon_2\left(\boldsymbol{p}^*, \frac{(\alpha_2\rho_2)^0}{\alpha_2^*}\right)$

Multiphase model study

- 6 equation model (velocity relaxation model, finally $p - v$ relxation)
  - Solution with thermal and chemical relaxation terms
    - Mechanical relaxation time $\ll$ thermal-chemical relaxation time
      - Thermal and chemical relaxation occur **under mechanical relaxation (pressure equilibrium)**.
    - Stiff thermal relaxation solver (ODEs) (step 3) – represented superscript **
      - the limit $H \to \infty$, $T_\ell = T_v = T$, at only liquid – vapour interfaces

$$\partial_t q = \psi_\mu(q) + \boldsymbol{\psi_H}(\boldsymbol{q})$$

$$\partial_t \alpha_1 = \mu(p_1 - p_2)$$

$$\partial_t(\alpha_k \rho_k) = 0, \qquad \partial_t(\rho \boldsymbol{u}) = 0$$

$$\partial_t(\alpha_1 E_1) = \mu p_I(p_2 - p_1) + H(T_2 - T_1), \qquad \partial_t(\alpha_2 E_2) = \mu p_I(p_1 - p_2) + H(T_1 - T_2)$$

- The initial values are coming from pressure relaxation solver.
- Metastable condition, $T_\ell^{**} > T_{sat}(p^{**})$, is verified through the updated values (with superscript **).
- The partial densities $(\alpha_k \rho_k)$ (of course, mixture density ρ), mixture momentum $(\rho \boldsymbol{u})$, total energy (E),internal energy $(\rho\varepsilon)$ remain constant because these aren't related to **thermal relaxation term ($\boldsymbol{H}$)** as well as mechanical relaxation term (μ).

→ $(\alpha_k \rho_k)^0 = (\alpha_k \rho_k)^* = (\alpha_k \rho_k)^{**},\ (\rho \boldsymbol{u})^0 = (\rho \boldsymbol{u})^* = (\rho \boldsymbol{u})^{**},\ E^0 = E^* = E^{**}, \varepsilon^0 = \varepsilon^* = \varepsilon^{**}$

➔ Using algebraic system (in case of SGEOS, quadratic eq.), equilibrium pressure (p^{**}) can be obtained. Then, also equilibrium values $\alpha_1^{**}(p^{**}), T^{**}(\alpha_1^{**})$ are obtained.

Multiphase model study

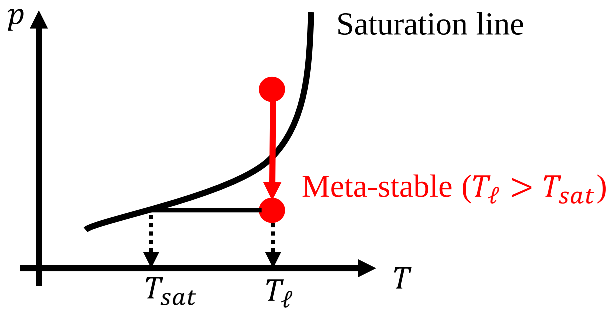
- **6 equation model (velocity relaxation model, finally $p - v$ relxation)**
  - **Solution with thermal and chemical relaxation terms**
    - Stiff thermal-chemical relaxation solver (ODEs) (step 4) – represented superscript ***
      - Under metastable region which is checked from the step 3, the limit $\nu \to \infty$, $g_\ell = g_v$, at only liquid vapour interfaces

$$\partial_t q = \psi_\mu(q) + \boldsymbol{\psi_H}(\boldsymbol{q}) + \boldsymbol{\psi_\nu}(\boldsymbol{q})$$

$$\partial_t \alpha_1 = \mu(p_1 - p_2) + \nu \frac{g_2 - g_1}{\rho_I}, \qquad \partial_t(\rho \boldsymbol{u}) = 0$$

$$\partial_t(\alpha_1\rho_1) = \nu(g_2 - g_1),$$
$$\partial_t(\alpha_2\rho_2) = \nu(g_1 - g_2)$$

$$\partial_t(\alpha_1 E_1) = \mu p_I(p_2 - p_1) + H(T_2 - T_1) + \nu \boldsymbol{e_I}(g_2 - g_1),$$
$$\partial_t(\alpha_2 E_2) = \mu p_I(p_1 - p_2) + H(T_1 - T_2) + +\nu \boldsymbol{e_I}(g_1 - g_2)$$



- The initial values are coming from pressure-temperature relaxation solver.
- The mixture density (ρ) (not partial densities, $\alpha_k\rho_k$, due to $\dot{m} = \nu(g_2 - g_1)$), momentum ($\rho\boldsymbol{u}$), total energy (E),internal energy (ε) remain constant because these aren't related to thermal (H) and **chemical relaxation (ν) terms** as well as mechanical relaxation term (μ).

→ $\rho^0 = \rho^* = \rho^{**} = \rho^{***},\ (\rho\boldsymbol{u})^0 = (\rho\boldsymbol{u})^* = (\rho\boldsymbol{u})^{**} = (\rho\boldsymbol{u})^{***},\ E^0 = E^* = E^{**} = E^{***},\ \varepsilon^0 = \varepsilon^* = \varepsilon^{**} = \varepsilon^{***}$

→ $\rho^0 = \Sigma\alpha_k^{***}\rho_k^{***},\ \varepsilon^0 = \Sigma\alpha_k^{***}\varepsilon_k^{***}$

- In these equations, interface variables ($\rho_I,\ \boldsymbol{e_I}$) doesn't need to be specified.

➔ Using algebraic system (in case of SGEOS, quadratic eq.), equilibrium pressure (p^{***}) can be obtained. Then, also equilibrium values $T^{***}(p^{***}),\ \rho^{***}(p^{***}, T^{***}),\ \alpha_1^{***}(\rho^{***})$ are obtained.

- **5 equation model (pressure-velocity relaxation model)**
  - **Asymptotic limit with stiff pressure relaxation ($\mu \to \infty$)**
    - The equation that contain relaxation parameter (μ) are changed only.
      - Volume fraction equation

$$\frac{\partial \alpha_1}{\partial t} + \vec{u} \cdot \nabla \alpha_1 = \mu(p_1 - p_2) \Rightarrow \boldsymbol{\frac{d\alpha_1}{dt} = \mu(p_1 - p_2)}$$

      - Each phasic internal energy equations (with mass balance equation)

$$\frac{\partial \alpha_1 \rho_1 e_1}{\partial t} + \frac{\partial}{\partial x}(\alpha_1 \rho_1 e_1 \vec{u}) + \alpha_1 p_1 \frac{\partial \vec{u}}{\partial x} = \mu p_I (p_2 - p_1), \qquad \frac{d}{dt}(\alpha_1 \rho_1) + \alpha_1 \rho_1 \frac{\partial \vec{u}}{\partial x} = 0$$

$$\Rightarrow \boldsymbol{\alpha_1 \rho_1 \frac{de_1}{dt} + \alpha_1 p_1 \frac{d\vec{u}}{dx} = -p_I \mu(p_1 - p_2)}$$

$$\frac{\partial \alpha_2 \rho_2 e_2}{\partial t} + \frac{\partial}{\partial x}(\alpha_2 \rho_2 e_2 \vec{u}) + \alpha_2 p_2 \frac{\partial \vec{u}}{\partial x} = \mu p_I (p_1 - p_2), \qquad \frac{d}{dt}(\alpha_2 \rho_2) + \alpha_2 \rho_2 \frac{\partial \vec{u}}{\partial x} = 0$$

$$\Rightarrow \boldsymbol{\alpha_2 \rho_2 \frac{de_2}{dt} + \alpha_2 p_2 \frac{d\vec{u}}{dx} = p_I \mu(p_1 - p_2)}$$

    - Internal energy equations can be expressed as **pressure evolution equations** using $e_1 = e_1(\rho_1, p_1)$.

$$\alpha_1 \rho_1 \left(\left.\frac{\partial e_1}{\partial \rho_1}\right|_{p_1} \frac{d\rho_1}{dt} + \left.\frac{\partial e_1}{\partial p_1}\right|_{\rho_1} \frac{dp_1}{dt} + \frac{p_1}{\rho_1}\frac{\partial u}{\partial x} \right) = -p_I \mu (p_1 - p_2)$$

- **5 equation model (pressure-velocity relaxation model)**
  - **Asymptotic limit with stiff pressure relaxation ($\mu \to \infty$)**
    - Mass balance equation for phase 1 with volume fraction equation.

$$\frac{d}{dt}(\alpha_1\rho_1) + \alpha_1\rho_1\frac{\partial\vec{u}}{\partial x} = 0, \qquad \frac{d\alpha_1}{dt} = \mu(p_1 - p_2) \quad \Rightarrow \quad \frac{d\rho_1}{dt} = -\frac{\rho_1}{\alpha_1}\mu(p_1 - p_2) - \rho_1\frac{\partial\vec{u}}{\partial x}$$

$$\frac{dp_1}{dt} + \rho_1\frac{\frac{p_1}{\rho_1^2} - \left.\frac{\partial e_1}{\partial\rho_1}\right|_{p_1}}{\left.\frac{\partial e_1}{\partial p_1}\right|_{\rho_1}}\frac{\partial\vec{u}}{\partial x} = -\frac{\rho_1}{\alpha_1}\frac{\frac{p_I}{\rho_1^2} - \left.\frac{\partial e_1}{\partial\rho_1}\right|_{p_1}}{\left.\frac{\partial e_1}{\partial p_1}\right|_{\rho_1}}\mu(p_1 - p_2)$$

    - Sound speed definitions

$$c_1^2 = \frac{\frac{p_1}{\rho_1^2} - \left.\frac{\partial e_1}{\partial\rho_1}\right|_{p_1}}{\left.\frac{\partial e_1}{\partial p_1}\right|_{\rho_1}}, \qquad c_{1,I}^2 = \frac{\frac{p_I}{\rho_1^2} - \left.\frac{\partial e_1}{\partial\rho_1}\right|_{p_1}}{\left.\frac{\partial e_1}{\partial p_1}\right|_{\rho_1}}$$

    - Final form

$$\because \boldsymbol{\frac{dp_1}{dt} + \rho_1 c_1^2\frac{\partial\vec{u}}{\partial x} = -\frac{\rho_1}{\alpha_1}c_{1,I}^2\mu(p_1 - p_2)}$$

$$\boldsymbol{\frac{dp_2}{dt} + \rho_2 c_2^2\frac{\partial\vec{u}}{\partial x} = \frac{\rho_2}{\alpha_2}c_{2,I}^2\mu(p_1 - p_2)}$$

Appendix A

- **5 equation model (pressure-velocity relaxation model)**
  - **Asymptotic limit with stiff pressure relaxation ($\mu \rightarrow \infty$)**
    - Asymptotic expansion, $f = f^0 + \epsilon f^1$
      - f^0 : equilibrium state
      - f^1 : small perturbation around this state
      - $\epsilon \rightarrow 0^+$: Stiff pressure relaxation

$$\frac{dp_1}{dt} + \rho_1 c_1^2 \frac{\partial \vec{u}}{\partial x} = -\frac{\rho_1}{\alpha_1} c_{1,I}^2 \mu (p_1 - p_2)$$

$$\Rightarrow \left(\frac{dp_1^0}{dt} + \epsilon \frac{dp_1^1}{dt}\right) + (\rho_1^0 + \epsilon \rho_1^1)(c_1^0 + \epsilon c_1^1)^2 \left(\frac{\partial \vec{u}^0}{\partial x} + \epsilon \frac{\partial \vec{u}^1}{\partial x}\right) = -\frac{(\rho_1^0 + \epsilon \rho_1^1)}{(\alpha_1^0 + \epsilon \alpha_1^1)} (c_{1,I}^0 + \epsilon c_{1,I}^1)^2 \frac{1}{\epsilon} (p_1^0 + \epsilon p_1^1 - p_2^0 - \epsilon p_2^1)$$

$$\boldsymbol{\frac{dp_1^0}{dt} + \rho_1^0 {c_1^0}^2 \frac{\partial \vec{u}^0}{\partial x} = -\frac{\rho_1^0}{\alpha_1^0} {c_{1,I}^0}^2 \frac{1}{\epsilon} (p_1^0 + \epsilon p_1^1 - p_2^0 - \epsilon p_2^1)}$$

- Order $1/\epsilon$

$$\frac{1}{\epsilon}(p_1^0 - p_2^0) = 0$$

→ $p_1^0 = p_2^0 = p^0 = p_I^0$

→ ${c_1^0}^2 = {c_{1,I}^0}^2$, ${c_2^0}^2 = {c_{2,I}^0}^2$

Appendix A

- **5 equation model (pressure-velocity relaxation model)**
  - **Asymptotic limit with stiff pressure relaxation ($\mu \rightarrow \infty$)**
    - Asymptotic expansion, $f = f^0 + \epsilon f^1$
      - Zero – order

$$\frac{dp^0}{dt} + \rho_1^0 {c_1^0}^2 \frac{\partial \vec{u}^0}{\partial x} = -\frac{\rho_1^0}{\alpha_1^0} {c_1^0}^2 (p_1^1 - p_2^1)$$

$$\frac{dp^0}{dt} + \rho_2^0 {c_2^0}^2 \frac{\partial \vec{u}^0}{\partial x} = \frac{\rho_2^0}{\alpha_2^0} {c_2^0}^2 (p_1^1 - p_2^1)$$

$$\Rightarrow p_1^1 - p_2^1 = \frac{\rho_2^0 {c_2^0}^2 - \rho_1^0 {c_1^0}^2}{\frac{\rho_2^0}{\alpha_2^0} {c_2^0}^2 + \frac{\rho_1^0}{\alpha_1^0} {c_1^0}^2} \frac{\partial \vec{u}^0}{\partial x}$$

- In the limit $\mu \rightarrow \infty$, volume fraction equation

$$\because \boldsymbol{\frac{d\alpha_1}{dt} = \frac{\rho_2 c_2^2 - \rho_1 c_1^2}{\frac{\rho_2}{\alpha_2} c_2^2 + \frac{\rho_1}{\alpha_1} c_1^2} \frac{\partial \vec{u}}{\partial x}}$$

Appendix B

- **Method of Characteristics**
  - **1D, unsteady isentropic flow**
    - Differential equation
      - Mass equation

$$\frac{d\rho}{dt} + \rho \frac{\partial u}{\partial x} = 0$$

      - Momentum equation

$$\rho \frac{du}{dt} = -p \frac{\partial p}{\partial x}$$

      - Energy equation (isentropic equation)

$$\frac{ds}{dt} = 0$$

    - Using these equations, it can be expressed by characteristics line form.
      - Non-linear differential equations.

$$\frac{\partial}{\partial t}\left(u + \frac{2}{\gamma - 1}a\right) + (u + a)\frac{\partial}{\partial x}\left(u + \frac{2}{\gamma - 1}a\right) = 0$$

$$\frac{\partial}{\partial t}\left(u - \frac{2}{\gamma - 1}a\right) + (u - a)\frac{\partial}{\partial x}\left(u - \frac{2}{\gamma - 1}a\right) = 0$$

        - Because a propagation velocity is different at each point on the wave, wave form are changed. → **shock formation in finite compression region.**

Method of Characteristics

1D, unsteady isentropic flow

- If assuming small perturbance (weak wave), it has linearity. → **acoustic equations**

$$\frac{\partial}{\partial t}\left(\frac{u}{a}\right)+a\frac{\partial}{\partial x}\left(\frac{\rho'}{\rho}\right)=0 \qquad \frac{\partial}{\partial t}\left(\frac{\rho'}{\rho}\right)+a\frac{\partial}{\partial x}\left(\frac{u}{a}\right)=0$$

- Wave equations

$$\frac{\partial^2}{\partial t^2}\left(\frac{u}{a}\right)-a^2\frac{\partial^2}{\partial x^2}\left(\frac{u}{a}\right)=0 \qquad \frac{\partial^2}{\partial t^2}\left(\frac{\rho'}{\rho}\right)-a^2\frac{\partial^2}{\partial x^2}\left(\frac{\rho'}{\rho}\right)=0$$

- Equations can be expressed by other variables ($\eta = x + at, \zeta = x - at$)
  - Chain rule

$$\frac{\partial}{\partial t}=\frac{\partial}{\partial \zeta}\frac{\partial \zeta}{\partial t}+\frac{\partial}{\partial \eta}\frac{\partial \eta}{\partial t}=-a\frac{\partial}{\partial \zeta}+a\frac{\partial}{\partial \eta}$$

$$\frac{\partial}{\partial x}=\frac{\partial}{\partial \zeta}\frac{\partial \zeta}{\partial x}+\frac{\partial}{\partial \eta}\frac{\partial \eta}{\partial x}=\frac{\partial}{\partial \zeta}+\frac{\partial}{\partial \eta}$$

$$\frac{\partial^2}{\partial t^2}=\frac{\partial}{\partial t}\left(\frac{\partial}{\partial t}\right)=\frac{\partial}{\partial \zeta}\left(\frac{\partial}{\partial t}\right)\frac{\partial \zeta}{\partial t}+\frac{\partial}{\partial \eta}\left(\frac{\partial}{\partial t}\right)\frac{\partial \eta}{\partial t}=-a\left(-a\frac{\partial}{\partial \zeta}+a\frac{\partial}{\partial \eta}\right)\frac{\partial}{\partial \zeta}+a\left(a\frac{\partial}{\partial \zeta}+a\frac{\partial}{\partial \eta}\right)\frac{\partial}{\partial \eta}=a^2\left(\frac{\partial^2}{\partial \zeta^2}-2\frac{\partial^2}{\partial \zeta \partial \eta}+\frac{\partial^2}{\partial \eta^2}\right)$$

$$\frac{\partial^2}{\partial x^2}=\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}\right)=\frac{\partial}{\partial \zeta}\left(\frac{\partial}{\partial x}\right)\frac{\partial \zeta}{\partial x}+\frac{\partial}{\partial \eta}\left(\frac{\partial}{\partial x}\right)\frac{\partial \eta}{\partial x}=\left(\frac{\partial}{\partial \zeta}+\frac{\partial}{\partial \eta}\right)\frac{\partial}{\partial \zeta}+\left(\frac{\partial}{\partial \zeta}+\frac{\partial}{\partial \eta}\right)\frac{\partial}{\partial \eta}=\frac{\partial^2}{\partial \zeta^2}+2\frac{\partial^2}{\partial \zeta \partial \eta}+\frac{\partial^2}{\partial \eta^2}$$

Appendix B

- **Method of Characteristics**
  - **1D, unsteady isentropic flow**
    - Equations can be expressed by other variables ($\eta = x + at$, $\zeta = x - at$)

$$\frac{\partial^2}{\partial\zeta\partial\eta}\left(\frac{u}{a}\right) = 0 \qquad \frac{\partial^2}{\partial\zeta\partial\eta}\left(\frac{\rho'}{\rho}\right) = 0$$

- Solution

$$\frac{u}{a} = \int \frac{dF(\zeta)}{d\zeta} d\zeta + G(\eta) = F(\zeta) + G(\eta) = F(x - at) + G(x + at)$$

$$\frac{\rho'}{\rho} = \int \frac{df(\zeta)}{d\zeta} d\zeta + g(\eta) = f(\zeta) + g(\eta) = f(x - at) + g(x + at)$$

- Substitute to acoustic equations

$$-af' + ag' + a(F' + G') = 0 \qquad -aF' + aG' + a(f + g') = 0$$

$$\Rightarrow G(\eta) = g(\eta), \qquad F(\zeta) = f(\zeta)$$

- Final form

$$\frac{u}{a} = f(x - at) - g(x + at) \qquad \frac{\rho'}{\rho} = f(x - at) + g(x + at)$$

  - u/a, ρ'/ρ are right or left facing waves propagated at constant velocity ($dx/dt = a$).
  - Because this equations have linearity, wave form does not changed.

Method of Characteristics

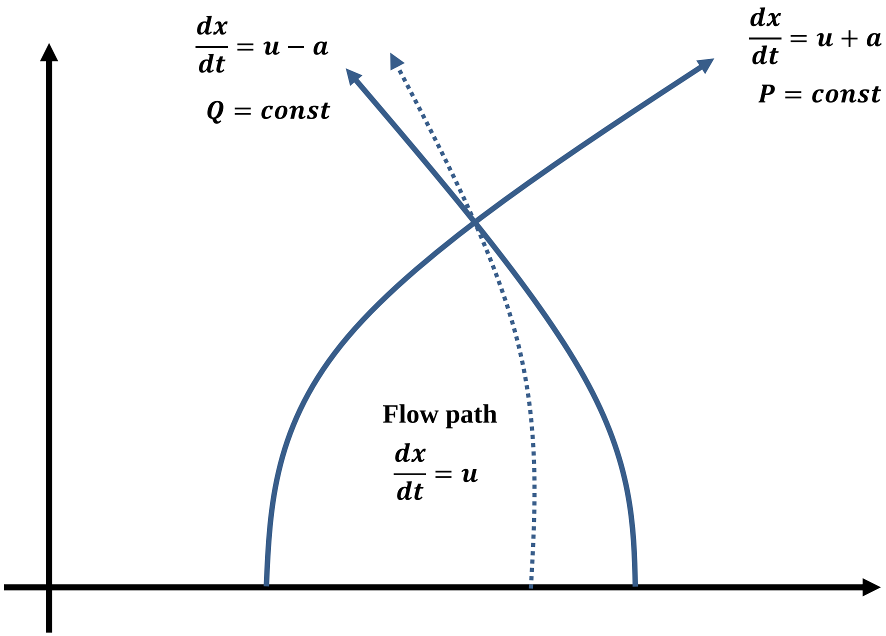
1D, unsteady isentropic flow

- Finite wave (non-linear differential equations).

$$\frac{\partial P}{\partial t} + (u+a)\frac{\partial P}{\partial x} = 0 \qquad \frac{\partial Q}{\partial t} + (u-a)\frac{\partial Q}{\partial x} = 0$$

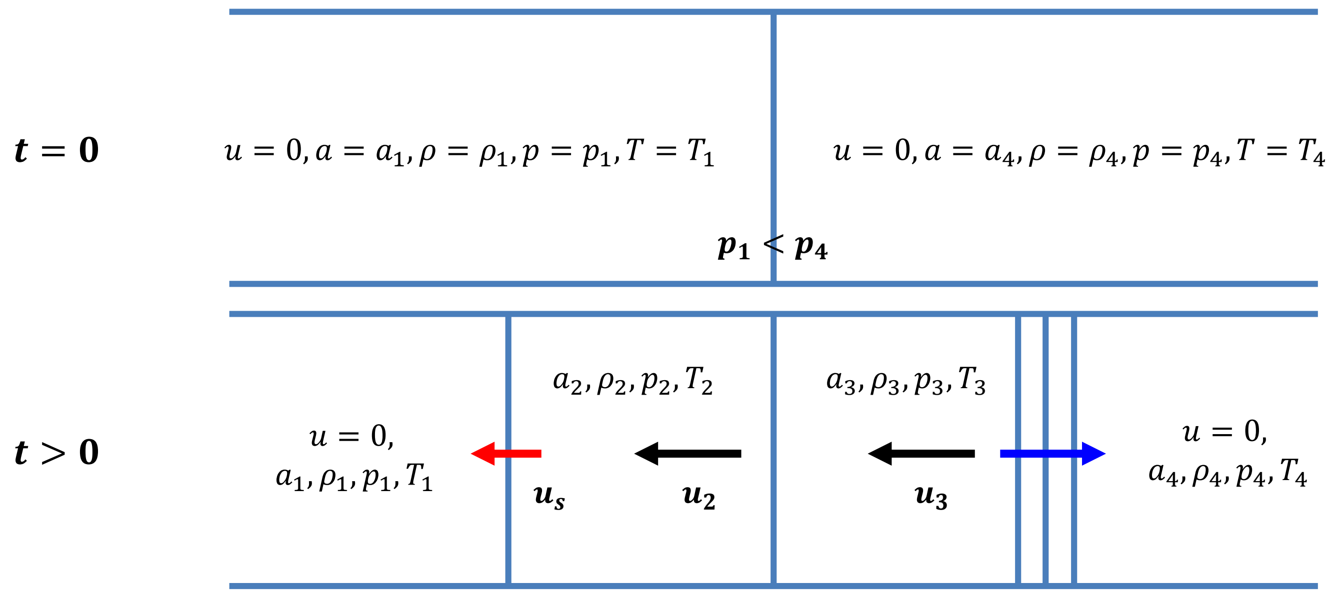
- Where P, Q are Riemann invariants which mean constant value along the characteristics line.

$$P = u + \frac{2}{\gamma - 1}a, \qquad Q = u - \frac{2}{\gamma - 1}a$$



Appendix C

Shock tube problem (Riemann problem)



- Across the contact wave, there are different fluids.
  - After diaphragm raptured, fluids does not penetrated each other (not mixed)
  - In other to contact wave is maintained, pressure and normal velocity have to same across the contact wave.

$$p_2 = p_3, \qquad u_2 = u_3$$

Appendix C

- **HLL approximate Riemann solvers**
  - **Across the contact wave, there are different fluids.**
    - After diaphragm raptured, fluids does not penetrated each other (not mixed)
    - In other to contact wave is maintained, pressure and normal velocity have to same across the contact wave.