November, 2011

Modelling and Simulation of Liquid-Vapor Phase Transition

A contribution to the study of the boiling crisis

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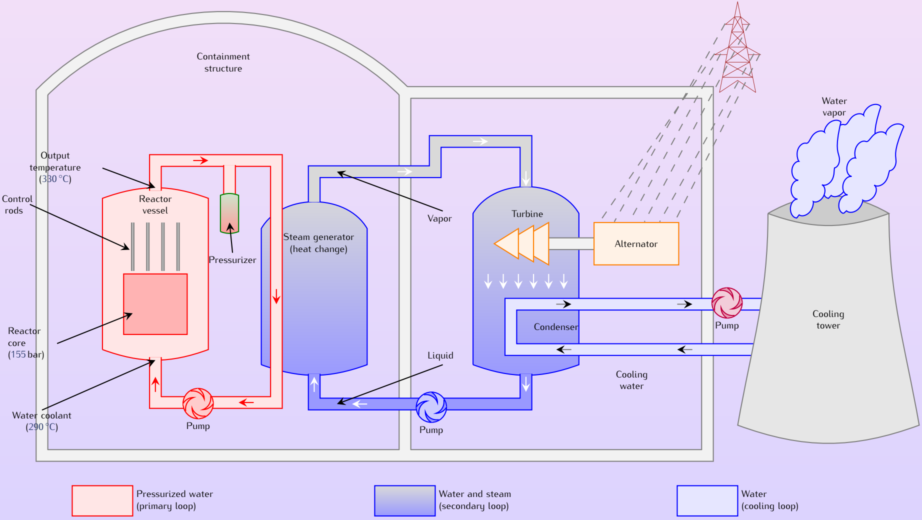
Outline

Pressurized Water Reactor



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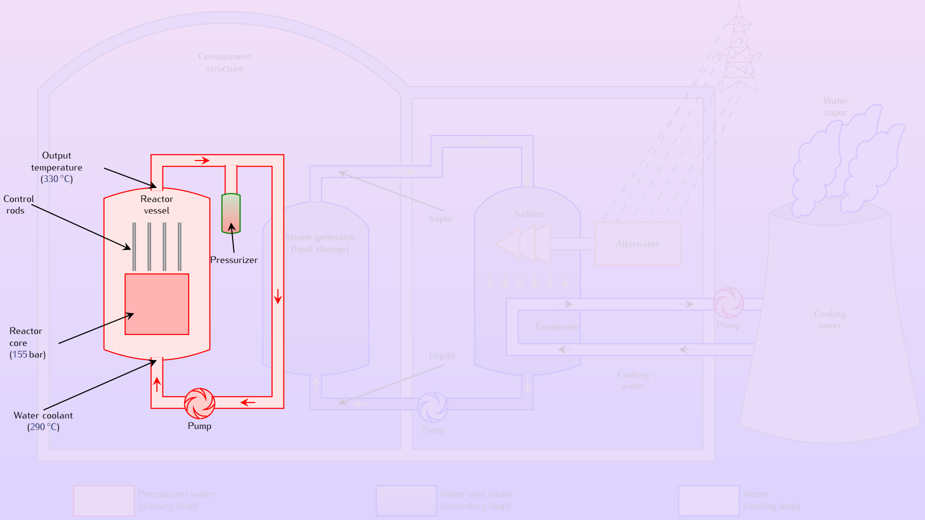

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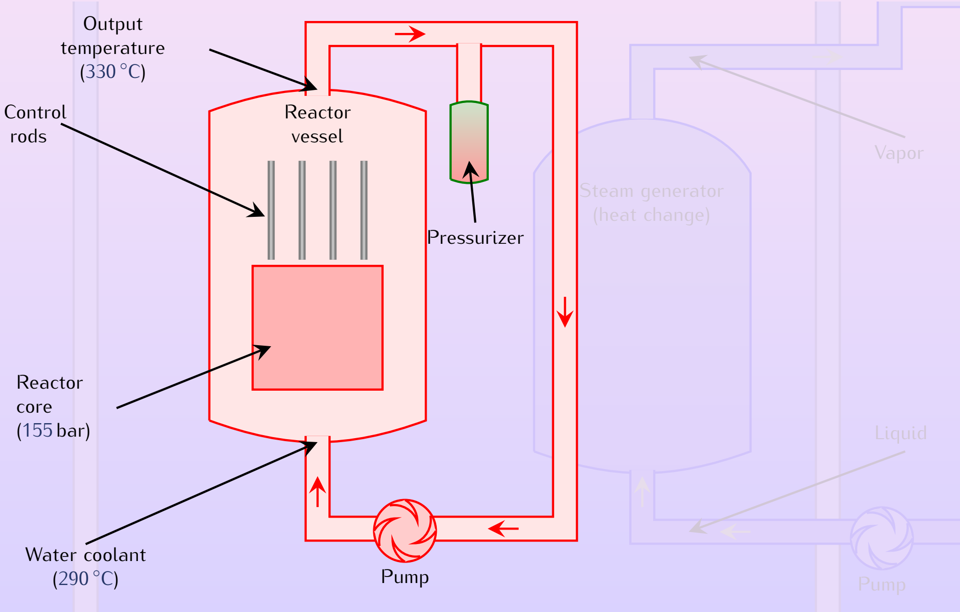
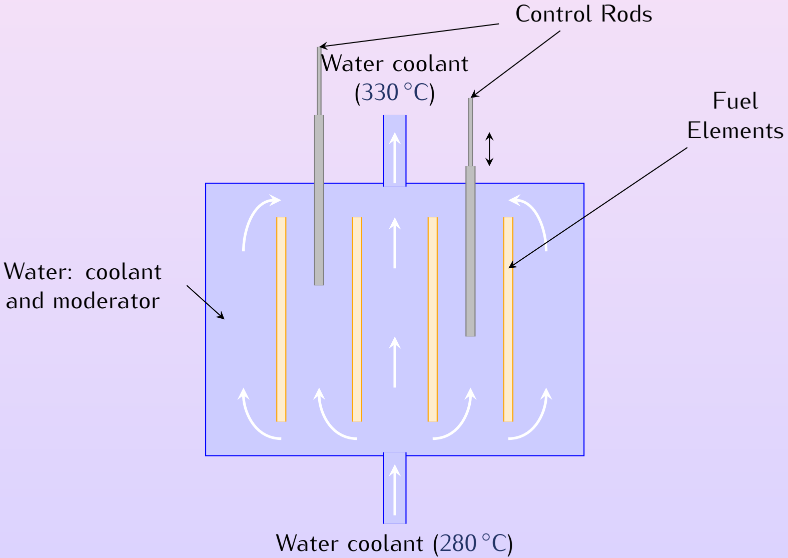


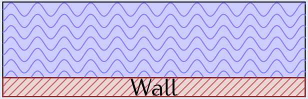
Core of a Pressurized Water Reactor



Boiling Crisis

Phenomenon

Liquid phase heated by a wall at a fixed temperature T^{wall}.
When T^{wall} increases, we switch from a Nucleate Boiling to a Film Boiling.



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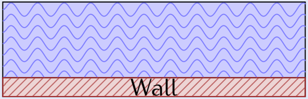

Nucleate Boiling

source: http://www.spaceflight.esa.int/users/fluids/TT_boiling.htm

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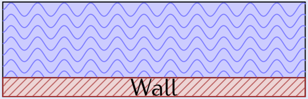

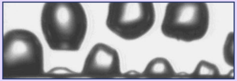

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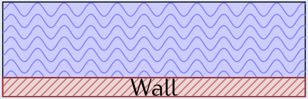

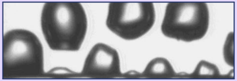

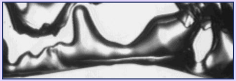

Nucleate Boiling → Film Boiling

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Outline

"Ingredients" of the Model

- Simulating all bubbles (no mixture),
- System of PDEs for the fluid flow (monophasic or diphasic),
- Phase transition (pressure and/or temperature variations),

- Heat Diffusion,
- Surface Tension,
- Gravity.

Outline

Euler System

$$
\begin{cases}
\partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0,\\
\partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u}\otimes \mathbf{u} + P\, \mathbb{I}) = \mathfrak{V}_{\text{vf}} - \mathfrak{S}_{\text{sf}},\\
\partial_t\left(\varrho\left(\frac{|\mathbf{u}|^2}{2}+\varepsilon\right)\right) + \operatorname{div}\left(\varrho\left(\frac{|\mathbf{u}|^2}{2}+\varepsilon\right)\mathbf{u} + P\,\mathbf{u}\right) = (\mathfrak{V}_{\text{vf}} - \mathfrak{S}_{\text{sf}})\cdot\mathbf{u} - \operatorname{div}(q).
\end{cases}
$$

Unknowns:

- $(\mathbf{x}, t) \mapsto \varrho$ specific density,
- $(\mathbf{x}, t) \mapsto \varepsilon$ specific internal energy,
- $(\mathbf{x}, t) \mapsto \mathbf{u}$ velocity;

Source terms:

- $(\varrho, \varepsilon) \mapsto \mathfrak{V}_{\text{vf}}$ body forces,
- $(\varrho, \varepsilon) \mapsto \mathfrak{S}_{\text{sf}}$ surface forces,
- $(\varrho, \varepsilon) \mapsto \operatorname{div}(q)$ heat transfer.

EOS: $(\varrho, \varepsilon) \mapsto P$

Euler System

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Outline

EOS OF EACH PHASE $\alpha = \text{liq}, \text{vap}$

$\tau = 1/\varrho$ specific volume

ε specific internal energy

$(\tau, \varepsilon) \mapsto s_\alpha$ specific entropy (Hessian matrix neg. def.);

$$\begin{cases} T_\alpha \stackrel{\text{def}}{=} \left(\left.\dfrac{\partial s_\alpha}{\partial \varepsilon}\right|_\tau \right)^{-1} > 0 & \text{temperature,} \\ P_\alpha \stackrel{\text{def}}{=} T_\alpha \left.\dfrac{\partial s_\alpha}{\partial \tau}\right|_\varepsilon > 0 & \text{pressure,} \\ g_\alpha \stackrel{\text{def}}{=} \varepsilon + P_\alpha \tau - T_\alpha s_\alpha & \text{free enthalpy (Gibbs potential),} \\ (c_\alpha)^2 \stackrel{\text{def}}{=} \tau^2 \left(P_\alpha \left.\dfrac{\partial P_\alpha}{\partial \varepsilon}\right|_\tau - \left.\dfrac{\partial P_\alpha}{\partial \tau}\right|_\varepsilon \right) & \text{speed of sound.} \end{cases}$$

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Example: stiffened gas

$$(\tau,\varepsilon)\mapsto s_\alpha = c_{v_\alpha}\ln(\varepsilon - q_\alpha - \pi_\alpha\tau) + c_{v_\alpha}(\gamma_\alpha - 1)\ln\tau + m_\alpha$$

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$$c_\alpha^2 = \gamma_\alpha(\gamma_\alpha - 1)(\varepsilon - q_\alpha - \pi_\alpha\tau) = \gamma_\alpha(P_\alpha + \pi_\alpha)\tau = \gamma_\alpha(\gamma_\alpha - 1)c_{v_\alpha}T_\alpha > 0.$$

Phase	c_v [J kg^{-1} K^{-1}]	γ	π [Pa]	q [J kg^{-1}]	m [J kg^{-1} K^{-1}]
Liquid	1816.2	2.35	10^9	-1167.056×10^3	-32765.55596
Vapor	1040.14	1.43	0	2030.255×10^3	-33265.65947

Table: Parameters proposed by [O. Le Metayer] for water and steam: $\gamma > 1$ adiabatic coefficient, π molecular attraction, q binding energy.

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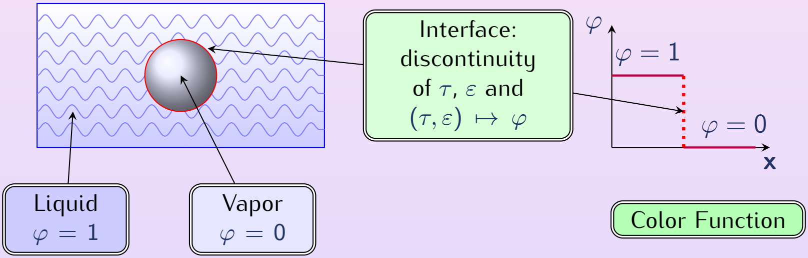
Liquid–Vapor Interface



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- Goal ①: define $(\tau,\varepsilon)\mapsto\varphi$ for physical values of (τ,ε)
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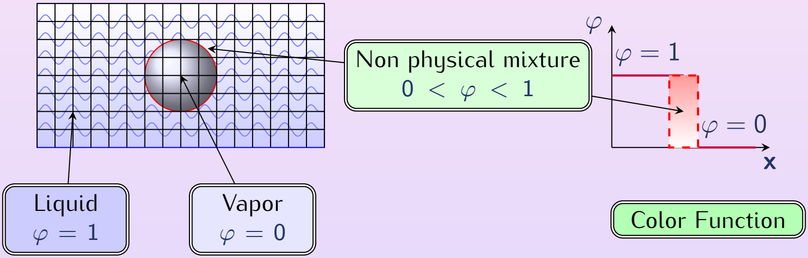

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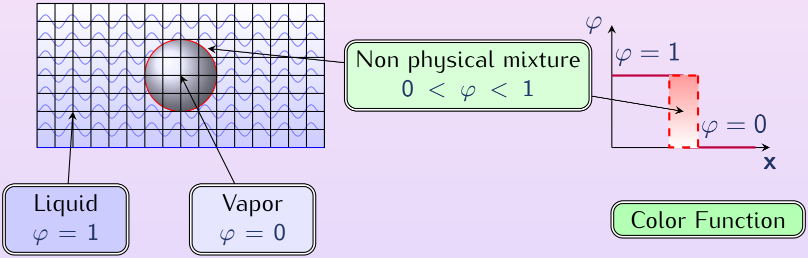

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EOS of a Mixture

- y mass fraction
- $\begin{cases} \tau \stackrel{\text{def}}{=} y\tau_{\text{liq}} + (1-y)\tau_{\text{vap}} \\ \varepsilon \stackrel{\text{def}}{=} y\varepsilon_{\text{liq}} + (1-y)\varepsilon_{\text{vap}} \end{cases}$
- z volume fraction s.t. $y\tau_{\text{liq}} = z\tau$
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Entropy without phase change

$$\sigma \stackrel{\text{def}}{=} ys_{\text{liq}}(\tau_{\text{liq}}, \varepsilon_{\text{liq}}) + (1-y)s_{\text{vap}}(\tau_{\text{vap}}, \varepsilon_{\text{vap}})$$

$$= ys_{\text{liq}}\left(\frac{z}{y}\tau, \frac{\psi}{y}\varepsilon\right) + (1-y)s_{\text{vap}}\left(\frac{1-z}{1-y}\tau, \frac{1-\psi}{1-y}\varepsilon\right)$$

$$P = \left(\left.\frac{\partial\sigma}{\partial\varepsilon}\right|_{\tau;y,z,\psi}\right)^{-1} \left.\frac{\partial\sigma}{\partial\tau}\right|_{\varepsilon;y,z,\psi}$$

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EOS of Phase Change

Entropy at equilibrium

$$(\tau,\varepsilon) \mapsto s^{\text{eq}}(\tau,\varepsilon) = \sigma(\tau,\varepsilon,z^{\text{eq}}(\tau,\varepsilon),y^{\text{eq}}(\tau,\varepsilon),\psi^{\text{eq}}(\tau,\varepsilon))$$

Definition [H. Callen, Ph. Helluy ...]

Optimization Problem:

$$s^{\text{eq}}(\tau,\varepsilon) \stackrel{\text{def}}{=} \max_{z,y,\psi\in[0,1]^3} \sigma(\tau,\varepsilon,z,y,\psi)$$

Optimality Condition: $\begin{cases} T_{\text{liq}}(z,y,\psi) = T_{\text{vap}}(z,y,\psi) \\ P_{\text{liq}}(z,y,\psi) = P_{\text{vap}}(z,y,\psi) \\ g_{\text{liq}}(z,y,\psi) = g_{\text{vap}}(z,y,\psi) \end{cases}$

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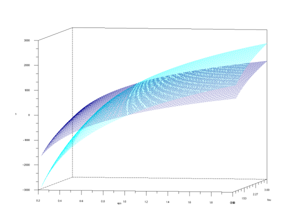

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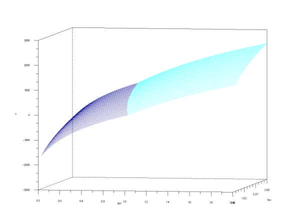

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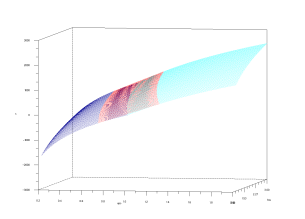

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Optimization Problem:

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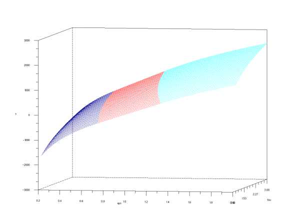
$$= \text{co}\left\{ \max\left\{ s_{\text{liq}}(\tau,\varepsilon), s_{\text{vap}}(\tau,\varepsilon)\right\}\right\}$$



Optimality Condition: $\begin{cases} T_{\text{liq}}(z,y,\psi) = T_{\text{vap}}(z,y,\psi) \\ P_{\text{liq}}(z,y,\psi) = P_{\text{vap}}(z,y,\psi) \\ g_{\text{liq}}(z,y,\psi) = g_{\text{vap}}(z,y,\psi) \end{cases}$

Analytical EOS

(τ, ε) fixed

$(\tau_{\text{liq}}, \varepsilon_{\text{liq}}, \tau_{\text{vap}}, \varepsilon_{\text{vap}}, y)$ solution of

$$\begin{cases} P_{\text{liq}}(\tau_{\text{liq}}, \varepsilon_{\text{liq}}) = P_{\text{vap}}(\tau_{\text{vap}}, \varepsilon_{\text{vap}}) \\ T_{\text{liq}}(\tau_{\text{liq}}, \varepsilon_{\text{liq}}) = T_{\text{vap}}(\tau_{\text{vap}}, \varepsilon_{\text{vap}}) \\ g_{\text{liq}}(\tau_{\text{liq}}, \varepsilon_{\text{liq}}) = g_{\text{vap}}(\tau_{\text{vap}}, \varepsilon_{\text{vap}}) \\ \tau = y\tau_{\text{liq}} + (1-y)\tau_{\text{vap}} \\ \varepsilon = y\varepsilon_{\text{liq}} + (1-y)\varepsilon_{\text{vap}} \end{cases}$$

(P, T) solution of

$$\begin{cases} \tau_\alpha = \tau_\alpha(P, T) \\ \varepsilon_\alpha = \varepsilon_\alpha(P, T) \\ g_{\text{liq}}(P, T) = g_{\text{vap}}(P, T) \\ \\ y = \dfrac{\tau - \tau_{\text{vap}}(P, T)}{\tau_{\text{liq}}(P, T) - \tau_{\text{vap}}(P, T)} = \dfrac{\varepsilon - \varepsilon_{\text{vap}}(P, T)}{\varepsilon_{\text{liq}}(P, T) - \varepsilon_{\text{vap}}(P, T)} \end{cases}$$

$$T \mapsto P = P^{\text{sat}}(T)$$

T solution of

$$\frac{\tau - \tau_{\text{vap}}^{\text{sat}}(T)}{\tau_{\text{liq}}^{\text{sat}}(T) - \tau_{\text{vap}}^{\text{sat}}(T)} = \frac{\varepsilon - \varepsilon_{\text{vap}}^{\text{sat}}(T)}{\varepsilon_{\text{liq}}^{\text{sat}}(T) - \varepsilon_{\text{vap}}^{\text{sat}}(T)} \quad \text{where} \quad \begin{pmatrix} \tau \\ \varepsilon \end{pmatrix}_\alpha^{\text{sat}}(T) \stackrel{\text{def}}{=} \begin{pmatrix} \tau \\ \varepsilon \end{pmatrix}_\alpha (P^{\text{sat}}(T), T)$$

Analytical EOS

(τ, ε) fixed

$(\tau_{\text{liq}}, \varepsilon_{\text{liq}}, \tau_{\text{vap}}, \varepsilon_{\text{vap}}, y)$ SOLUTION OF

$$\begin{cases} P_{\text{liq}}(\tau_{\text{liq}}, \varepsilon_{\text{liq}}) = P_{\text{vap}}(\tau_{\text{vap}}, \varepsilon_{\text{vap}}) \\ T_{\text{liq}}(\tau_{\text{liq}}, \varepsilon_{\text{liq}}) = T_{\text{vap}}(\tau_{\text{vap}}, \varepsilon_{\text{vap}}) \\ g_{\text{liq}}(\tau_{\text{liq}}, \varepsilon_{\text{liq}}) = g_{\text{vap}}(\tau_{\text{vap}}, \varepsilon_{\text{vap}}) \\ \tau = y\tau_{\text{liq}} + (1-y)\tau_{\text{vap}} \\ \varepsilon = y\varepsilon_{\text{liq}} + (1-y)\varepsilon_{\text{vap}} \end{cases}$$

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$T \mapsto P = P^{\text{sat}}(T)$

T SOLUTION OF

$$\frac{\tau - \tau^{\text{sat}}_{\text{vap}}(T)}{\tau^{\text{sat}}_{\text{liq}}(T) - \tau^{\text{sat}}_{\text{vap}}(T)} = \frac{\varepsilon - \varepsilon^{\text{sat}}_{\text{vap}}(T)}{\varepsilon^{\text{sat}}_{\text{liq}}(T) - \varepsilon^{\text{sat}}_{\text{vap}}(T)} \quad \text{where} \quad \begin{pmatrix}\tau \\ \varepsilon\end{pmatrix}^{\text{sat}}_\alpha (T) \stackrel{\text{def}}{=} \begin{pmatrix}\tau \\ \varepsilon\end{pmatrix}_\alpha (P^{\text{sat}}(T), T)$$

Analytical EOS

(τ, ε) fixed

$(\tau_{\text{liq}}, \varepsilon_{\text{liq}}, \tau_{\text{vap}}, \varepsilon_{\text{vap}}, y)$ SOLUTION OF

$$\begin{cases} P_{\text{liq}}(\tau_{\text{liq}}, \varepsilon_{\text{liq}}) = P_{\text{vap}}(\tau_{\text{vap}}, \varepsilon_{\text{vap}}) \\ T_{\text{liq}}(\tau_{\text{liq}}, \varepsilon_{\text{liq}}) = T_{\text{vap}}(\tau_{\text{vap}}, \varepsilon_{\text{vap}}) \\ g_{\text{liq}}(\tau_{\text{liq}}, \varepsilon_{\text{liq}}) = g_{\text{vap}}(\tau_{\text{vap}}, \varepsilon_{\text{vap}}) \\ \tau = y\tau_{\text{liq}} + (1-y)\tau_{\text{vap}} \\ \varepsilon = y\varepsilon_{\text{liq}} + (1-y)\varepsilon_{\text{vap}} \end{cases}$$

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Analytical EOS

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$(\tau_{liq}, \varepsilon_{liq}, \tau_{vap}, \varepsilon_{vap}, y)$ solution of

$$\begin{cases} P_{liq}(\tau_{liq}, \varepsilon_{liq}) = P_{vap}(\tau_{vap}, \varepsilon_{vap}) \\ T_{liq}(\tau_{liq}, \varepsilon_{liq}) = T_{vap}(\tau_{vap}, \varepsilon_{vap}) \\ g_{liq}(\tau_{liq}, \varepsilon_{liq}) = g_{vap}(\tau_{vap}, \varepsilon_{vap}) \\ \tau = y\tau_{liq} + (1-y)\tau_{vap} \\ \varepsilon = y\varepsilon_{liq} + (1-y)\varepsilon_{vap} \end{cases}$$

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Speed of sound

Theorem

If $\tau^*_{\text{liq}} \neq \tau^*_{\text{vap}}$ and $\varepsilon^*_{\text{liq}} \neq \varepsilon^*_{\text{vap}}$ (first order phase transition) then $c^{\text{eq}}(\tau,\varepsilon) > 0$.

$$(c^{\text{eq}})^2 \stackrel{\text{def}}{=} \tau^2 \left(P^{\text{eq}} \left.\frac{\partial P^{\text{eq}}}{\partial \varepsilon}\right|_{\tau} - \left.\frac{\partial P^{\text{eq}}}{\partial \tau}\right|_{\varepsilon} \right) = \underbrace{-\tau^2 T^{\text{eq}}}_{<0} \underbrace{\begin{bmatrix} P^{\text{eq}}, -1 \end{bmatrix} \begin{bmatrix} s^{\text{eq}}_{\varepsilon\varepsilon} & s^{\text{eq}}_{\tau\varepsilon} \\ s^{\text{eq}}_{\tau\varepsilon} & s^{\text{eq}}_{\tau\tau} \end{bmatrix} \begin{bmatrix} P^{\text{eq}} \\ -1 \end{bmatrix}}_{\leq 0}$$

Hessian matrix of $(\tau,\varepsilon) \mapsto s^{\text{eq}}$

- for all (τ,ε) pure phase state

$$\mathbf{v}^T \, \mathrm{d}^2 s^{\text{eq}}(\tau,\varepsilon) \, \mathbf{v} < 0 \quad \forall \, \mathbf{v} \neq \mathbf{0},$$

- for all (τ,ε) equilibrium mixture state

$$\exists \, \mathbf{v}(\tau,\varepsilon) \neq \mathbf{0} \ \text{ s.t. } \mathbf{v}^T \, \mathrm{d}^2 s^{\text{eq}}(\tau,\varepsilon) \, \mathbf{v} = 0.$$

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$$\forall (\tau,\varepsilon) \text{ equilibrium mixture state, } \mathbf{v}(\tau,\varepsilon) \stackrel{?}{\equiv} [P^{\text{eq}}(\tau,\varepsilon), -1]$$

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Outline

Outline

1. Context
2. Model
   - Governing equations
   - Equation of State
3. Numerical Approximation and Example
   - Conservation Laws
   - Numerical Scheme
   - Numerical Example
4. Conclusion

Dynamic Liquid–Vapor Phase Change

Euler System

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0, \\ \partial_t (\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u} + P^{\text{eq}}\, \mathbb{I}) = 0 \\ \partial_t \left(\varrho \left(\frac{|\mathbf{u}|^2}{2} + \varepsilon \right) \right) + \operatorname{div} \left(\varrho \left(\frac{|\mathbf{u}|^2}{2} + \varepsilon \right) \mathbf{u} + P^{\text{eq}} \mathbf{u} \right) = 0 \end{cases} \quad \text{with} \quad P^{\text{eq}} \stackrel{\text{def}}{=} \frac{s_\tau^{\text{eq}}}{s_\varepsilon^{\text{eq}}}.$$

Mathematical Properties

If $\tau^*_{\text{liq}} \neq \tau^*_{\text{vap}}$ and $\varepsilon^*_{\text{liq}} \neq \varepsilon^*_{\text{vap}}$ (first order phase transition) then

1. Euler system: strict hyperbolicity ($\sim$ p-system),
2. Riemann problem: multitude of entropy (Lax) solutions [R. Menikoff, B. J. Plohr], uniqueness of Liu solution.

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Outline

Numerical Scheme based on Relaxation Approach

$\sigma(y, z, \psi, \tau, \varepsilon)$ —Optimization→ $s^{\text{eq}}(\tau, \varepsilon)$

Off Equilibrium

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0 \\ \partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u} + P\,\mathbb{I}) = 0 \\ \partial_t(\varrho e) + \operatorname{div}((\varrho e + P)\mathbf{u}) = 0 \\ \partial_t z + \mathbf{u} \cdot \mathbf{grad}\, z = \\ \partial_t y + \mathbf{u} \cdot \mathbf{grad}\, y = \\ \partial_t \psi + \mathbf{u} \cdot \mathbf{grad}\, \psi = \end{cases}$$

$\xrightarrow[\mu_j \to \infty]{}$

Equilibrium

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0 \\ \partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u} + P^{\text{eq}}\,\mathbb{I}) = 0 \\ \partial_t(\varrho e) + \operatorname{div}((\varrho e + P^{\text{eq}})\mathbf{u}) = 0 \end{cases}$$

$$P^{\text{eq}}(\varrho, \varepsilon) = \frac{s^{\text{eq}}_\tau}{s^{\text{eq}}_\varepsilon}$$

Two Steps:

1. Hydrodynamic (+ gravity, surface tension, heat diffusion, ...)
2. Projection by solving the Phase-Change Equation

Numerical Scheme based on Relaxation Approach

$\sigma(y,z,\psi,\tau,\varepsilon)$ $\xrightarrow{\text{Optimization}}$ $s^{\text{eq}}(\tau,\varepsilon)$

Off Equilibrium

$$\begin{cases}\partial_t\varrho+\operatorname{div}(\varrho\mathbf{u})=0\\ \partial_t(\varrho\mathbf{u})+\operatorname{div}(\varrho\mathbf{u}\otimes\mathbf{u}+P\,\mathbb{I})=0\\ \partial_t(\varrho e)+\operatorname{div}((\varrho e+P)\mathbf{u})=0\\ \partial_t z+\mathbf{u}\cdot\mathbf{grad}\,z=\mu_z(z^{\text{eq}}-z)\\ \partial_t y+\mathbf{u}\cdot\mathbf{grad}\,y=\mu_y(y^{\text{eq}}-y)\\ \partial_t\psi+\mathbf{u}\cdot\mathbf{grad}\,\psi=\mu_\psi(\psi^{\text{eq}}-\psi)\end{cases}$$

$$P(\varrho,\varepsilon,z,y,\psi)=\frac{\sigma_\tau}{\sigma_\varepsilon}$$

$\xrightarrow[\mu_j\to\infty]{}$

Equilibrium

$$\begin{cases}\partial_t\varrho+\operatorname{div}(\varrho\mathbf{u})=0\\ \partial_t(\varrho\mathbf{u})+\operatorname{div}(\varrho\mathbf{u}\otimes\mathbf{u}+P^{\text{eq}}\,\mathbb{I})=0\\ \partial_t(\varrho e)+\operatorname{div}((\varrho e+P^{\text{eq}})\mathbf{u})=0\end{cases}$$

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Two Steps:

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Numerical Scheme based on Relaxation Approach

$\sigma(y, z, \psi, \tau, \varepsilon)$ → Optimization → $s^{eq}(\tau, \varepsilon)$

Off Equilibrium

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0 \\ \partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u} + P\,\mathbb{I}) = 0 \\ \partial_t(\varrho e) + \operatorname{div}((\varrho e + P)\mathbf{u}) = 0 \\ \partial_t z + \mathbf{u} \cdot \mathbf{grad}\, z = 0 \\ \partial_t y + \mathbf{u} \cdot \mathbf{grad}\, y = 0 \\ \partial_t \psi + \mathbf{u} \cdot \mathbf{grad}\, \psi = 0 \end{cases}$$

$$P(\varrho, \varepsilon, z, y, \psi) = \frac{\sigma_\tau}{\sigma_\varepsilon}$$

$\mu_j \to \infty$

Equilibrium

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0 \\ \partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u} + P^{eq}\,\mathbb{I}) = 0 \\ \partial_t(\varrho e) + \operatorname{div}((\varrho e + P^{eq})\mathbf{u}) = 0 \end{cases}$$

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Two Steps:

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Numerical Scheme based on Relaxation Approach

$\sigma(y,z,\psi,\tau,\varepsilon)$ —Optimization→ $s^{eq}(\tau,\varepsilon)$

Off Equilibrium

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0 \\ \partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u} + P\,\mathbb{I}) = 0 \\ \partial_t(\varrho e) + \operatorname{div}((\varrho e + P)\mathbf{u}) = 0 \\ \partial_t z + \mathbf{u} \cdot \mathbf{grad}\, 0 = \mu_z(z^{eq} - z) \\ \partial_t y + \mathbf{u} \cdot \mathbf{grad}\, 0 = \mu_y(y^{eq} - y) \\ \partial_t \psi + \mathbf{u} \cdot \mathbf{grad}\, 0 = \mu_\psi(\psi^{eq} - \psi) \end{cases}$$

$$P(\varrho,\varepsilon,z,y,\psi) = \frac{\sigma_\tau}{\sigma_\varepsilon}$$

$\xrightarrow{\mu_j \to \infty}$

Equilibrium

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0 \\ \partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u} + P^{eq}\,\mathbb{I}) = 0 \\ \partial_t(\varrho e) + \operatorname{div}((\varrho e + P^{eq})\mathbf{u}) = 0 \end{cases}$$

$$P^{eq}(\varrho,\varepsilon) = \frac{s^{eq}_\tau}{s^{eq}_\varepsilon}$$

Two Steps:

1. Hydrodynamic (+ gravity, surface tension, heat diffusion, ...)
2. Projection by solving the Phase-Change Equation

Off equilibrium systems

1. Lagrangian: $\mathcal{L}(\varrho, \mathbf{u}, \sigma, y, z, \psi) \stackrel{\text{def}}{=} \varrho\left(\frac{|\mathbf{u}|^2}{2} - \varepsilon(\varrho, \sigma, y, z, \psi)\right)$

   Action: $\mathcal{A}(\nu) \stackrel{\text{def}}{=} \int_{t_1}^{t_2} \int_{\widehat{\Omega}(t;\nu)} \mathcal{L}(\widehat{\varrho}, \widehat{\varrho\mathbf{u}}, \widehat{s}, \widehat{y}, \widehat{z}, \widehat{\psi})(\widehat{\mathbf{x}}, t; \nu)\, \mathrm{d}\widehat{\mathbf{x}}\, \mathrm{d}\, t$

   Minimization of the Action: $\frac{\mathrm{d}\,\mathcal{A}}{\mathrm{d}\,\nu}(\nu = 0) = 0$
2. Energy: $\varepsilon \stackrel{\text{def}}{=} \sum_\alpha y_\alpha \varepsilon_\alpha\left(\frac{z_\alpha}{y_\alpha}\frac{1}{\varrho}, \frac{\psi_\alpha}{y_\alpha}\sigma\right)$
3. Positive Entropy Production: $\mathrm{D}_t\sigma \geq 0$

$$\begin{cases} \partial_t\varrho + \operatorname{div}(\varrho\mathbf{u}) = 0 \\ \partial_t(\varrho\mathbf{u}) + \operatorname{div}(\varrho\mathbf{u}\otimes\mathbf{u} + P\,\mathbb{I}) = 0 \\ \partial_t(\varrho e) + \operatorname{div}((\varrho e + P)\mathbf{u}) = 0 \\ \partial_t z + \mathbf{u}\cdot\mathbf{grad}\, z = \mu_z(z^{\text{eq}} - z) \\ \partial_t y + \mathbf{u}\cdot\mathbf{grad}\, y = \mu_y(y^{\text{eq}} - y) \\ \partial_t\psi + \mathbf{u}\cdot\mathbf{grad}\,\psi = \mu_\psi(\psi^{\text{eq}} - \psi) \end{cases}$$

$$P(\varrho, \varepsilon, z, y, \psi) = \frac{\sigma_\tau}{\sigma_\varepsilon}$$

$$\begin{cases} \partial_t\varrho + \operatorname{div}(\varrho\mathbf{u}) = 0 \\ \partial_t(\varrho\mathbf{u}) + \operatorname{div}(\varrho\mathbf{u}\otimes\mathbf{u} + P\,\mathbb{I}) = 0 \\ \partial_t(\varrho e) + \operatorname{div}((\varrho e + P)\mathbf{u}) = 0 \\ \partial_t z + \mathbf{u}\cdot\mathbf{grad}\, z = \mu_z(z^{\text{eq}} - z) \\ \partial_t y + \mathbf{u}\cdot\mathbf{grad}\, y = \mu_y(y^{\text{eq}} - y) \end{cases}$$

$T^{\text{liq}} = T^{\text{vap}}$ in the mixture

$$P(\tau, \varepsilon, z, y, \psi^{\text{eq}}(\tau, \varepsilon)) = \frac{\sigma_\tau}{\sigma_\varepsilon}$$

Off equilibrium systems

1. Lagrangian: $\mathcal{L}(\varrho,\mathbf{u},\sigma,y,z,\psi)\stackrel{\text{def}}{=}\varrho\left(\frac{|\mathbf{u}|^2}{2}-\varepsilon(\varrho,\sigma,y,z,\psi)\right)$

   Action: $\mathcal{A}(\nu)\stackrel{\text{def}}{=}\int_{t_1}^{t_2}\int_{\widehat{\Omega}(t;\nu)}\mathcal{L}(\widehat{\varrho},\widehat{\varrho\mathbf{u}},\widehat{s},\widehat{y},\widehat{z},\widehat{\psi})(\widehat{\mathbf{x}},t;\nu)\,\mathrm{d}\widehat{\mathbf{x}}\,\mathrm{d}t$

   Minimization of the Action: $\frac{\mathrm{d}\mathcal{A}}{\mathrm{d}\nu}(\nu=0)=0$
2. Energy: $\varepsilon\stackrel{\text{def}}{=}\sum_\alpha y_\alpha\varepsilon_\alpha\left(\frac{z_\alpha}{y_\alpha}\frac{1}{\varrho},\frac{\psi_\alpha}{y_\alpha}\sigma\right)$
3. Positive Entropy Production: $\mathrm{D}_t\sigma\geq 0$

$$\begin{cases}\partial_t\varrho+\operatorname{div}(\varrho\mathbf{u})=0\\ \partial_t(\varrho\mathbf{u})+\operatorname{div}(\varrho\mathbf{u}\otimes\mathbf{u}+P\,\mathbb{I})=0\\ \partial_t(\varrho e)+\operatorname{div}((\varrho e+P)\mathbf{u})=0\\ \partial_t z+\mathbf{u}\cdot\mathbf{grad}\,z=\mu_z(z^{\text{eq}}-z)\\ \partial_t y+\mathbf{u}\cdot\mathbf{grad}\,y=\mu_y(y^{\text{eq}}-y)\\ \partial_t\psi+\mathbf{u}\cdot\mathbf{grad}\,\psi=\mu_\psi(\psi^{\text{eq}}-\psi)\end{cases}$$

$$P(\varrho,\varepsilon,z,y,\psi)=\frac{\sigma_\tau}{\sigma_\varepsilon}$$

$$\begin{cases}\partial_t\varrho+\operatorname{div}(\varrho\mathbf{u})=0\\ \partial_t(\varrho\mathbf{u})+\operatorname{div}(\varrho\mathbf{u}\otimes\mathbf{u}+P\,\mathbb{I})=0\\ \partial_t(\varrho e)+\operatorname{div}((\varrho e+P)\mathbf{u})=0\\ \partial_t z+\mathbf{u}\cdot\mathbf{grad}\,z=\mu_z(z^{\text{eq}}-z)\\ \partial_t y+\mathbf{u}\cdot\mathbf{grad}\,y=\mu_y(y^{\text{eq}}-y)\end{cases}$$

$T^{\text{liq}}=T^{\text{vap}}$ in the mixture

$$P(\tau,\varepsilon,z,y,\psi^{\text{eq}}(\tau,\varepsilon))=\frac{\sigma_\tau}{\sigma_\varepsilon}$$

Hydrodynamic step

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0 \\ \partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u} + P\,\mathbb{I}) = 0 \\ \partial_t(\varrho e) + \operatorname{div}((\varrho e + P)\mathbf{u}) = 0 \\ \partial_t z + \mathbf{u} \cdot \mathbf{grad}\, z = 0 \\ \partial_t y + \mathbf{u} \cdot \mathbf{grad}\, y = 0 \end{cases}$$

$T^{\text{liq}} = T^{\text{vap}}$ in the mixture

$$P(\varrho, \varepsilon, z, y) = \frac{\sigma_\tau}{\sigma_\varepsilon}$$

Scheme:
Roe quasi-conservative [S. Kokh]

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0 \\ \partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u} + P\,\mathbb{I}) = 0 \\ \partial_t(\varrho e) + \operatorname{div}((\varrho e + P)\mathbf{u}) = 0 \\ \partial_t z + \mathbf{u} \cdot \mathbf{grad}\, z = 0 \\ \partial_t y + \mathbf{u} \cdot \mathbf{grad}\, y = 0 \end{cases}$$

$P^{\text{liq}} = P^{\text{vap}}$ in the mixture

$$P(\varrho, \varepsilon, z, y) = \frac{\sigma_\tau}{\sigma_\varepsilon}$$

Scheme:
antidiffusive [Lagoutière and Kokh]

Hydrodynamic step

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0 \\ \partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u} + P\,\mathbb{I}) = 0 \\ \partial_t(\varrho e) + \operatorname{div}((\varrho e + P)\mathbf{u}) = 0 \\ \partial_t z + \mathbf{u} \cdot \mathbf{grad}\, z = 0 \\ \partial_t y + \mathbf{u} \cdot \mathbf{grad}\, y = 0 \end{cases}$$

$T^{\text{liq}} = T^{\text{vap}}$ in the mixture

$$P(\varrho, \varepsilon, z, y) = \frac{\sigma_\tau}{\sigma_\varepsilon}$$

Scheme:
Roe quasi-conservative [S. Kokh]

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0 \\ \partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u} + P\,\mathbb{I}) = 0 \\ \partial_t(\varrho e) + \operatorname{div}((\varrho e + P)\mathbf{u}) = 0 \\ \partial_t z + \mathbf{u} \cdot \mathbf{grad}\, z = 0 \\ \partial_t y + \mathbf{u} \cdot \mathbf{grad}\, y = 0 \end{cases}$$

$P^{\text{liq}} = P^{\text{vap}}$ in the mixture

$$P(\varrho, \varepsilon, z, y) = \frac{\sigma_\tau}{\sigma_\varepsilon}$$

Scheme:
antidiffusive [Lagoutière and Kokh]

Projection step

In each cell, (τ, ε) is computed in the hydrodynamic step and we update the fractions as follows:

1. T^*: solution of the Phase-Change Equation:

$$\frac{\tau - \tau_{\text{vap}}(T, P^{\text{sat}}(T))}{\tau_{\text{liq}}(T, P^{\text{sat}}(T)) - \tau_{\text{vap}}(T, P^{\text{sat}}(T))} = \frac{\varepsilon - \varepsilon_{\text{vap}}(T, P^{\text{sat}}(T))}{\varepsilon_{\text{liq}}(T, P^{\text{sat}}(T)) - \varepsilon_{\text{vap}}(T, P^{\text{sat}}(T))}$$

2. $\tau^*_\alpha \stackrel{\text{def}}{=} \tau_\alpha(T^*, P^{\text{sat}}(T^*)), \quad \varepsilon^*_\alpha \stackrel{\text{def}}{=} \varepsilon_\alpha(T^*, P^{\text{sat}}(T^*)), \quad y^* = y(T^*, P^{\text{sat}}(T^*)).$
3. 3.1. if $0 < y^* < 1$ then (τ, ε) is a saturated state and we set

$$y^{\text{eq}} = y^*, \qquad z^{\text{eq}} = y^* \tau^*_{\text{liq}}/\tau, \qquad \psi^{\text{eq}} = y^* \varepsilon^*_{\text{liq}}/\varepsilon,$$

   3.2. otherwise, if y^* is outside the range $(0, 1)$,

   3.2.1. if $s_{\text{liq}}(\tau, \varepsilon) > s_{\text{vap}}(\tau, \varepsilon)$ then (τ, ε) is a liquid state, therefore we set

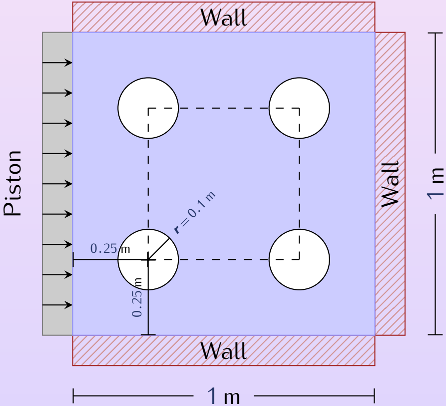
$$y^{\text{eq}}(\tau, \varepsilon) = 1, \qquad z^{\text{eq}}(\tau, \varepsilon) = 1, \qquad \psi^{\text{eq}}(\tau, \varepsilon) = 1,$$

   3.2.2. if $s_{\text{liq}}(\tau, \varepsilon) < s_{\text{vap}}(\tau, \varepsilon)$ then τ, ε is a vapor state, therefore we set

$$y^{\text{eq}}(\tau, \varepsilon) = 0, \qquad z^{\text{eq}}(\tau, \varepsilon) = 0, \qquad \psi^{\text{eq}}(\tau, \varepsilon) = 0,$$

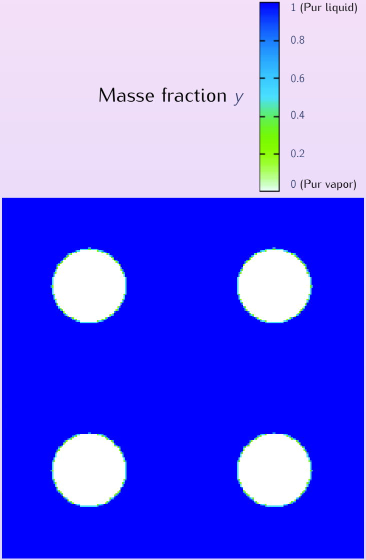
Outline

Compression of Vapor Bubbles

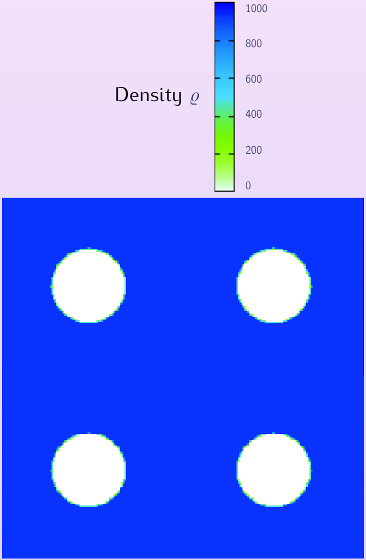


Compression of Vapor Bubbles

Masse fraction y

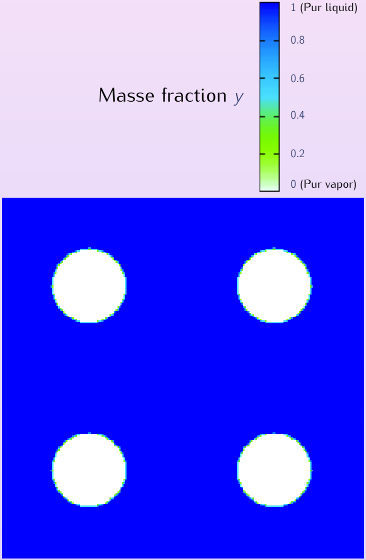


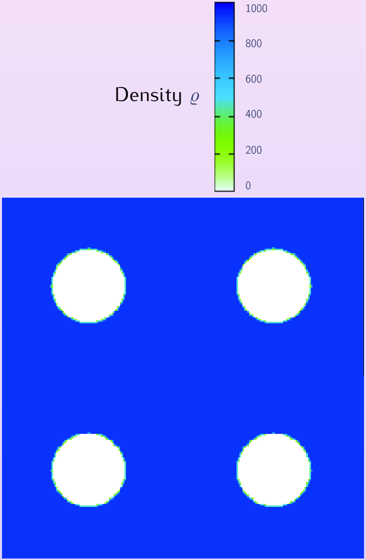
Density ϱ



◂ Geometry ▸ Play ▸▸ Skip

Compression of Vapor Bubbles





◂ Geometry ▸ Play ▸▸ Skip

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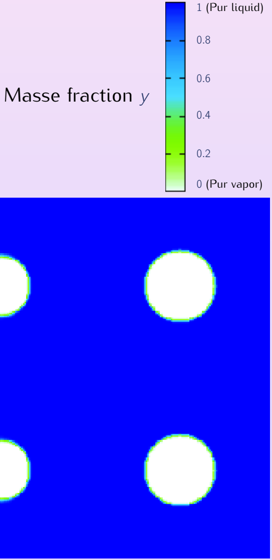

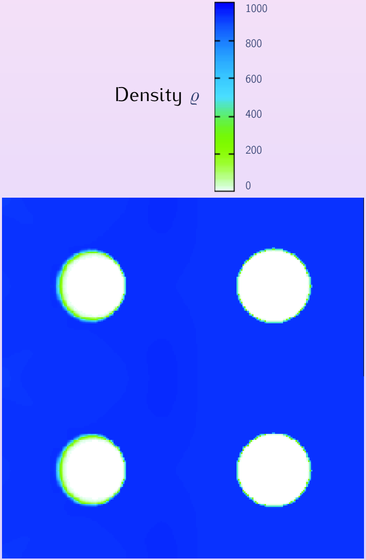

◂ Geometry ▸ Play ▸▸ Skip

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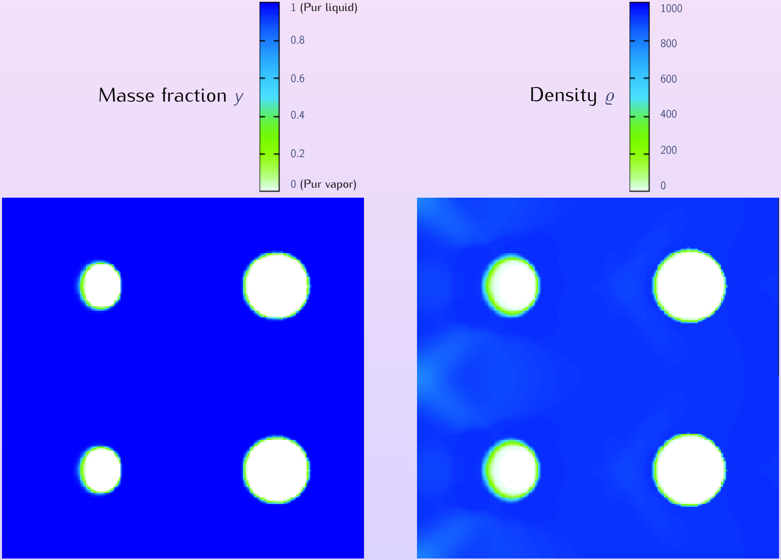

◂ Geometry ▸ Play ▸▸ Skip

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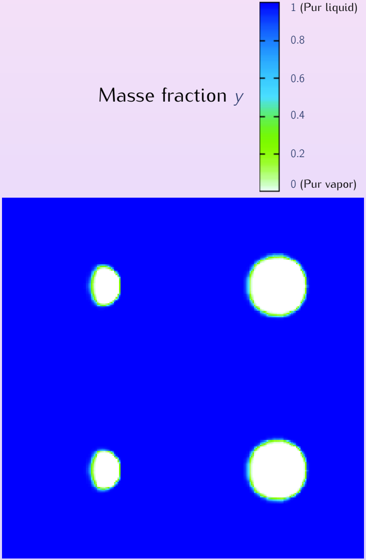

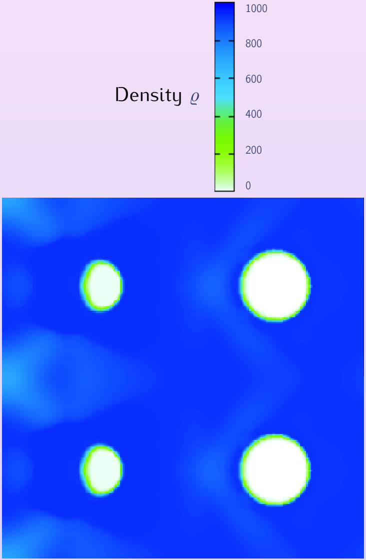

◂ Geometry ▸ Play ▸▸ Skip

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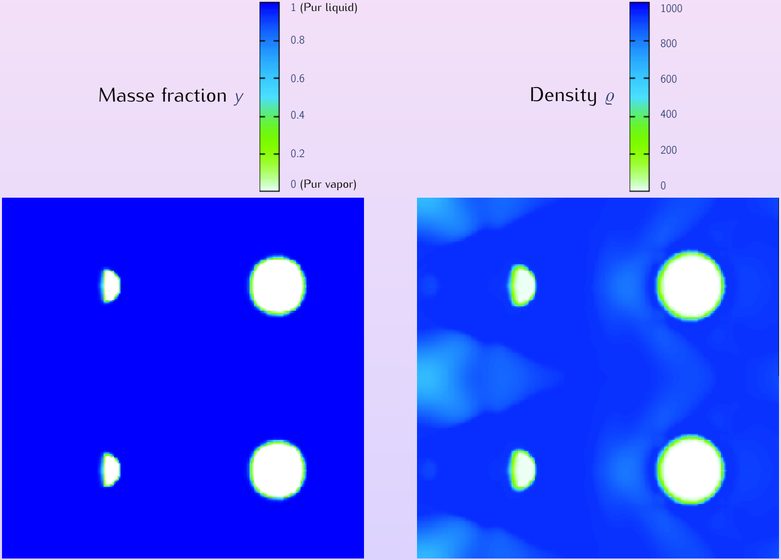
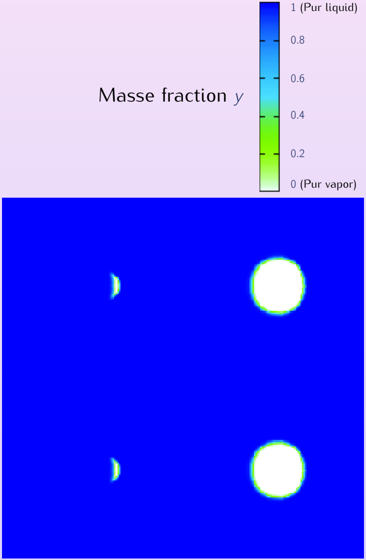


◂ Geometry ▸ Play ▸▸ Skip

Compression of Vapor Bubbles

Masse fraction y



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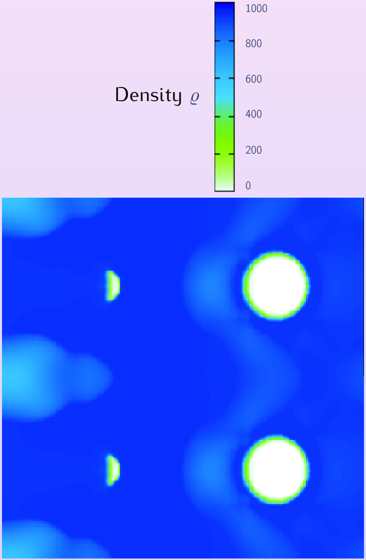
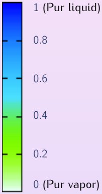


Geometry Play Skip

Compression of Vapor Bubbles

Masse fraction y



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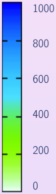
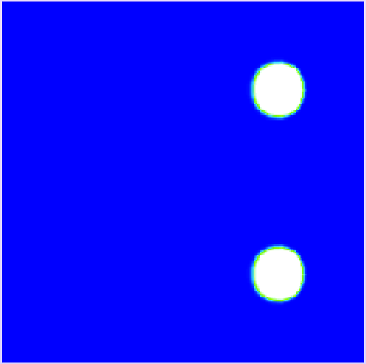
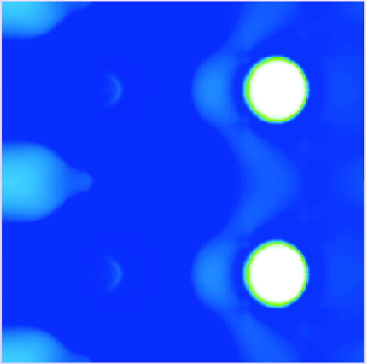
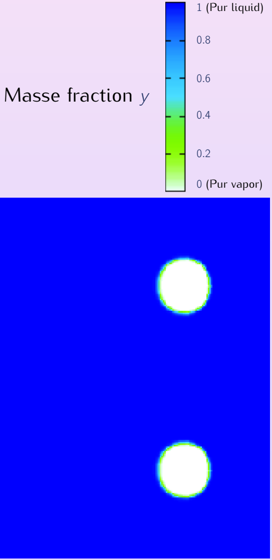


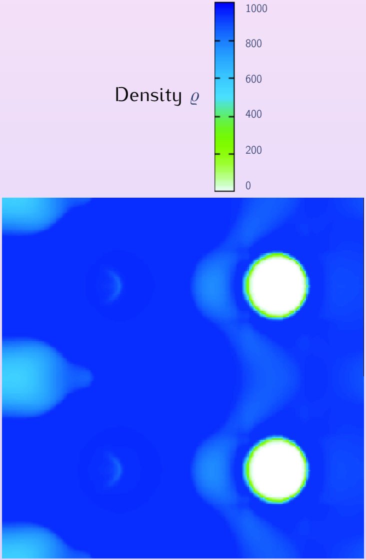




Geometry Play Skip

Compression of Vapor Bubbles





Geometry Play Skip

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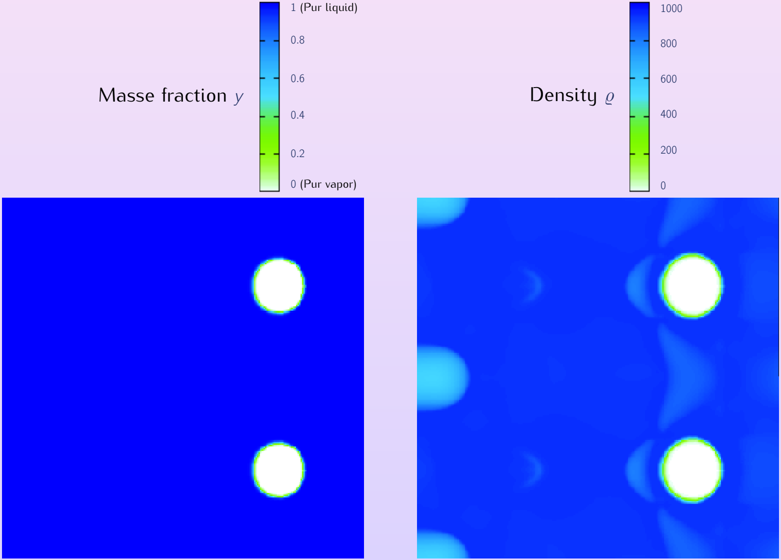
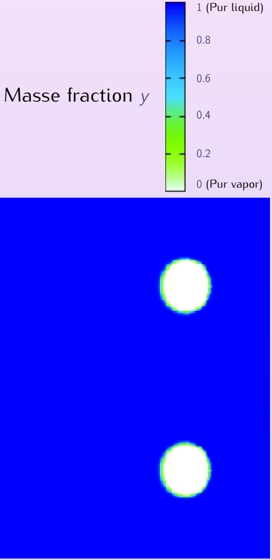
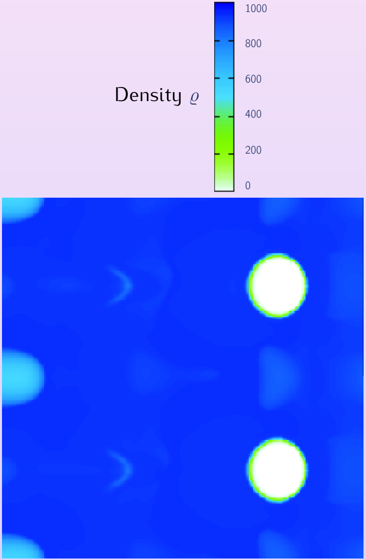


Geometry Play Skip

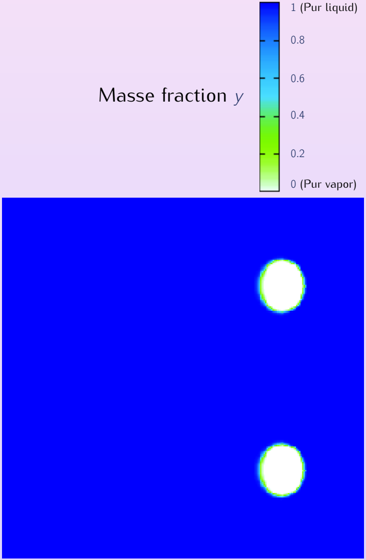
Compression of Vapor Bubbles

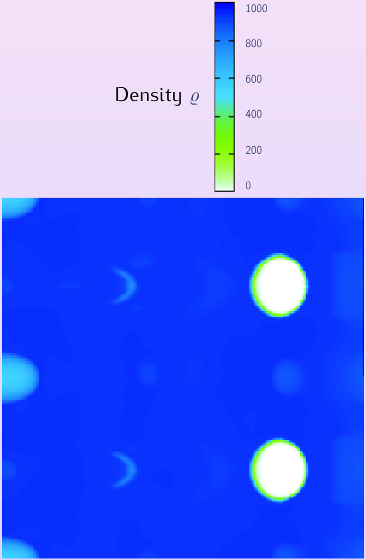




◀ Geometry ▶ Play ▶▶ Skip

Compression of Vapor Bubbles





◂ Geometry ▸ Play ▸▸ Skip

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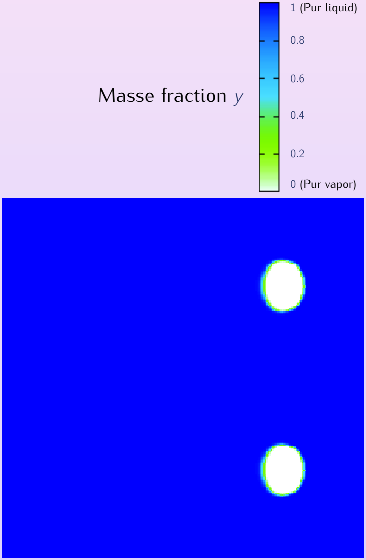

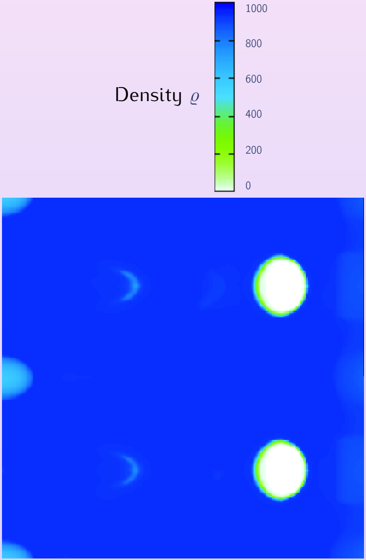

◀ Geometry ▶ Play ▶▶ Skip

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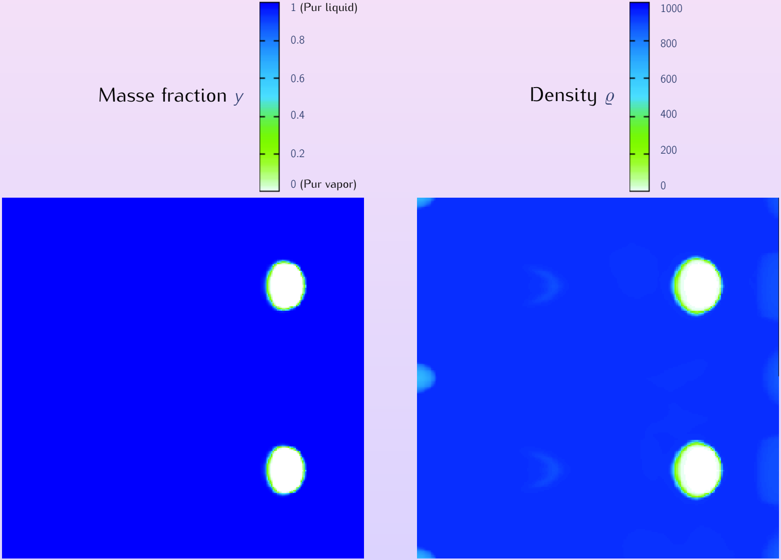
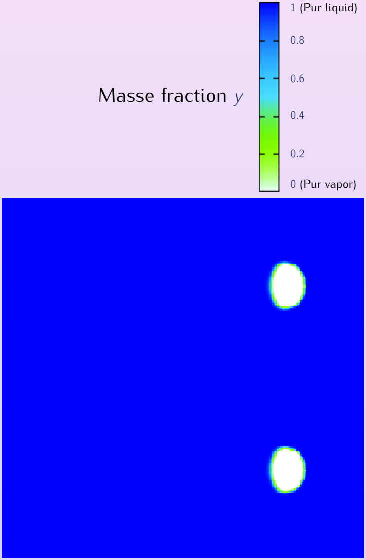


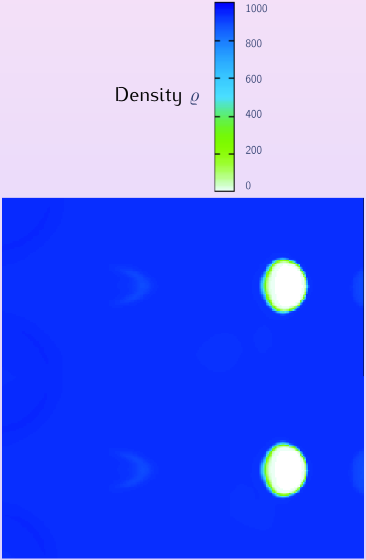
◂ Geometry ▸ Play ▸▸ Skip

Compression of Vapor Bubbles

Masse fraction y



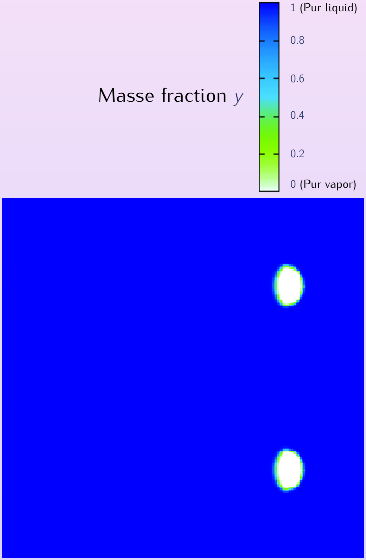
Density ϱ



Geometry Play Skip

Compression of Vapor Bubbles

Masse fraction y



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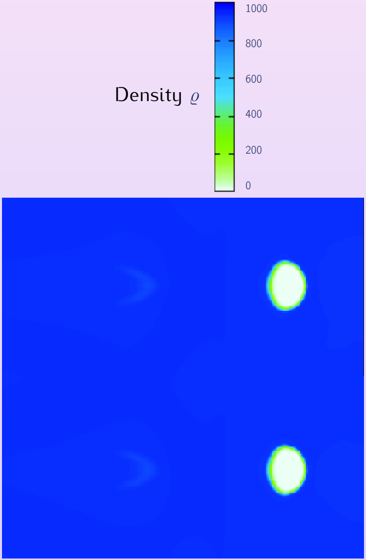

Geometry Play Skip

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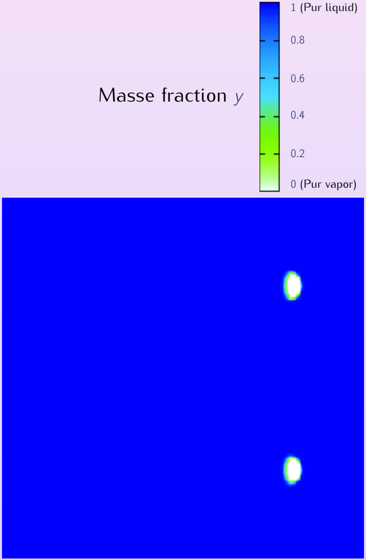
Masse fraction y



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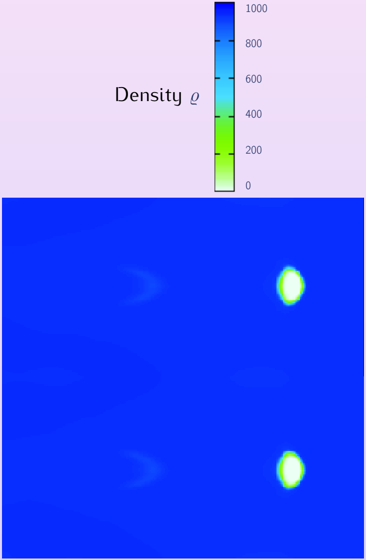
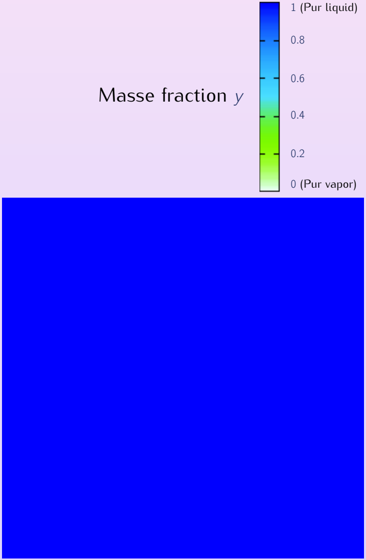
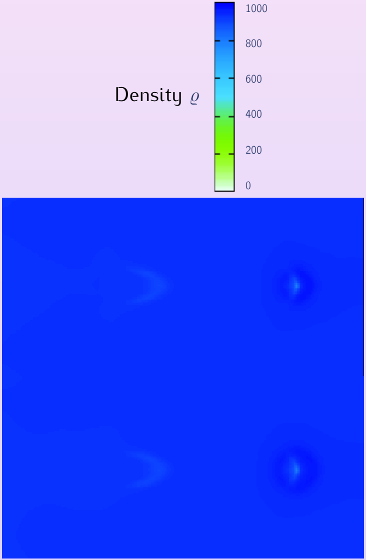


◂ Geometry ▸ Play ▸▸ Skip

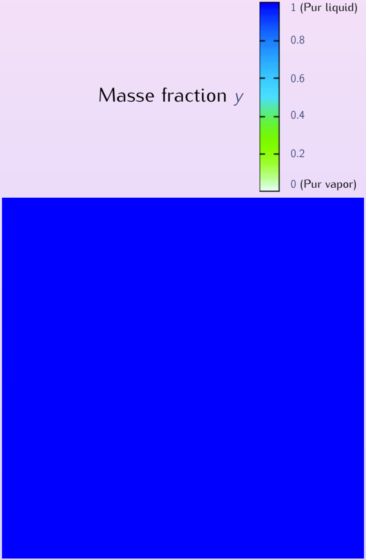
Compression of Vapor Bubbles

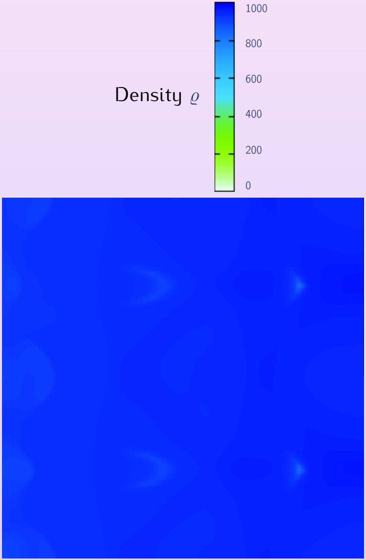




◂ Geometry ▸ Play ▸▸ Skip

Compression of Vapor Bubbles

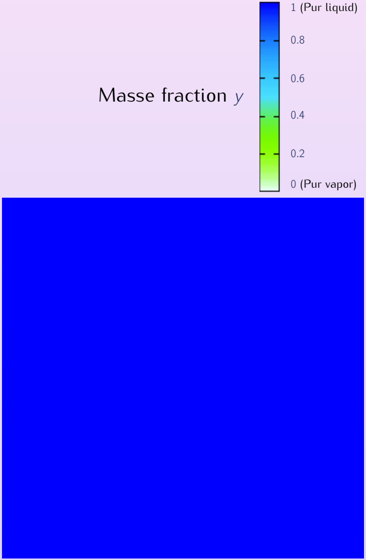




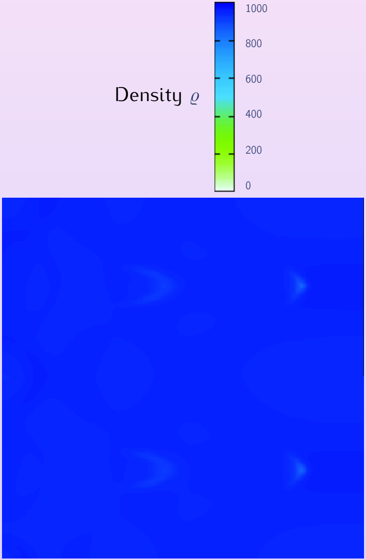
Geometry Play Skip

Compression of Vapor Bubbles

Masse fraction y

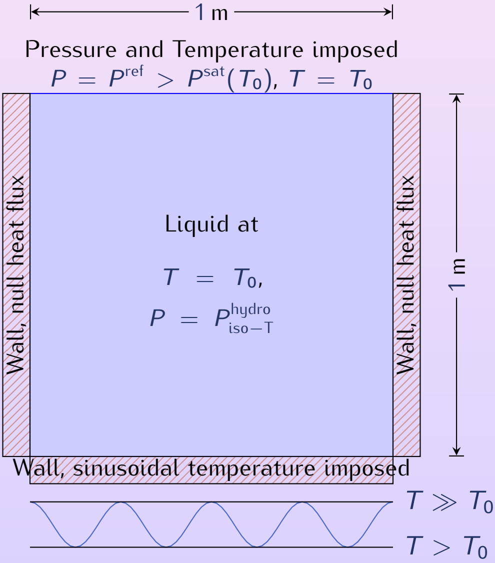


Density ϱ

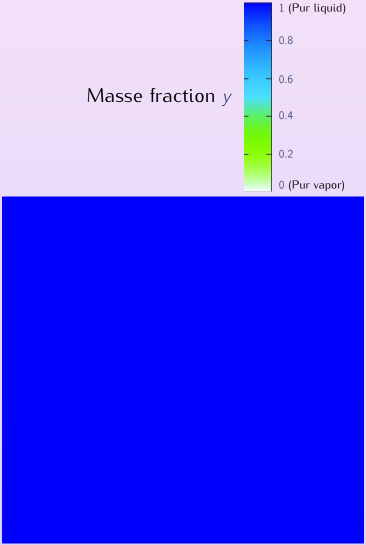


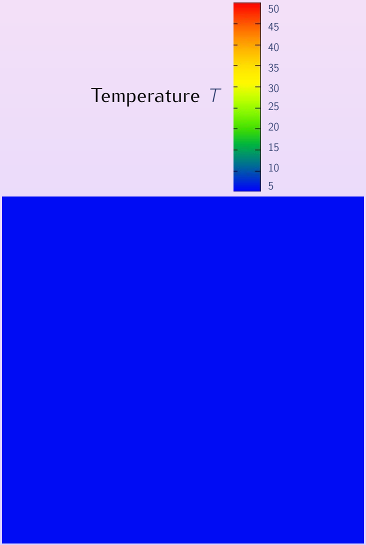
◂ Geometry ▸ Play ▸▸ Skip

Transition to a Film Boiling



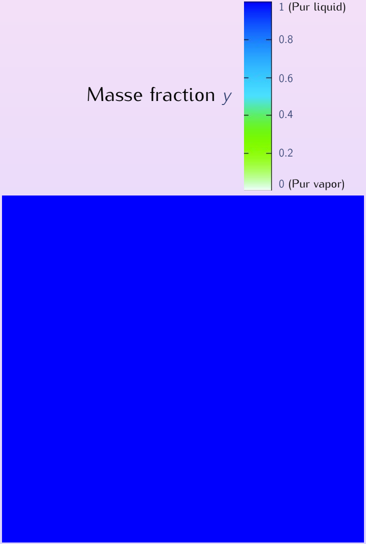
Transition to a Film Boiling

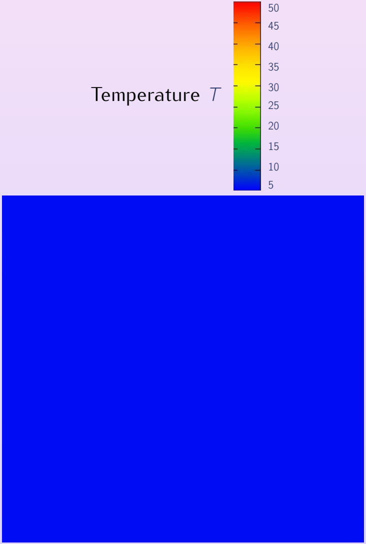




Geometry Play Skip

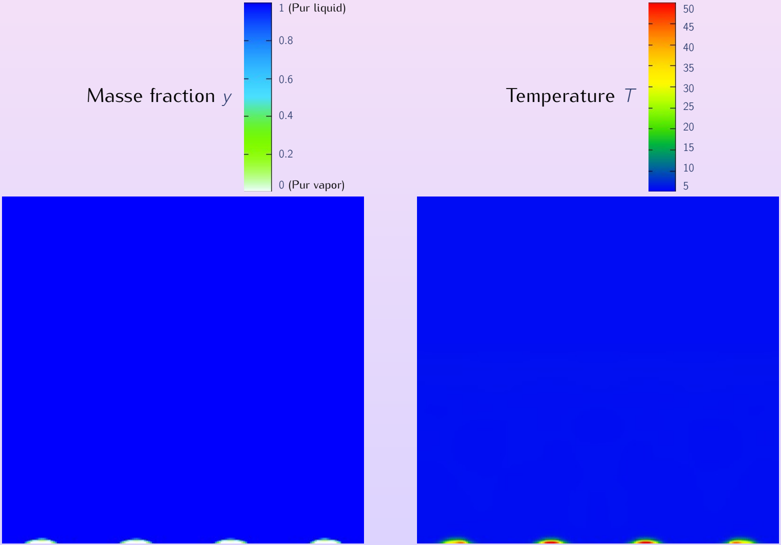
Transition to a Film Boiling





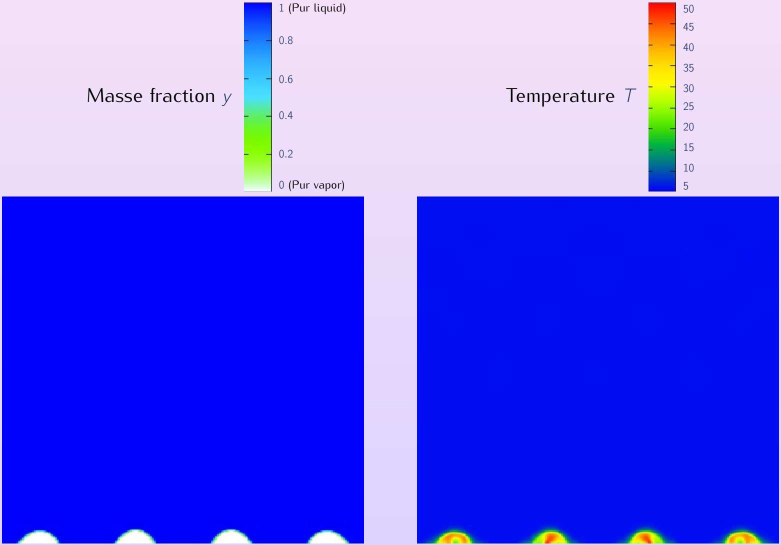
◂ Geometry ▸ Play ▸▸ Skip

Transition to a Film Boiling



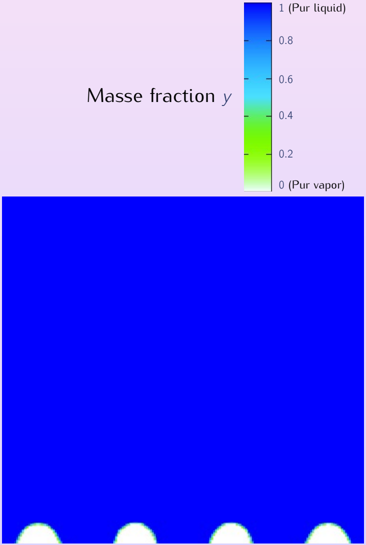
Geometry Play Skip

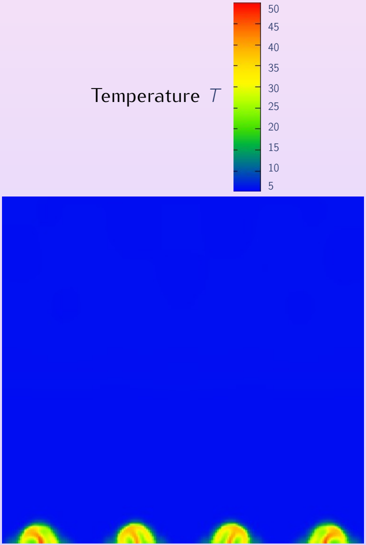
Transition to a Film Boiling



Geometry Play Skip

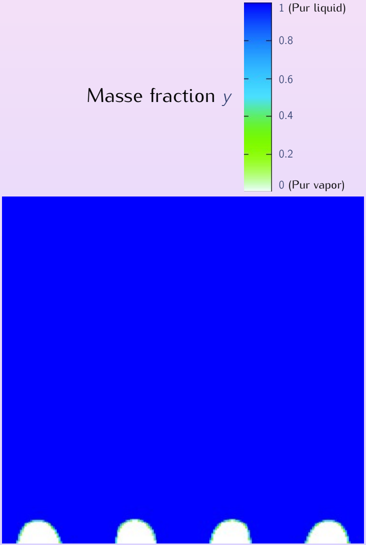
Transition to a Film Boiling

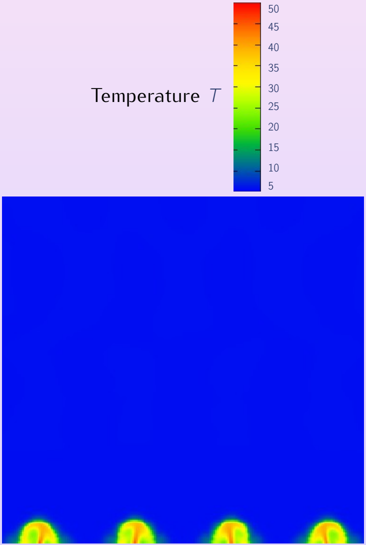




Geometry Play Skip

Transition to a Film Boiling

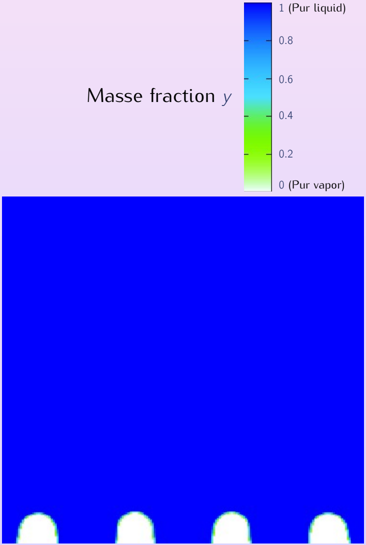




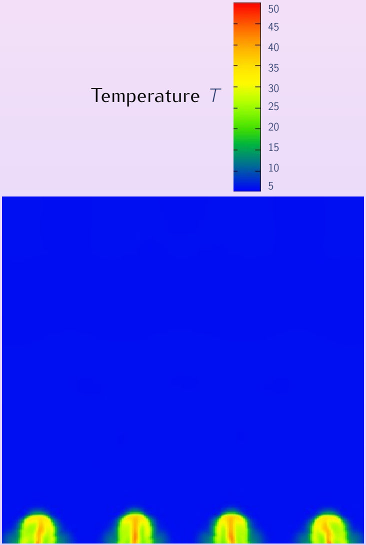
◂ Geometry ▸ Play ▸▸ Skip

Transition to a Film Boiling

Masse fraction y

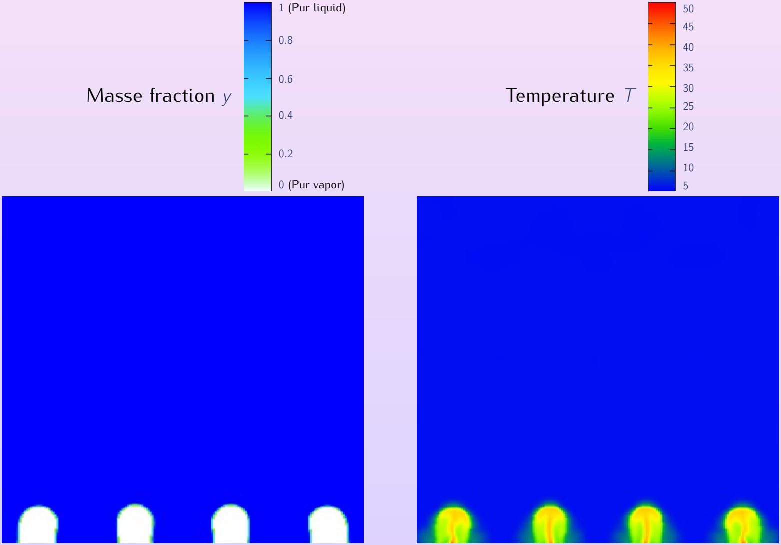


Temperature T



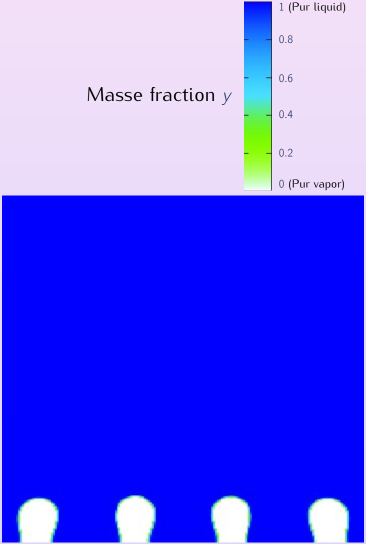
◀ Geometry ▶ Play ⏩ Skip

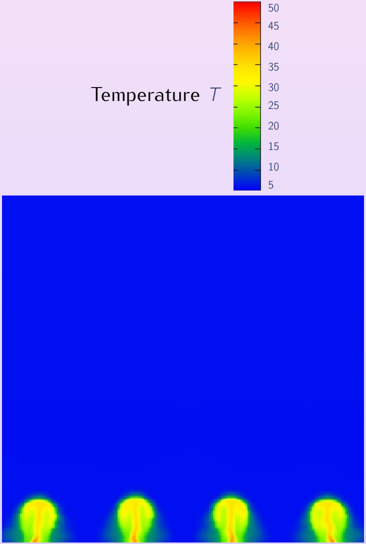
Transition to a Film Boiling



◂ Geometry ▸ Play ▸▸ Skip

Transition to a Film Boiling





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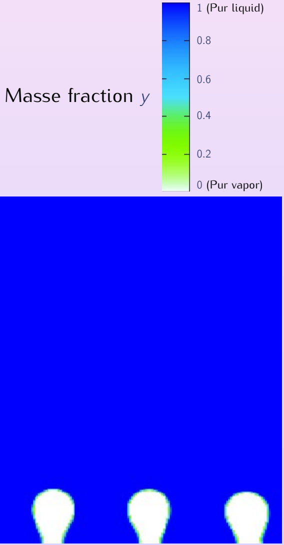
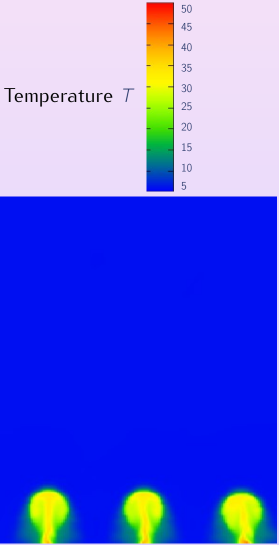
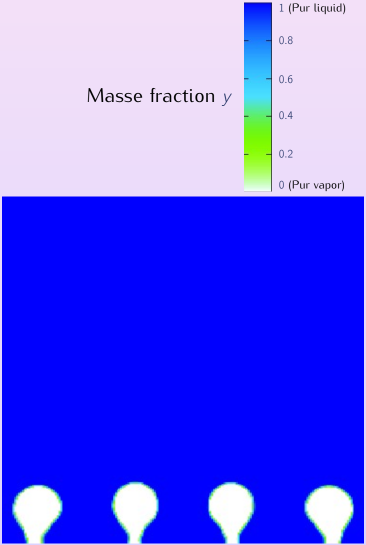
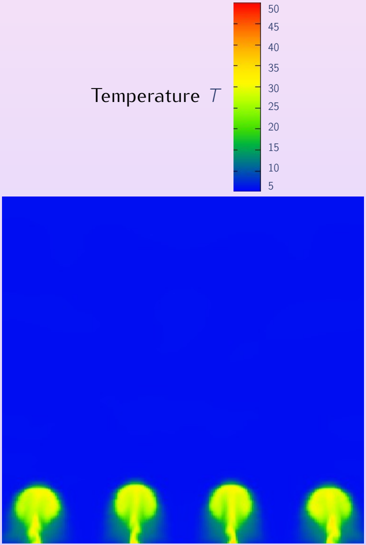




Geometry Play Skip

Transition to a Film Boiling

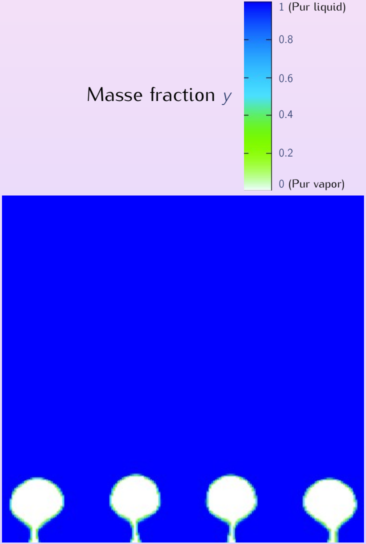




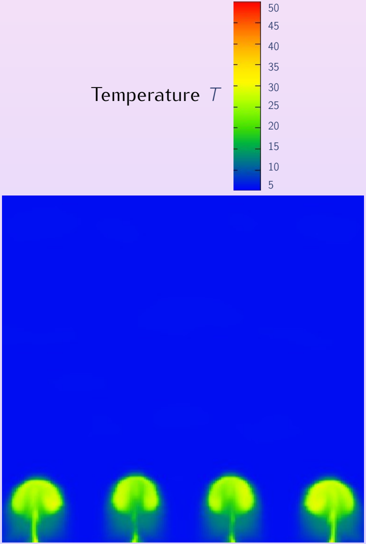
Geometry Play Skip

Transition to a Film Boiling

Masse fraction y



Temperature T



Geometry Play Skip

Transition to a Film Boiling

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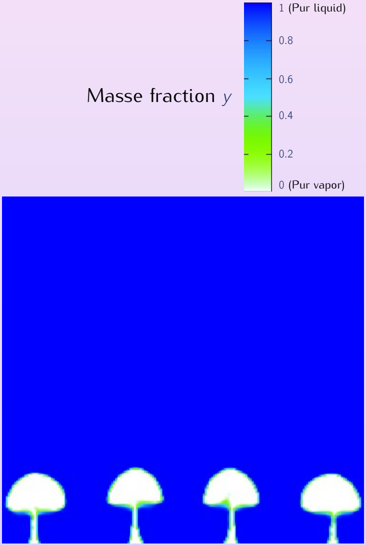
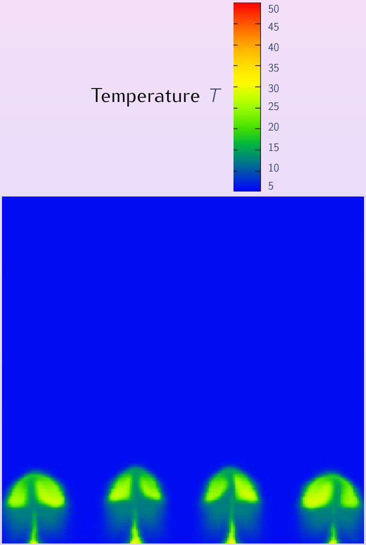
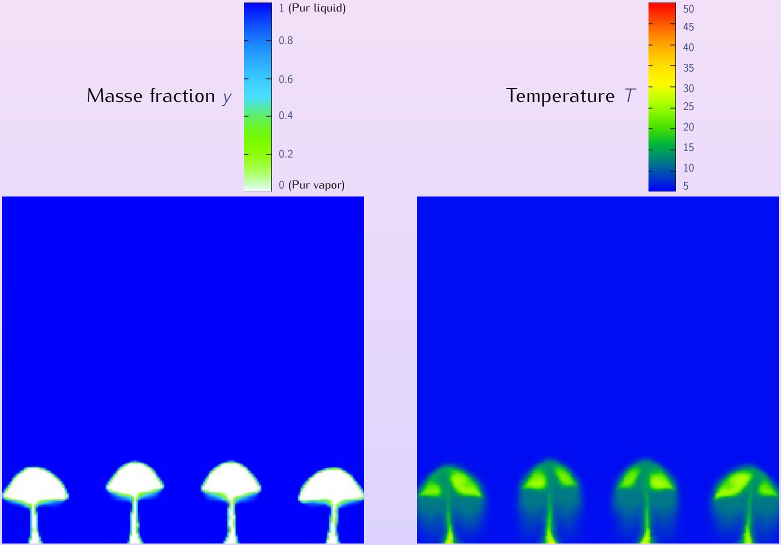


Temperature T



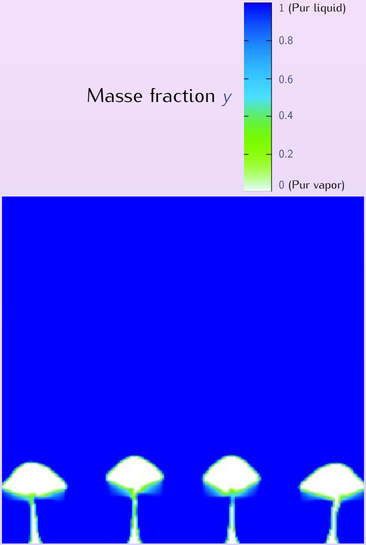
Geometry Play Skip

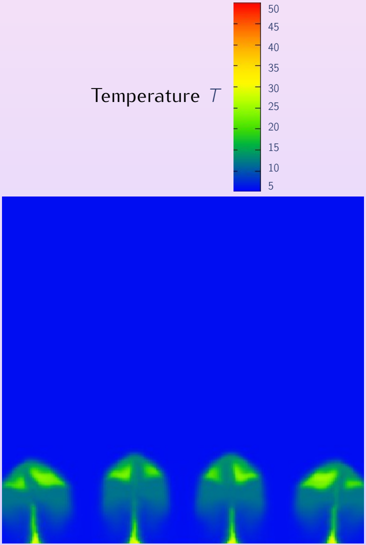
Transition to a Film Boiling



Geometry Play Skip

Transition to a Film Boiling





◀ Geometry ▶ Play ▶▶ Skip

Transition to a Film Boiling

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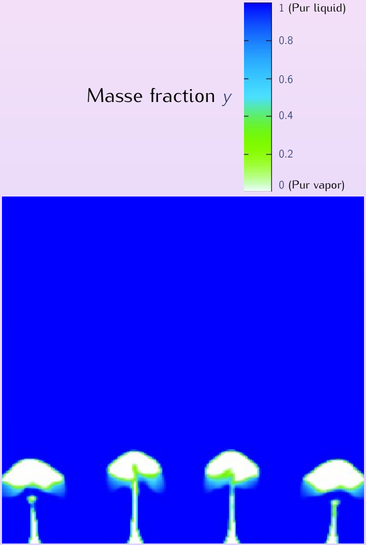
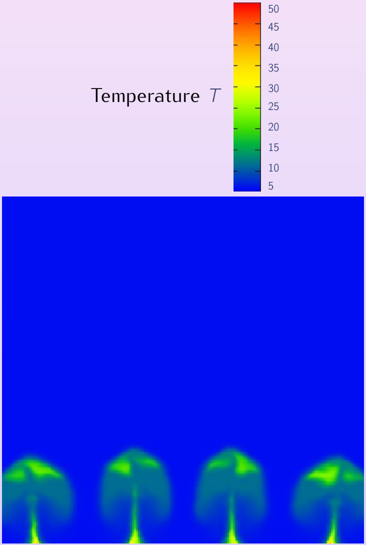
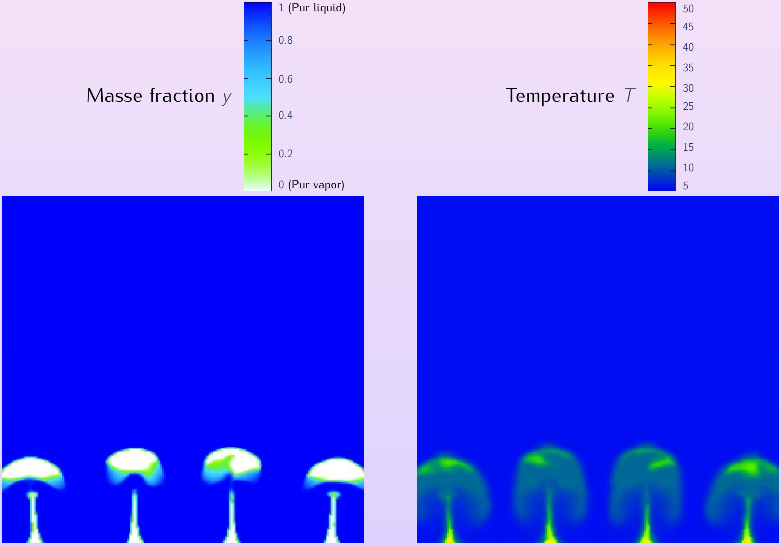


Temperature T



◀ Geometry ▶ Play ▶▶ Skip

Transition to a Film Boiling



◂ Geometry ▸ Play ▸▸ Skip

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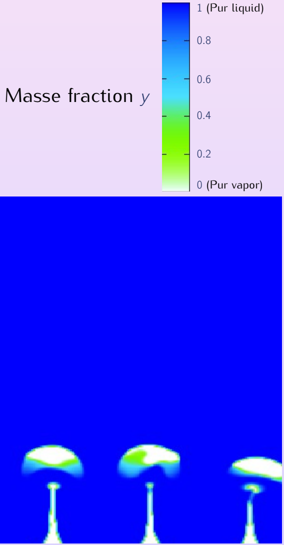

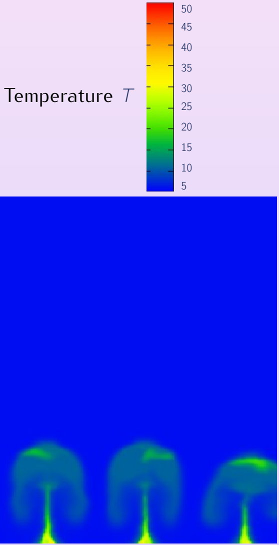

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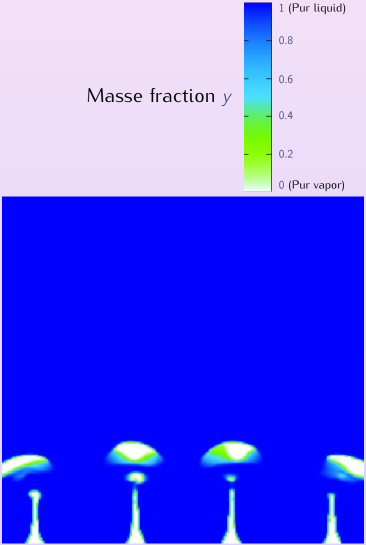

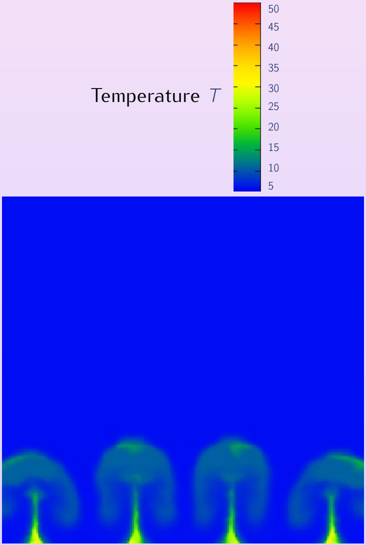

◂ Geometry ▸ Play ▸▸ Skip

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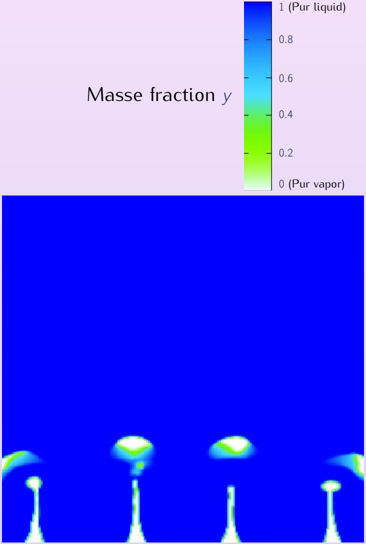
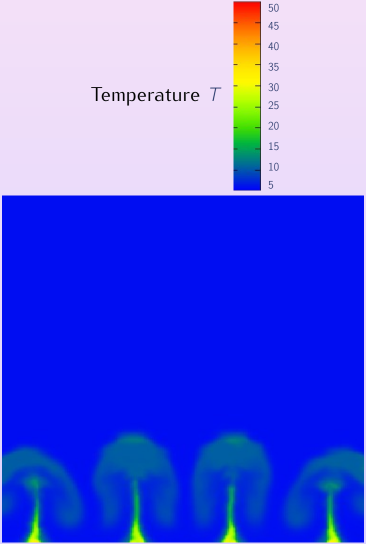
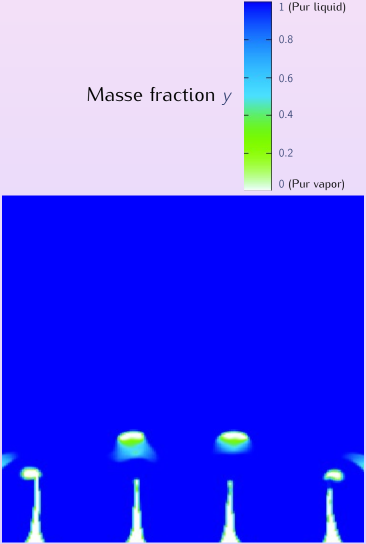


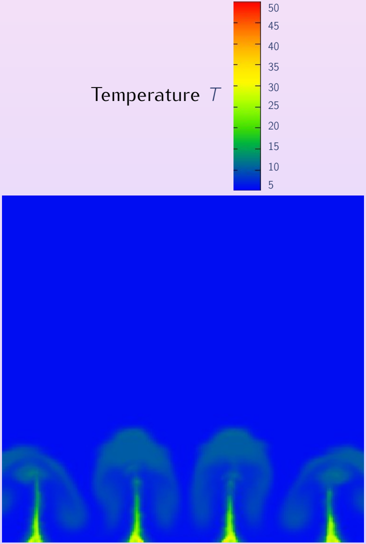
Temperature T



◂ Geometry ▸ Play ▸▸ Skip

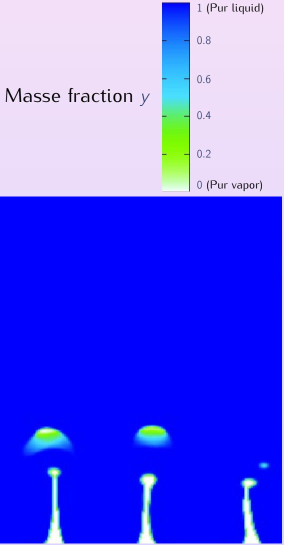
Transition to a Film Boiling

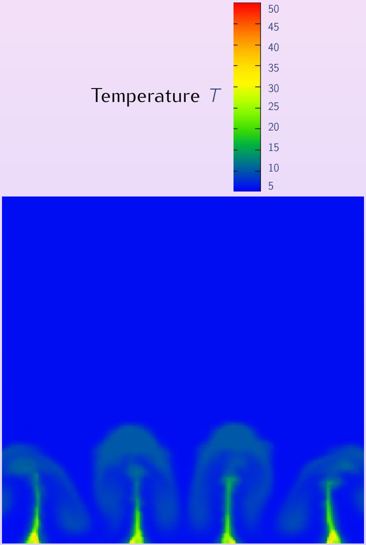




Geometry Play Skip

Transition to a Film Boiling





Geometry Play Skip

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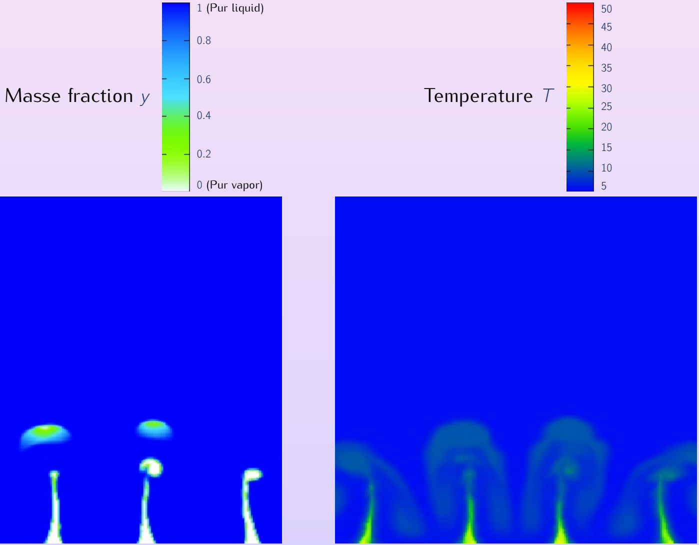
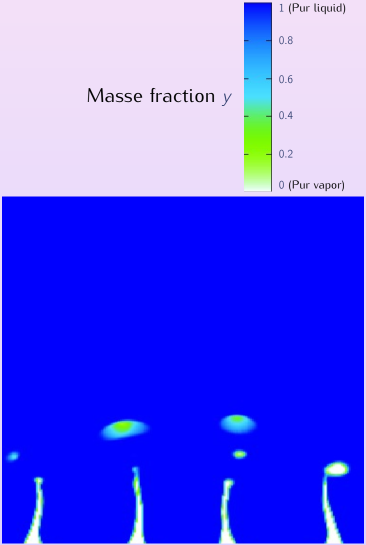
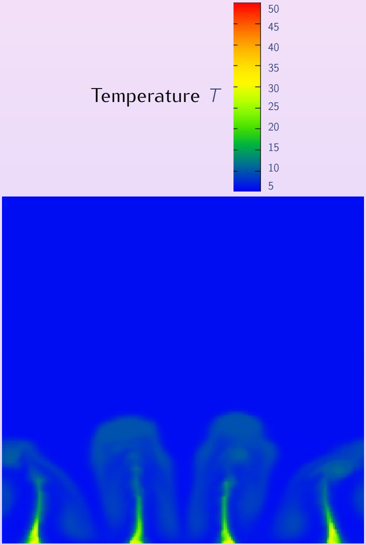


Geometry Play Skip

Transition to a Film Boiling





◂ Geometry ▸ Play ▸▸ Skip

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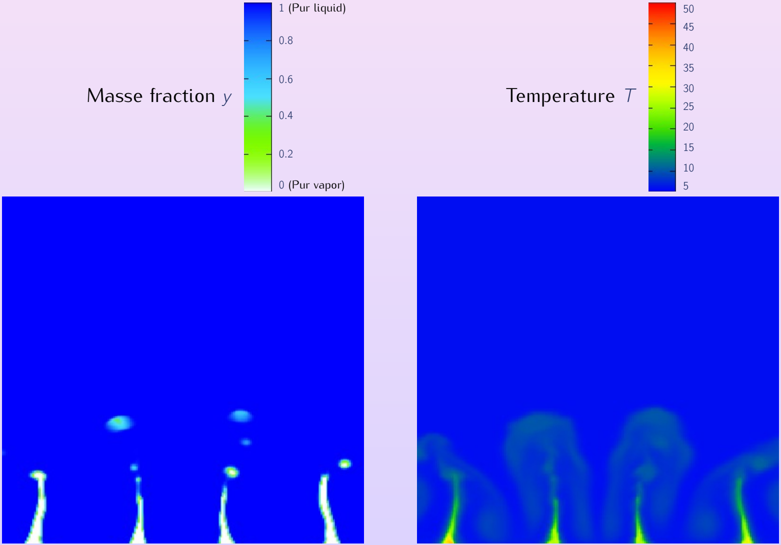

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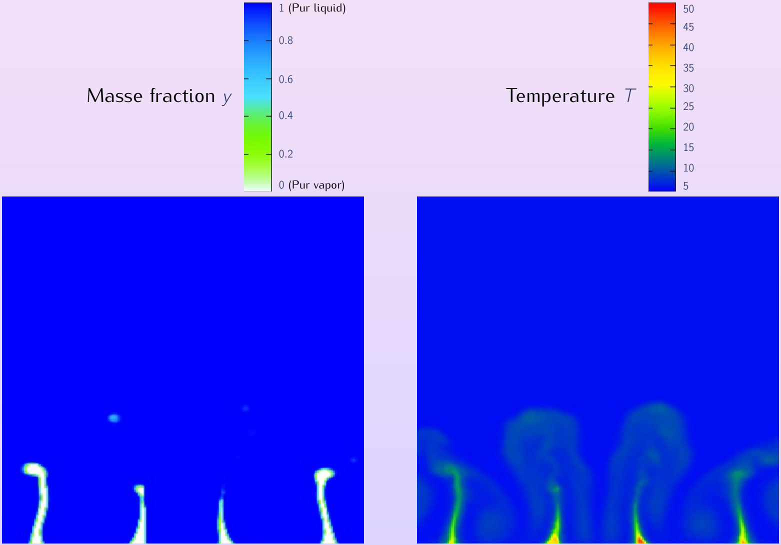

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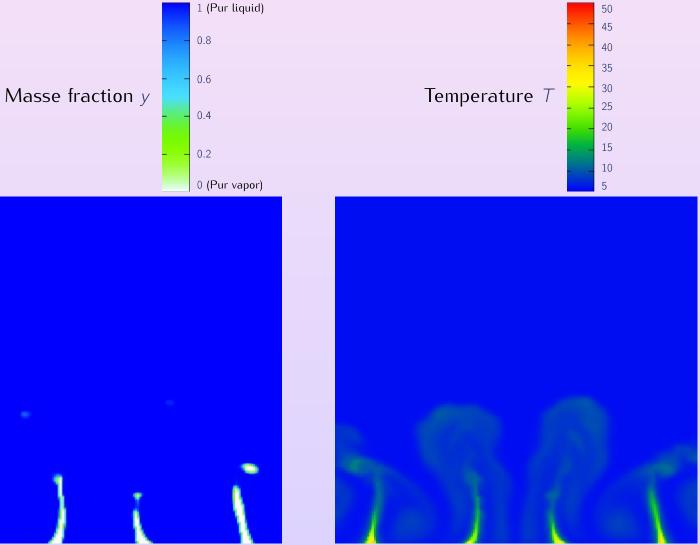

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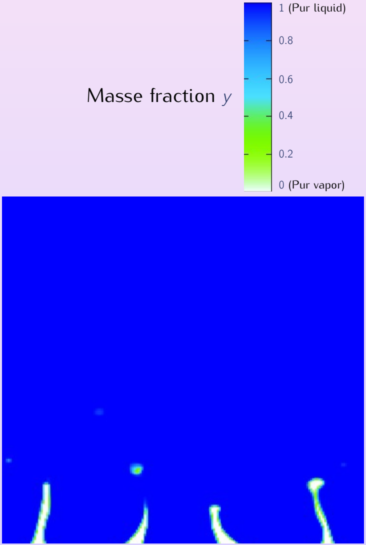

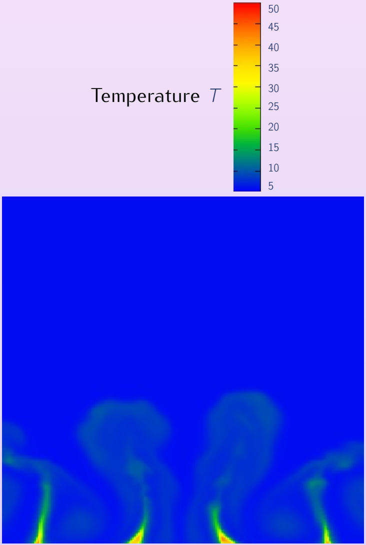

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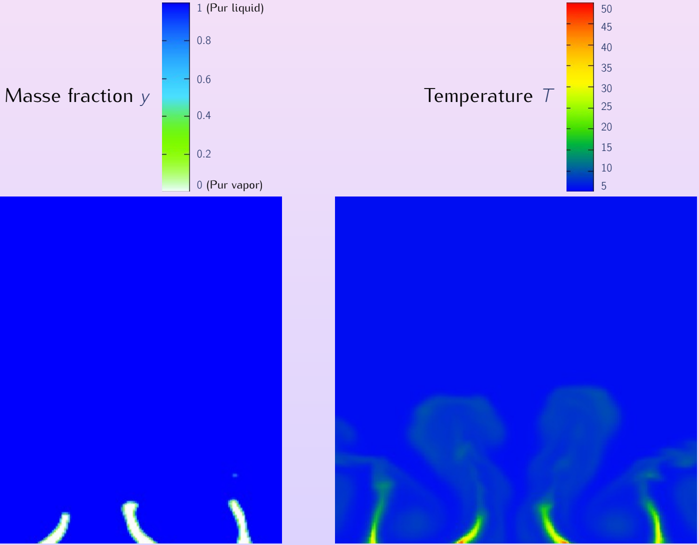

Geometry Play Skip

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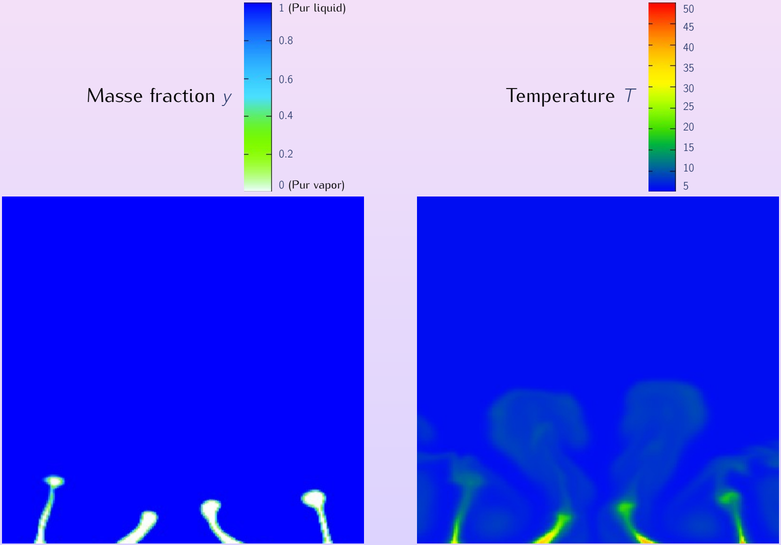

Geometry Play Skip

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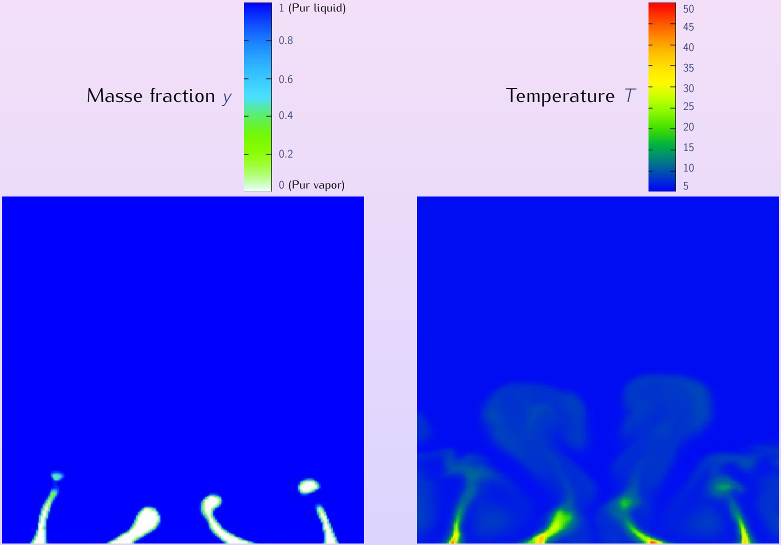
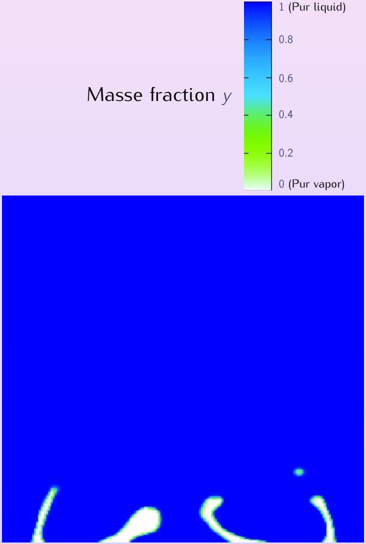


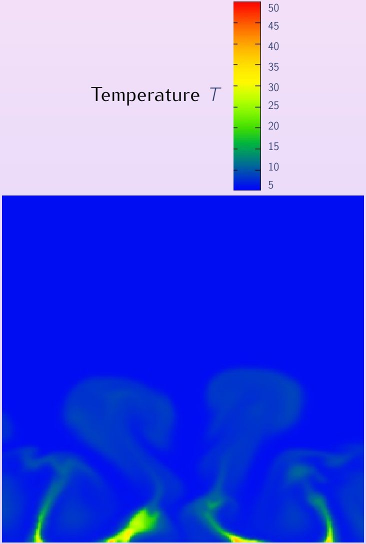
Geometry Play Skip

Transition to a Film Boiling

Masse fraction y



Temperature T



◂ Geometry ▸ Play ▸▸ Skip

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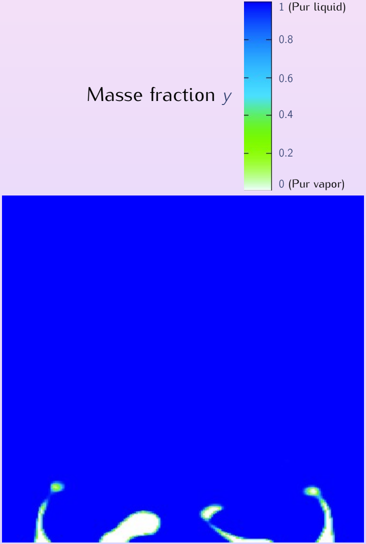

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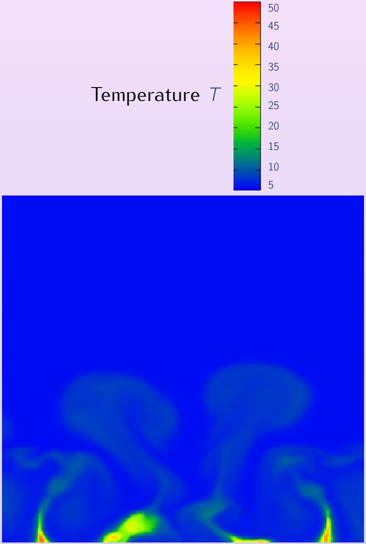
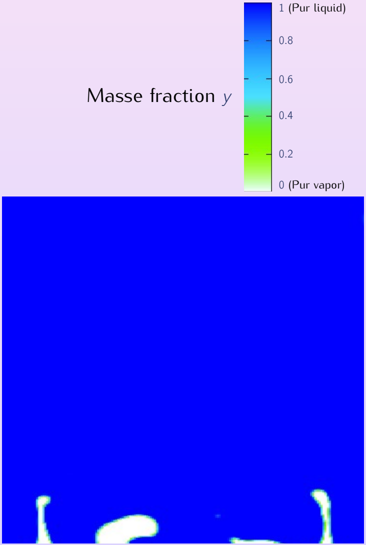
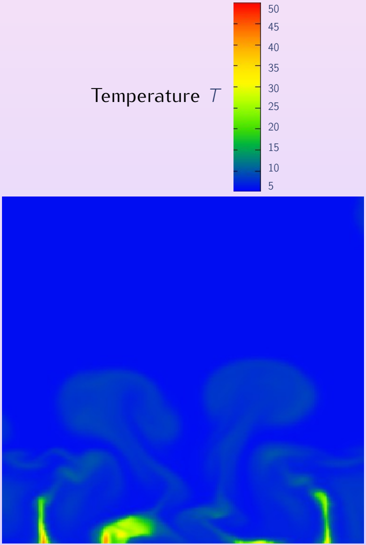


◂ Geometry ▸ Play ▸▸ Skip

Transition to a Film Boiling





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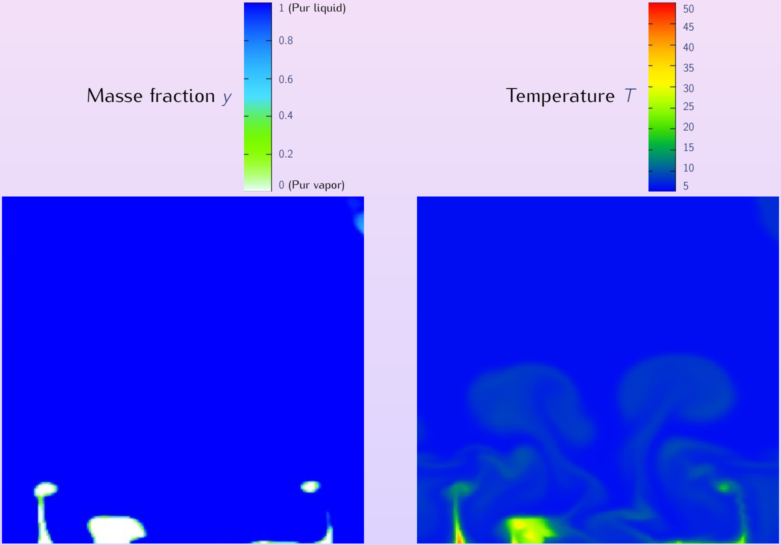

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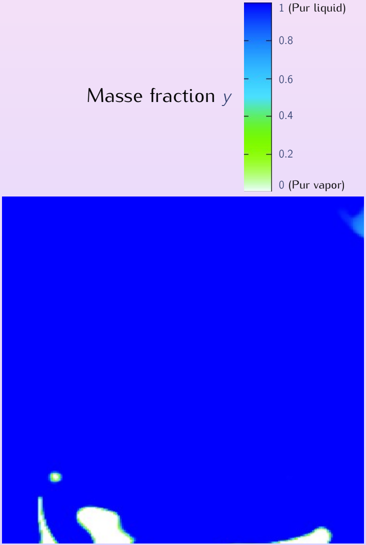

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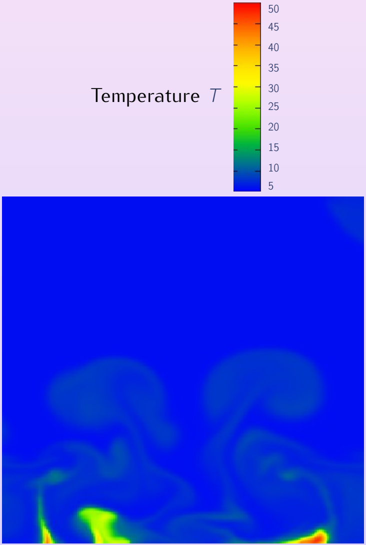

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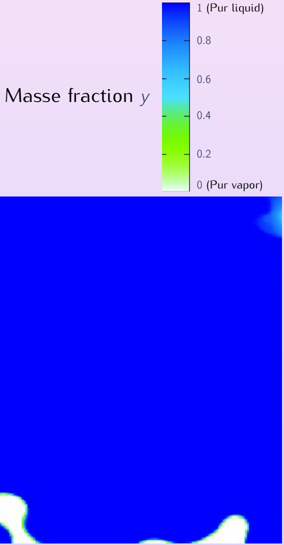

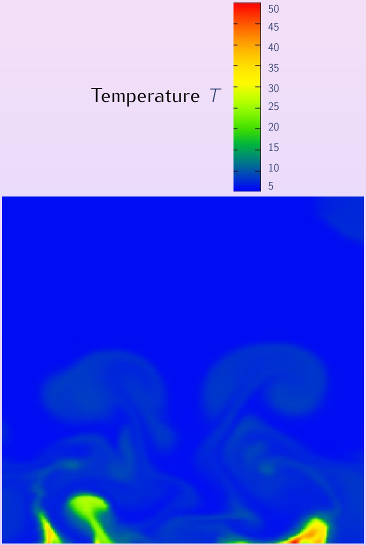

◀ Geometry ▶ Play ⏩ Skip

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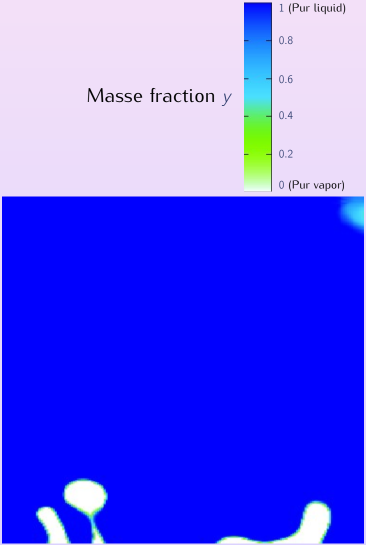

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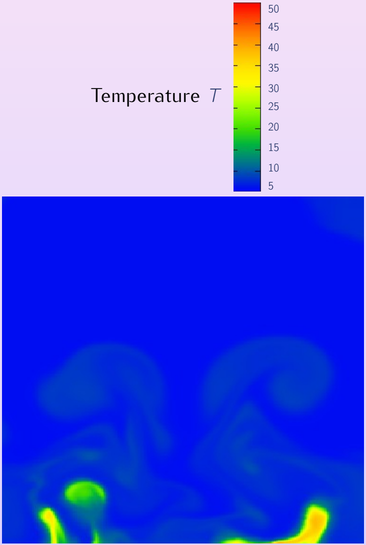

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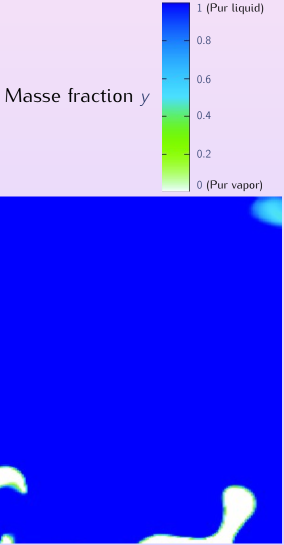

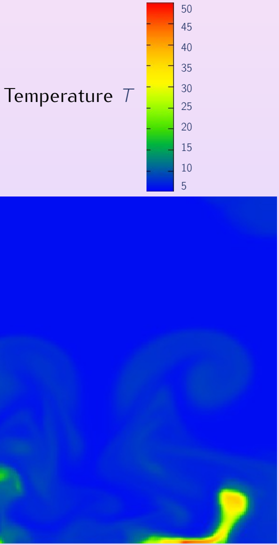

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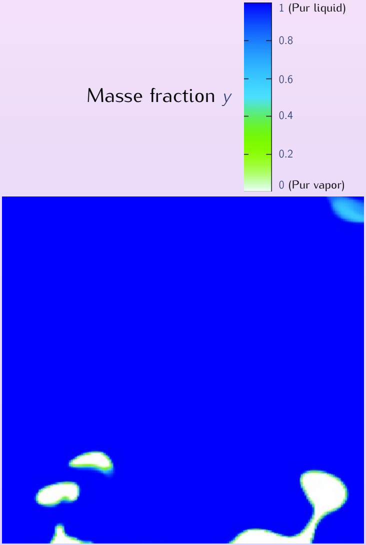

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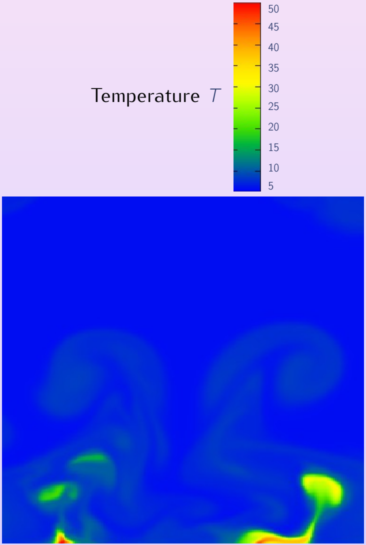

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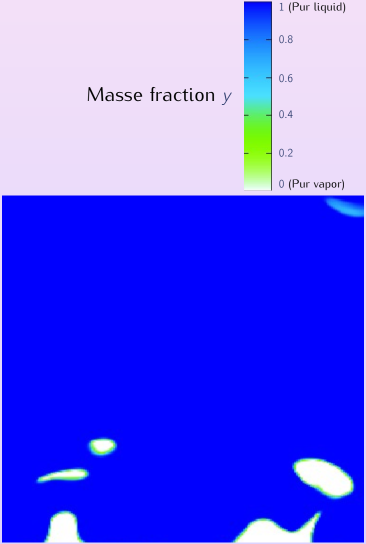

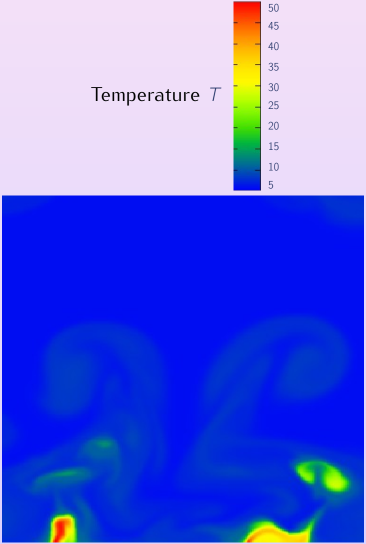

◂ Geometry ▸ Play ▸▸ Skip

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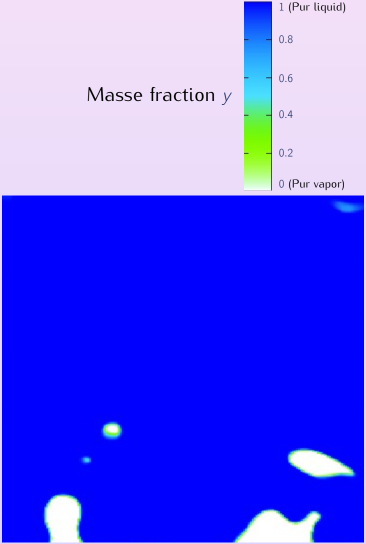
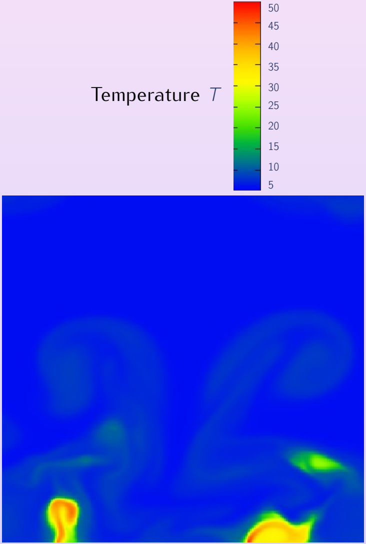


Temperature T



◂ Geometry ▸ Play ▸▸ Skip

Outline

1. Context
2. Model
   - Governing equations
   - Equation of State
3. Numerical Approximation and Example
   - Conservation Laws
   - Numerical Scheme
   - Numerical Example
4. Conclusion

Summary & Perspectives

- Model
  - ✓ based on a general construction of the Equilibrium EOS (also for tabulated data),
- Numerical Method based on the relaxation approach: off-equilibrium systems with relaxation terms
  - ✓ preliminary results: dynamic generation of a phase in a 2D-flow in a pure phase with surface tension, gravity and heat diffusion,
  - ✓ transition: liquid phase → nucleating boiling → "film" boiling

SUMMARY & PERSPECTIVES

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  - ✗ quantitative simulations: tabulated EOS for pure phases, implicit transport step or Adam-Bashfort refinement (CFL condition), 3D (parallelization).

Appendix

From $\mathbf{w} \mapsto s^{\text{eq}}$ to $\mathbf{w} \mapsto P^{\text{eq}}$

For all $\widetilde{\mathbf{w}}$ fixed, we seek $(\mathbf{w}^*_{\text{liq}}, \mathbf{w}^*_{\text{vap}}, y^*)$ as the solution of the system

$$\begin{cases} P_{\text{liq}}(\mathbf{w}_{\text{liq}}) = P_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ T_{\text{liq}}(\mathbf{w}_{\text{liq}}) = T_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ g_{\text{liq}}(\mathbf{w}_{\text{liq}}) = g_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ \widetilde{\mathbf{w}} = y\mathbf{w}_{\text{liq}} + (1-y)\mathbf{w}_{\text{vap}} \end{cases}$$

1. if $y^* \in]0,1[$ then $\widetilde{\mathbf{w}}$ is an **equilibrium mixture state**

$$s^{\text{eq}}(\widetilde{\mathbf{w}}) = y^* s_{\text{liq}}(\mathbf{w}^*_{\text{liq}}) + (1-y^*) s_{\text{vap}}(\mathbf{w}^*_{\text{vap}}),$$

2. if the system has no solution or $y^* \notin]0,1[$ then $\widetilde{\mathbf{w}}$ is a **monophasic pure state**

$$s^{\text{eq}}(\widetilde{\mathbf{w}}) = \max\{s_{\text{liq}}(\widetilde{\mathbf{w}}), s_{\text{vap}}(\widetilde{\mathbf{w}})\},$$
$$P^{\text{eq}}(\widetilde{\mathbf{w}}) = P_\alpha(\widetilde{\mathbf{w}}).$$

From $\mathbf{w} \mapsto s^{eq}$ to $\mathbf{w} \mapsto P^{eq}$

For all $\widetilde{\mathbf{w}}$ fixed, we seek $(\mathbf{w}_{liq}^*, \mathbf{w}_{vap}^*, y^*)$ as the solution of the system

$$\begin{cases} P_{liq}(\mathbf{w}_{liq}) = P_{vap}(\mathbf{w}_{vap}) \\ T_{liq}(\mathbf{w}_{liq}) = T_{vap}(\mathbf{w}_{vap}) \\ g_{liq}(\mathbf{w}_{liq}) = g_{vap}(\mathbf{w}_{vap}) \\ \widetilde{\mathbf{w}} = y\mathbf{w}_{liq} + (1-y)\mathbf{w}_{vap} \end{cases}$$

1. if $y^* \in]0,1[$ then $\widetilde{\mathbf{w}}$ is an **equilibrium mixture state**

$$s^{eq}(\widetilde{\mathbf{w}}) = y^* s_{liq}(\mathbf{w}_{liq}^*) + (1-y^*) s_{vap}(\mathbf{w}_{vap}^*),$$

$$P^{eq}(\widetilde{\mathbf{w}}) = P_{liq}(\mathbf{w}_{liq}^*) = P_{vap}(\mathbf{w}_{vap}^*);$$

2. if the system has no solution or $y^* \notin]0,1[$ then $\widetilde{\mathbf{w}}$ is a **monophasic pure state**

$$s^{eq}(\widetilde{\mathbf{w}}) = \max\{s_{liq}(\widetilde{\mathbf{w}}), s_{vap}(\widetilde{\mathbf{w}})\},$$

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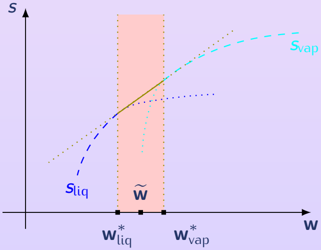

From $\mathbf{w} \mapsto s^{\text{eq}}$ to $\mathbf{w} \mapsto P^{\text{eq}}$

For all $\widetilde{\mathbf{w}}$ fixed, we seek $(\mathbf{w}^*_{\text{liq}}, \mathbf{w}^*_{\text{vap}}, y^*)$ as the solution of the system

$$\begin{cases} P_{\text{liq}}(\mathbf{w}_{\text{liq}}) = P_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ T_{\text{liq}}(\mathbf{w}_{\text{liq}}) = T_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ g_{\text{liq}}(\mathbf{w}_{\text{liq}}) = g_{\text{vap}}(\mathbf{w}_{\text{vap}}) \\ \widetilde{\mathbf{w}} = y\mathbf{w}_{\text{liq}} + (1-y)\mathbf{w}_{\text{vap}} \end{cases}$$

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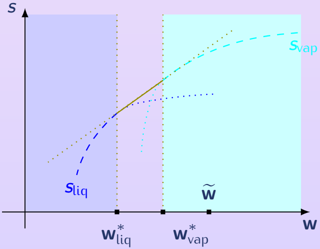

From $\mathbf{w} \mapsto s^{\mathrm{eq}}$ to $\mathbf{w} \mapsto P^{\mathrm{eq}}$

For all $\widetilde{\mathbf{w}}$ fixed, we seek $(\mathbf{w}^*_{\mathrm{liq}}, \mathbf{w}^*_{\mathrm{vap}}, y^*)$ as the solution of the system

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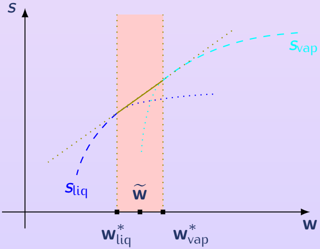

From $\mathbf{w} \mapsto s^{\mathrm{eq}}$ to $\mathbf{w} \mapsto P^{\mathrm{eq}}$

For all $\widetilde{\mathbf{w}}$ fixed, we seek $(\mathbf{w}^*_{\mathrm{liq}}, \mathbf{w}^*_{\mathrm{vap}}, y^*)$ as the solution of the system

$$\begin{cases} P_{\mathrm{liq}}(\mathbf{w}_{\mathrm{liq}}) = P_{\mathrm{vap}}(\mathbf{w}_{\mathrm{vap}}) \\ T_{\mathrm{liq}}(\mathbf{w}_{\mathrm{liq}}) = T_{\mathrm{vap}}(\mathbf{w}_{\mathrm{vap}}) \\ g_{\mathrm{liq}}(\mathbf{w}_{\mathrm{liq}}) = g_{\mathrm{vap}}(\mathbf{w}_{\mathrm{vap}}) \\ \widetilde{\mathbf{w}} = y\mathbf{w}_{\mathrm{liq}} + (1-y)\mathbf{w}_{\mathrm{vap}} \end{cases}$$

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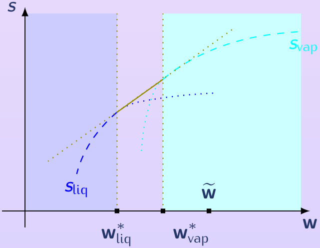

Projection step: Analytical EOS

(τ, ε) fixed

$(\tau_{liq}, \varepsilon_{liq}, \tau_{vap}, \varepsilon_{vap}, y)$ solution of

$$\begin{cases} P_{liq}(\tau_{liq}, \varepsilon_{liq}) = P_{vap}(\tau_{vap}, \varepsilon_{vap}) \\ T_{liq}(\tau_{liq}, \varepsilon_{liq}) = T_{vap}(\tau_{vap}, \varepsilon_{vap}) \\ g_{liq}(\tau_{liq}, \varepsilon_{liq}) = g_{vap}(\tau_{vap}, \varepsilon_{vap}) \\ \tau = y\tau_{liq} + (1-y)\tau_{vap} \\ \varepsilon = y\varepsilon_{liq} + (1-y)\varepsilon_{vap} \end{cases}$$

(P, T) solution of

$$\begin{cases} \tau_\alpha = \tau_\alpha(P, T) \\ \varepsilon_\alpha = \varepsilon_\alpha(P, T) \\ g_{liq}(P, T) = g_{vap}(P, T) \\ y = \dfrac{\tau - \tau_{vap}(P, T)}{\tau_{liq}(P, T) - \tau_{vap}(P, T)} = \dfrac{\varepsilon - \varepsilon_{vap}(P, T)}{\varepsilon_{liq}(P, T) - \varepsilon_{vap}(P, T)} \end{cases}$$

$T \mapsto P = P^{sat}(T) \approx P^{sat}(T)$

T solution of

$$\frac{\tau - \tau_{vap}^{sat}(T)}{\tau_{liq}^{sat}(T) - \tau_{vap}^{sat}(T)} = \frac{\varepsilon - \varepsilon_{vap}^{sat}(T)}{\varepsilon_{liq}^{sat}(T) - \varepsilon_{vap}^{sat}(T)} \quad \text{where} \quad \begin{pmatrix} \tau \\ \varepsilon \end{pmatrix}_\alpha^{sat}(T) \stackrel{\text{def}}{=} \begin{pmatrix} \tau \\ \varepsilon \end{pmatrix}_\alpha (P^{sat}(T), T)$$

Projection step: Analytical EOS

(τ, ε) fixed

$(\tau_{\text{liq}}, \varepsilon_{\text{liq}}, \tau_{\text{vap}}, \varepsilon_{\text{vap}}, y)$ solution of

$$\begin{cases} P_{\text{liq}}(\tau_{\text{liq}}, \varepsilon_{\text{liq}}) = P_{\text{vap}}(\tau_{\text{vap}}, \varepsilon_{\text{vap}}) \\ T_{\text{liq}}(\tau_{\text{liq}}, \varepsilon_{\text{liq}}) = T_{\text{vap}}(\tau_{\text{vap}}, \varepsilon_{\text{vap}}) \\ g_{\text{liq}}(\tau_{\text{liq}}, \varepsilon_{\text{liq}}) = g_{\text{vap}}(\tau_{\text{vap}}, \varepsilon_{\text{vap}}) \\ \tau = y\tau_{\text{liq}} + (1-y)\tau_{\text{vap}} \\ \varepsilon = y\varepsilon_{\text{liq}} + (1-y)\varepsilon_{\text{vap}} \end{cases}$$

(P, T) solution of

$$\begin{cases} \tau_\alpha = \tau_\alpha(P, T) \\ \varepsilon_\alpha = \varepsilon_\alpha(P, T) \\ g_{\text{liq}}(P, T) = g_{\text{vap}}(P, T) \\ y = \dfrac{\tau - \tau_{\text{vap}}(P, T)}{\tau_{\text{liq}}(P, T) - \tau_{\text{vap}}(P, T)} = \dfrac{\varepsilon - \varepsilon_{\text{vap}}(P, T)}{\varepsilon_{\text{liq}}(P, T) - \varepsilon_{\text{vap}}(P, T)} \end{cases}$$

$$T \mapsto P = \widehat{P}^{\text{sat}}(T) \approx P^{\text{sat}}(T)$$

T solution of

$$\frac{\tau - \tau^{\text{sat}}_{\text{vap}}(T)}{\tau^{\text{sat}}_{\text{liq}}(T) - \tau^{\text{sat}}_{\text{vap}}(T)} = \frac{\varepsilon - \varepsilon^{\text{sat}}_{\text{vap}}(T)}{\varepsilon^{\text{sat}}_{\text{liq}}(T) - \varepsilon^{\text{sat}}_{\text{vap}}(T)} \quad \text{where} \quad \begin{pmatrix}\tau \\ \varepsilon\end{pmatrix}^{\text{sat}}_\alpha (T) \stackrel{\text{def}}{=} \begin{pmatrix}\tau \\ \varepsilon\end{pmatrix}_\alpha (\widehat{P}^{\text{sat}}(T), T)$$

Projection step: Tabulated EOS

		Volume ($m^3\,kg^{-1}$)		Internal Energy ($kJ\,kg^{-1}$)	
T (K)	P^{sat} (MPa)	τ_{liq}^{sat}	τ_{vap}^{sat}	ε_{liq}^{sat}	ε_{vap}^{sat}
275	0,00069845	0,0010001	181,60	7,7590	2377,5
278	0,00086349	0,0010001	148,48	20,388	2381,6
281	0,0010621	0,0010002	122,01	32,996	2385,7
284	0,0012999	0,0010004	100,74	45,586	2389,8
287	0,0015835	0,0010008	83,560	58,162	2393,9
290	0,0019200	0,0010012	69,625	70,727	2398,0
293	0,0023177	0,0010018	58,267	83,284	2402,1
296	0,0027856	0,0010025	48,966	95,835	2406,2
299	0,0033342	0,0010032	41,318	108,38	2410,3
302	0,0039745	0,0010041	35,002	120,92	2414,4
305	0,0047193	0,0010050	29,764	133,46	2418,4
308	0,0055825	0,0010060	25,403	146	2422,5
...	...	...	...	...	...

Source: `http://webbook.nist.gov/chemistry/fluid/`

Projection step: Tabulated EOS

(τ, ε) fixed

T solution of

$$\frac{\tau - \tau_{\text{vap}}^{\text{sat}}(T)}{\tau_{\text{liq}}^{\text{sat}}(T) - \tau_{\text{vap}}^{\text{sat}}(T)} = \frac{\varepsilon - \varepsilon_{\text{vap}}^{\text{sat}}(T)}{\varepsilon_{\text{liq}}^{\text{sat}}(T) - \varepsilon_{\text{vap}}^{\text{sat}}(T)} \quad \text{with} \quad \begin{pmatrix}\tau \\ \varepsilon\end{pmatrix}_{\alpha}^{\text{sat}}(T) \quad \text{tabulated}$$

$$\wr\wr$$

$$\frac{\tau - \widehat{\tau}_{\text{vap}}^{\text{sat}}(T)}{\widehat{\tau}_{\text{liq}}^{\text{sat}}(T) - \widehat{\tau}_{\text{vap}}^{\text{sat}}(T)} = \frac{\varepsilon - \widehat{\varepsilon}_{\text{vap}}^{\text{sat}}(T)}{\widehat{\varepsilon}_{\text{liq}}^{\text{sat}}(T) - \widehat{\varepsilon}_{\text{vap}}^{\text{sat}}(T)} \quad \text{with} \quad \begin{pmatrix}\widehat{\tau} \\ \widehat{\varepsilon}\end{pmatrix}_{\alpha}^{\text{sat}}(T)$$

Projection step: Tabulated EOS

(τ, ε) fixed

T solution of

$$\frac{\tau - \tau_{vap}^{sat}(T)}{\tau_{liq}^{sat}(T) - \tau_{vap}^{sat}(T)} = \frac{\varepsilon - \varepsilon_{vap}^{sat}(T)}{\varepsilon_{liq}^{sat}(T) - \varepsilon_{vap}^{sat}(T)}$$ with $\begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_{\alpha}^{sat}(T)$ tabulated

$\wr\wr$

$$\frac{\tau - \widehat{\tau}_{vap}^{sat}(T)}{\widehat{\tau}_{liq}^{sat}(T) - \widehat{\tau}_{vap}^{sat}(T)} = \frac{\varepsilon - \widehat{\varepsilon}_{vap}^{sat}(T)}{\widehat{\varepsilon}_{liq}^{sat}(T) - \widehat{\varepsilon}_{vap}^{sat}(T)}$$ with $\begin{pmatrix}\widehat{\tau}\\ \widehat{\varepsilon}\end{pmatrix}_{\alpha}^{sat}(T)$

least square approximations

Projection step: Tabulated EOS

(τ, ε) fixed

T solution of

$$\frac{\tau - \tau_{\text{vap}}^{\text{sat}}(T)}{\tau_{\text{liq}}^{\text{sat}}(T) - \tau_{\text{vap}}^{\text{sat}}(T)} = \frac{\varepsilon - \varepsilon_{\text{vap}}^{\text{sat}}(T)}{\varepsilon_{\text{liq}}^{\text{sat}}(T) - \varepsilon_{\text{vap}}^{\text{sat}}(T)}$$ with $$\begin{pmatrix}\tau \\ \varepsilon\end{pmatrix}_{\alpha}^{\text{sat}}(T)$$ tabulated

$\wr\wr$ ← least square approximations

$$\frac{\tau - \widehat{\tau}_{\text{vap}}^{\text{sat}}(T)}{\widehat{\tau}_{\text{liq}}^{\text{sat}}(T) - \widehat{\tau}_{\text{vap}}^{\text{sat}}(T)} = \frac{\varepsilon - \widehat{\varepsilon}_{\text{vap}}^{\text{sat}}(T)}{\widehat{\varepsilon}_{\text{liq}}^{\text{sat}}(T) - \widehat{\varepsilon}_{\text{vap}}^{\text{sat}}(T)}$$ with $$\begin{pmatrix}\widehat{\tau} \\ \widehat{\varepsilon}\end{pmatrix}_{\alpha}^{\text{sat}}(T)$$

Stiffened Gas for Water

Phase	c_v [J kg^{-1} K^{-1}]	γ	π [Pa]	q [J kg^{-1}]	m [J kg^{-1} K^{-1}]
Water	1816.2	2.35	10^9	-1167.056×10^3	-32765.55596
Steam	1040.14	1.43	0	2030.255×10^3	-33265.65947

Table: Parameters proposed by [O. Le Metayer] for water.

$$(\tau_\alpha, \varepsilon_\alpha) \mapsto s_\alpha = c_{v_\alpha} \ln(\varepsilon_\alpha - q_\alpha - \pi_\alpha \tau_\alpha) + c_{v_\alpha}(\gamma_\alpha - 1) \ln \tau_\alpha + m_\alpha$$

$$(P,T) \mapsto \varepsilon_\alpha = c_{v_\alpha} T \frac{P + \pi_\alpha \gamma_\alpha}{P + \pi_\alpha} + q_\alpha, \qquad (P,T) \mapsto \tau_\alpha = c_{v_\alpha}(\gamma_\alpha - 1)\frac{T}{P + \pi_\alpha}.$$

$$\left.\begin{aligned} &T^i = 278\,\mathrm{K} \ldots 610\,\mathrm{K}, \\ &g_{\mathrm{liq}}(P,T^i) = g_{\mathrm{vap}}(P,T^i) \Rightarrow P^{\mathrm{sat}}(T^i) \end{aligned}\right\} \Rightarrow \mathfrak{A} = \left\{\left(T^i, P^{\mathrm{sat}}(T^i)\right)\right\}_{i=0}^{83}$$

$\widehat{P}^{\mathrm{sat}}$ defined by using a least square approximation of $\mathfrak{A}$:

$$T \mapsto P^{\mathrm{sat}}(T) \approx \widehat{P}^{\mathrm{sat}}(T) \stackrel{\mathrm{def}}{=} \exp\left(\sum_{k=-8}^{k=8} a_k T^k\right)$$

Stiffened Gas for Water

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Stiffened Gas for Water

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Return

Stiffened Gas for Water

Phase	c_v [J kg^{-1} K^{-1}]	γ	π [Pa]	q [J kg^{-1}]	m [J kg^{-1} K^{-1}]
Water	1816.2	2.35	10^9	-1167.056×10^3	-32765.55596
Steam	1040.14	1.43	0	2030.255×10^3	-33265.65947

Table: Parameters proposed by [O. Le Metayer] for water.

$$(\tau_\alpha, \varepsilon_\alpha) \mapsto s_\alpha = c_{v_\alpha} \ln(\varepsilon_\alpha - q_\alpha - \pi_\alpha \tau_\alpha) + c_{v_\alpha}(\gamma_\alpha - 1) \ln \tau_\alpha + m_\alpha$$

$$(P, T) \mapsto \varepsilon_\alpha = c_{v_\alpha} T \frac{P + \pi_\alpha \gamma_\alpha}{P + \pi_\alpha} + q_\alpha, \qquad (P, T) \mapsto \tau_\alpha = c_{v_\alpha}(\gamma_\alpha - 1) \frac{T}{P + \pi_\alpha}.$$

$$\left.\begin{array}{l} T^i = 278\,\mathrm{K} \dots 610\,\mathrm{K}, \\ g_{\mathrm{liq}}(P, T^i) = g_{\mathrm{vap}}(P, T^i) \Rightarrow P^{\mathrm{sat}}(T^i) \end{array}\right\} \Rightarrow \mathfrak{A} = \left\{ \left(T^i, P^{\mathrm{sat}}(T^i) \right) \right\}_{i=0}^{83}$$

$\widehat{P}^{\mathrm{sat}}$ defined by using a least square approximation of $\mathfrak{A}$:

$$T \mapsto P^{\mathrm{sat}}(T) \approx \widehat{P}^{\mathrm{sat}}(T) \stackrel{\mathrm{def}}{=} \exp\left(\sum_{k=-8}^{k=8} a_k T^k \right)$$

Water Tabulated EOS

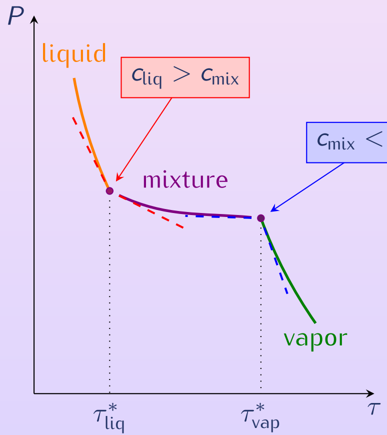
$$\left.\begin{array}{l} T^i = 278\,\mathrm{K}\ldots 610\,\mathrm{K}, \\ \varepsilon_\alpha^{\mathrm{sat}}(T^i),\ \tau_\alpha^{\mathrm{sat}}(T^i) \text{ found in the tables} \end{array}\right\} \Rightarrow \left\{\begin{array}{l} \mathfrak{A} = \left\{\left(T_i, \frac{1}{\varepsilon_{\mathrm{vap}}^{\mathrm{sat}}(T_i)}\right)\right\}_i \\ \mathfrak{B} = \left\{\left(T_i, \frac{\varepsilon_{\mathrm{liq}}^{\mathrm{sat}}(T_i)}{\varepsilon_{\mathrm{vap}}^{\mathrm{sat}}(T_i)}\right)\right\}_i \\ \mathfrak{C} = \left\{\left(T_i, \frac{1}{\tau_{\mathrm{vap}}^{\mathrm{sat}}(T_i)}\right)\right\}_i \\ \mathfrak{D} = \left\{\left(T_i, \frac{\tau_{\mathrm{liq}}^{\mathrm{sat}}(T_i)}{\tau_{\mathrm{vap}}^{\mathrm{sat}}(T_i)}\right)\right\}_i \end{array}\right.$$

$\widehat{\varepsilon}_\alpha^{\mathrm{sat}}$ and $\widehat{\tau}_\alpha^{\mathrm{sat}}$ defined by using a least square approximation of $\mathfrak{A}$, $\mathfrak{B}$, $\mathfrak{C}$ and $\mathfrak{D}$:

$$T \mapsto \varepsilon_{\mathrm{vap}}^{\mathrm{sat}} \approx \widehat{\varepsilon}_{\mathrm{vap}}^{\mathrm{sat}} \stackrel{\mathrm{def}}{=} \frac{1}{\sum_{k=0}^{6} a_k T^k} \qquad T \mapsto \varepsilon_{\mathrm{liq}}^{\mathrm{sat}} \approx \widehat{\varepsilon}_{\mathrm{liq}}^{\mathrm{sat}} \stackrel{\mathrm{def}}{=} \widehat{\varepsilon}_{\mathrm{vap}}^{\mathrm{sat}}(T) \sum_{k=0}^{6} b_k T^k$$

$$T \mapsto \tau_{\mathrm{vap}}^{\mathrm{sat}} \approx \widehat{\tau}_{\mathrm{vap}}^{\mathrm{sat}} \stackrel{\mathrm{def}}{=} \frac{1}{\sum_{k=0}^{8} c_k T^k} \qquad T \mapsto \tau_{\mathrm{liq}}^{\mathrm{sat}} \approx \widehat{\tau}_{\mathrm{liq}}^{\mathrm{sat}} \stackrel{\mathrm{def}}{=} \widehat{\tau}_{\mathrm{vap}}^{\mathrm{sat}}(T) \sum_{k=0}^{9} d_k T^k$$

Isentropic curves



$$\gamma \stackrel{\text{def}}{=} -\frac{\tau}{P}\left.\frac{\partial P}{\partial \tau}\right|_s$$

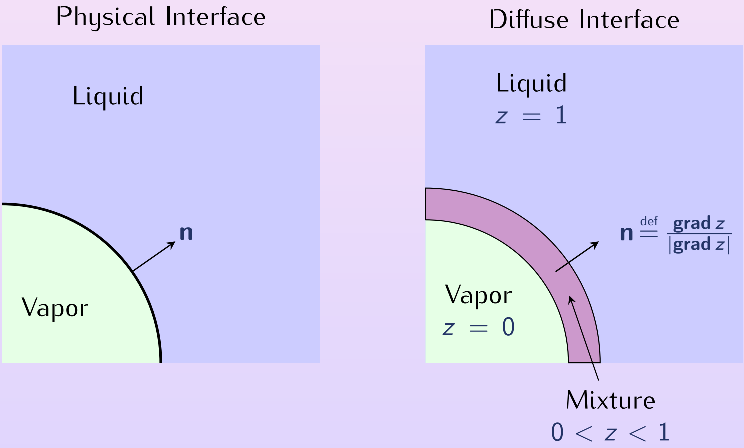
$$\Gamma \stackrel{\text{def}}{=} \tau \left.\frac{\partial P}{\partial \varepsilon}\right|_\tau$$

$$\mathfrak{G} \stackrel{\text{def}}{=} \frac{\tau^2}{2\gamma P}\left.\frac{\partial^2 P}{\partial \tau^2}\right|_s$$

- Pure Phases
  - (H) $\gamma > 0$
  - (H) $\Gamma > 0$
  - (H) $\mathfrak{G} > 0$
- Mixture
  - (P) $\gamma > 0$
  - (P) $\Gamma > 0$
  - (H) $\mathfrak{G} > 0$

- Regularity: [J. Correia, P.G. LeFloch, M.D. Thanh]
- Loss of convexity: [A. Voss]

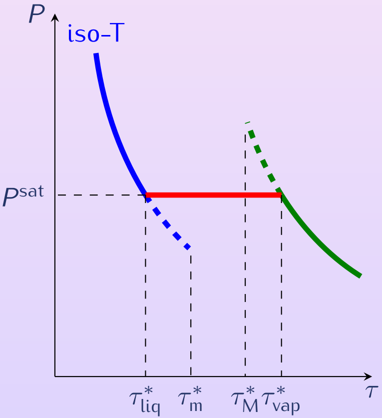
Continuum Surface Force (CSF) Approach



$$\Pi_{\text{tension}} = -\sigma\,\mathrm{div}(\mathbf{n})\mathbf{n}$$

[J.U. Brackbill, D.B. Kothe, C. Zemach]

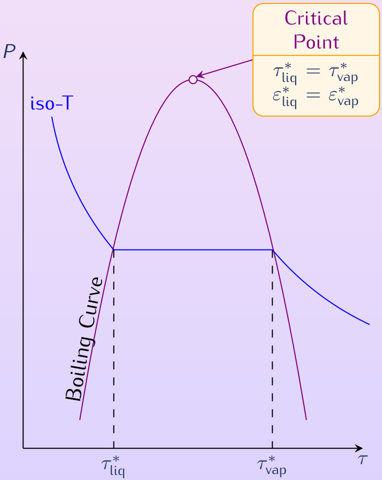
Metastability



$$P^{\text{eq}} = \begin{cases} P_{\text{liq}}, & \text{if } \tau < \tau^*_{\text{liq}}, \\ P^{\text{sat}}, & \text{if } \tau^*_{\text{liq}} < \tau < \tau^*_{\text{vap}}, \\ P_{\text{vap}}, & \text{if } \tau^*_{\text{vap}} < \tau. \end{cases}$$

$$P^{\text{met}} = \begin{cases} P_{\text{liq}}, & \text{if } \tau < \tau^*_{\text{liq}}, \\ [P^{\text{sat}} \text{ or } P_{\text{liq}}], & \text{if } \tau^*_{\text{liq}} < \tau < \tau^*_{\text{m}}, \\ P^{\text{sat}}, & \text{if } \tau^*_{\text{m}} < \tau < \tau^*_{\text{M}}, \\ [P^{\text{sat}} \text{ or } P_{\text{vap}}], & \text{if } \tau^*_{\text{M}} < \tau < \tau^*_{\text{vap}}, \\ P_{\text{vap}}, & \text{if } \tau^*_{\text{vap}} < \tau, \end{cases}$$

Critical Point



Physic

- 2 Pure Phases EOS $(\tau, \varepsilon) \mapsto P_\alpha$
- 1 Saturation EOS $\tau \mapsto P^{\text{sat}}$

Eq

EOS

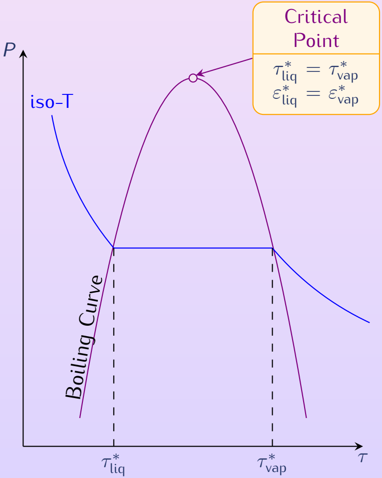
PG $\varepsilon^*_{\text{liq}} = \varepsilon^*_{\text{vap}} \Leftrightarrow c_{v_{\text{liq}}} = c_{v_{\text{vap}}}$ (indip. of T)

SG $\left\{\tau_i, P_i^{\text{sat,e}}\right\}_i \rightsquigarrow (\tau, \varepsilon) \mapsto P_\alpha \rightsquigarrow \tau \mapsto P^{\text{sat}}$

$\tau^*_{\text{liq}} = \tau^*_{\text{vap}}$ but $\varepsilon^*_{\text{liq}} \neq \varepsilon^*_{\text{vap}}$

TAB

Critical Point



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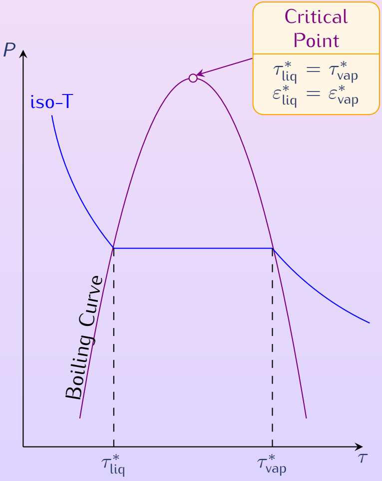

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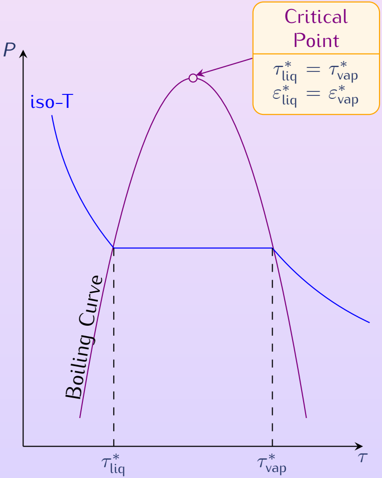

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Summary

Phase Change Equation

$$\frac{\tau - \tau_{\text{vap}}^{\text{sat}}}{\tau_{\text{liq}}^{\text{sat}} - \tau_{\text{vap}}^{\text{sat}}} = \frac{\varepsilon - \varepsilon_{\text{vap}}^{\text{sat}}}{\varepsilon_{\text{liq}}^{\text{sat}} - \varepsilon_{\text{vap}}^{\text{sat}}}$$

with

$$T \mapsto \begin{pmatrix} \tau \\ \varepsilon \end{pmatrix}_\alpha^{\text{sat}} (T) = \begin{pmatrix} \tau \\ \varepsilon \end{pmatrix}_\alpha (T, P^{\text{sat}}(T))$$

or

$$P \mapsto \begin{pmatrix} \tau \\ \varepsilon \end{pmatrix}_\alpha^{\text{sat}} (P) = \begin{pmatrix} \tau \\ \varepsilon \end{pmatrix}_\alpha (T^{\text{sat}}(P), P)$$

Summary

How to compute saturation functions τ_α^{sat} and $\varepsilon_\alpha^{\text{sat}}$

- Analytical EOS: we compute the saturation functions τ_α^{sat} and $\varepsilon_\alpha^{\text{sat}}$ by the Coexistence Curve:
  - Exact: $T \mapsto P^{\text{sat}}(T)$ or $P \mapsto T^{\text{sat}}(P)$

$$\begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_\alpha^{\text{sat}}(P) = \begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_\alpha (T^{\text{sat}}(P), P) \qquad \text{e.g. Simplified Stiffened Gases}$$

  - Approximated: $T \mapsto \widehat{P}^{\text{sat}}(T) \approx P^{\text{sat}}(T)$

$$\begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_\alpha^{\text{sat}}(T) \approx \begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_\alpha (T, \widehat{P}^{\text{sat}}(T)) \qquad \text{e.g. General Stiffened Gases}$$

- Tabulated EOS: the saturation functions τ_α^{sat} and $\varepsilon_\alpha^{\text{sat}}$ are given by experiments and we set

$$\begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_\alpha^{\text{sat}}(T \text{ or } P) \approx \begin{pmatrix}\widehat{\tau}\\ \widehat{\varepsilon}\end{pmatrix}_\alpha^{\text{sat}}(T \text{ or } P)$$

To Do

	EOS		Simulation		
	Pure Phases	Equilibrium	Cavitation	Boiling	Film
Virtual Fluid (SG)	✓	✓	✓	✓	①
Real Fluid (SG)	✓	✓	✓	②	③
Tabulated	④	✓	⑤	⑥	⑦