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Gloria FACCANONI[1] Grégoire ALLAIRE[2] Samuel KOKH[3]

MODELLING AND SIMULATION OF LIQUID-VAPOR PHASE TRANSITION

A CONTRIBUTION TO THE STUDY OF THE BOILING CRISIS

[1] IMATH – Université du Sud Toulon Var (France)

[2] CMAP – École Polytechnique (France)

[3] DEN/DANS/DM2S/SFME/LETR – CEA Saclay (France)

OUTLINE

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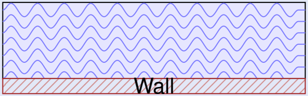
1. **Context**
2. **Model**
   - Equation of State WITHOUT Phase Change
   - Equation of State WITH Phase Change
   - The Phase Change Equation
   - Conservation Laws
3. **Numerical Approximation and Example**
4. **Conclusion**

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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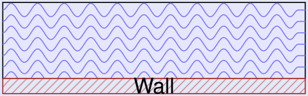

Nucleate Boiling

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

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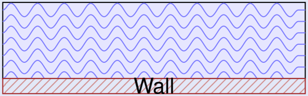

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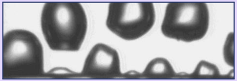

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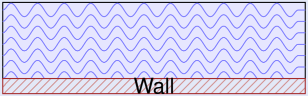

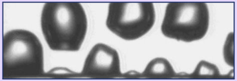

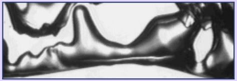

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“INGREDIENTS” OF THE MODEL

✔ Simulating all bubbles (DNS),

- System of PDEs for the fluid flow (monophasic or diphasic),
- Phase transition (pressure and/or temperature variations),
- Heat Diffusion,
- Surface Tension,
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EULER SYSTEM

$$
\begin{cases}
\partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = 0, \\
\partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + P\, \mathbb{I}) = \mathfrak{V}_{\mathrm{vf}} - \mathfrak{S}_{\mathrm{sf}}, \\
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\end{cases}
$$

- $(\mathbf{x}, t) \mapsto \rho$ specific density,
- $(\mathbf{x}, t) \mapsto \varepsilon$ specific internal energy,
- $(\mathbf{x}, t) \mapsto \mathbf{u}$ velocity;
- $(\rho, \varepsilon) \mapsto \mathfrak{V}_{\mathrm{vf}}$ body forces,
- $(\rho, \varepsilon) \mapsto \mathfrak{S}_{\mathrm{sf}}$ surface forces,
- $(\rho, \varepsilon) \mapsto \operatorname{div}(q)$ heat transfer.

$(\rho, \varepsilon) \mapsto P$ pressure law.

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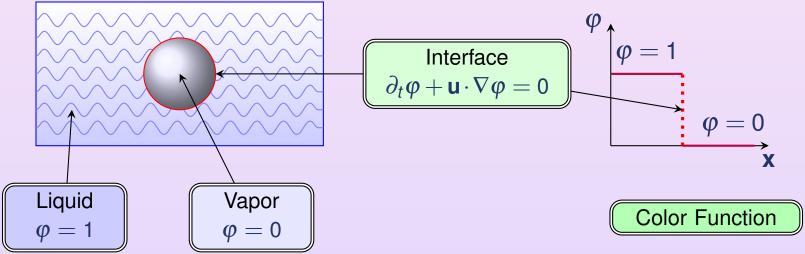
LIQUID-VAPOR INTERFACE



$$(\rho, \varepsilon) \mapsto P = \begin{cases} P^{\text{liq}} & \text{if } \varphi = 1; \\ P^{\text{vap}} & \text{if } \varphi = 0. \end{cases}$$

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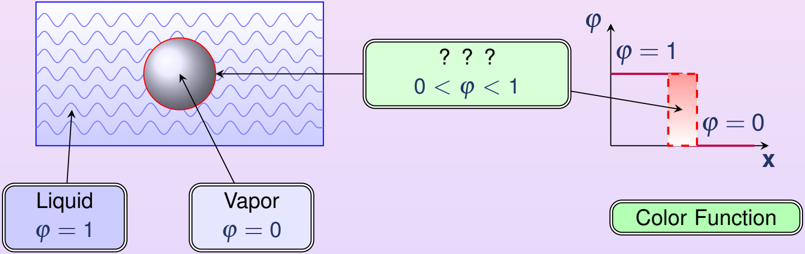

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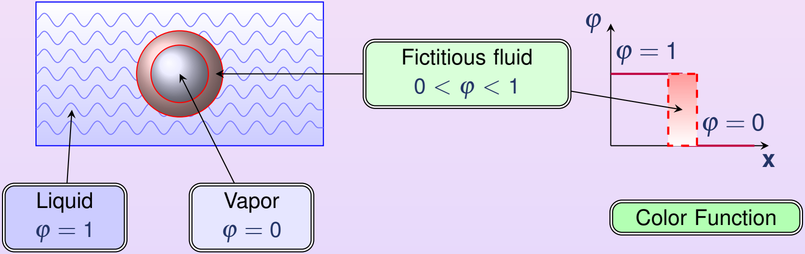

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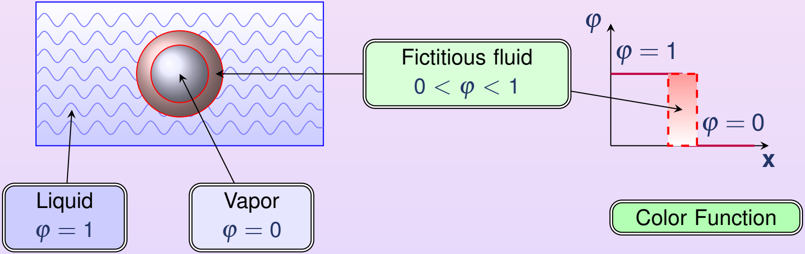
Liquid-Vapor Interface



Goal: define a global pressure law such that

- $(\rho, \varepsilon, \mathbf{u}, P)$ are continuous (3 zones)
- the interface position and the phase change are implicit (i.e. $\not\varphi$)
- coherence with classical thermodynamics [H. Callen]

EOS OF EACH PHASE $\alpha = 1, 2$

$$\left.\begin{array}{l}\tau_\alpha \text{ specific volume}\\ \varepsilon_\alpha \text{ specific internal energy}\end{array}\right\} \quad \Rightarrow \quad \mathbf{w}_\alpha \stackrel{\text{def}}{=} (\tau_\alpha, \varepsilon_\alpha);$$

$\mathbf{w}_\alpha \mapsto s_\alpha$ specific entropy (Hessian matrix neg. def.);

$$\hookrightarrow \begin{cases} T_\alpha \stackrel{\text{def}}{=} \left(\left.\dfrac{\partial s_\alpha}{\partial \varepsilon_\alpha}\right|_{\tau_\alpha} \right)^{-1} > 0 & \text{temperature,} \\ P_\alpha \stackrel{\text{def}}{=} T_\alpha \left.\dfrac{\partial s_\alpha}{\partial \tau_\alpha}\right|_{\varepsilon_\alpha} > 0 & \text{pressure,} \\ g_\alpha \stackrel{\text{def}}{=} \varepsilon_\alpha + P_\alpha \tau_\alpha - T_\alpha s_\alpha & \text{free enthalpy (Gibbs potential).} \end{cases}$$

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- $\mathbf{w} \stackrel{\text{def}}{=} y\mathbf{w}_1 + (1-y)\mathbf{w}_2$;
- y mass fraction;
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OUTLINE

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ENTROPY WITHOUT PH.CH.

$$(\mathbf{w}, z, y, \psi) \mapsto \sigma$$

→

ENTROPY AT EQUILIBRIUM

$$\mathbf{w} \mapsto s^{\mathrm{eq}}$$

DEFINITION [H. CALLEN, PH. HELLUY ...]

Optimization Problem:

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

Optimality Condition:

$$\begin{cases} T_1(z,y,\psi) = T_2(z,y,\psi) \\ P_1(z,y,\psi) = P_2(z,y,\psi) \\ g_1(z,y,\psi) = g_2(z,y,\psi) \\ z,y,\psi \in]0,1[^3 \end{cases}$$

Solution: (z^*, y^*, ψ^*)

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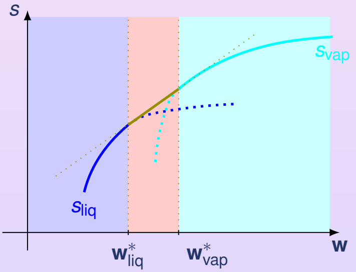

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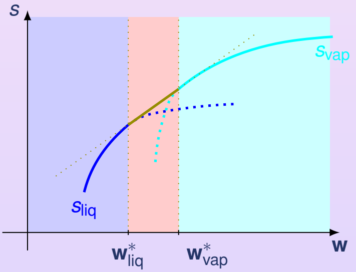

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EOS with Phase Change

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Entropy at equilibrium

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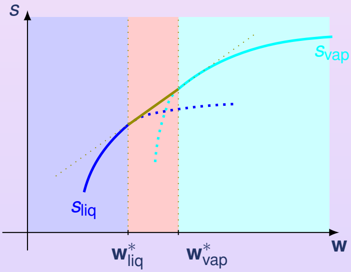

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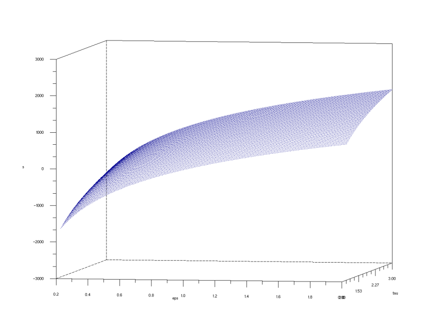
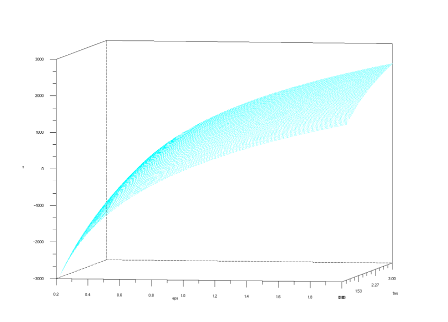
Concave Hull with two Perfect Gases

$$(\tau,\varepsilon) \mapsto s_{\text{liq}}$$



$$(\tau,\varepsilon) \mapsto s_{\text{vap}}$$



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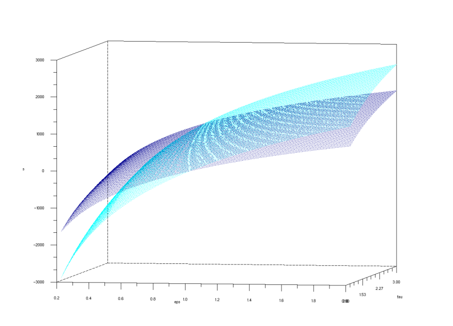

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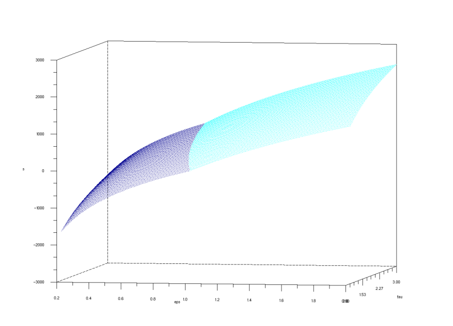

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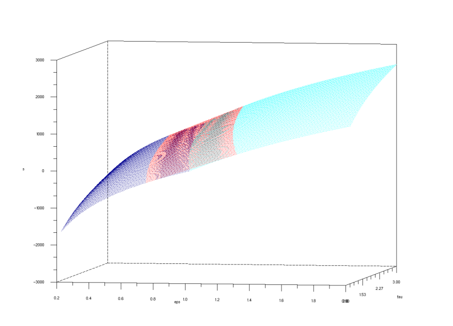

CONCAVE HULL WITH TWO PERFECT GASES

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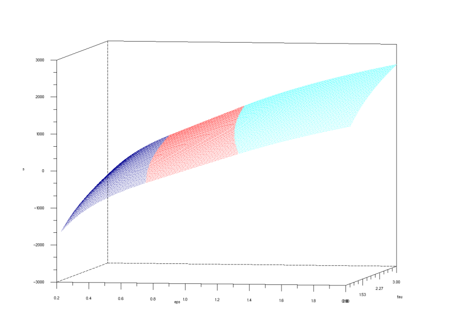

FROM $\mathbf{w} \mapsto s^{\text{eq}}$ TO $\mathbf{w} \mapsto P^{\text{eq}}$

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

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

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

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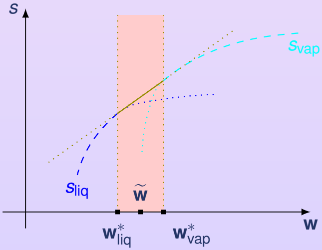

FROM $\mathbf{w} \mapsto s^{\text{eq}}$ TO $\mathbf{w} \mapsto P^{\text{eq}}$

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

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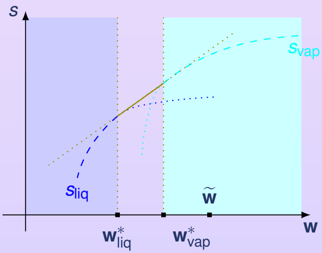

FROM $\mathbf{w} \mapsto s^{eq}$ TO $\mathbf{w} \mapsto P^{eq}$

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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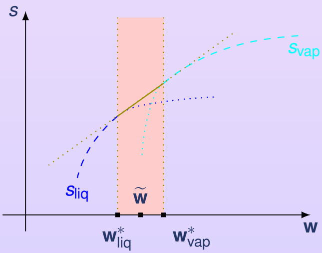

From $\mathbf{w} \mapsto s^{\text{eq}}$ to $\mathbf{w} \mapsto P^{\text{eq}}$

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

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

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

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

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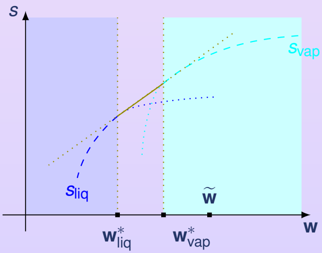

OUTLINE

Summary of the Model

$$\mathbf{w} \longmapsto s^{\text{eq}}$$

$$\begin{cases} g_1(\mathbf{w}_1)=g_2(\mathbf{w}_2) \\ P_1(\mathbf{w}_1)=P_2(\mathbf{w}_2) \\ T_1(\mathbf{w}_1)=T_2(\mathbf{w}_2) \\ \mathbf{w}=y\mathbf{w}_1+(1-y)\mathbf{w}_2 \end{cases}$$

Euler System

$$\mathbf{w} \longmapsto P^{\text{eq}}$$

Phase Change Equation

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

Summary of the Model

Euler System

$\mathbf{w} \longmapsto P^{\text{eq}}$

$\mathbf{w} \longmapsto s^{\text{eq}}$

$$\begin{cases} g_1(\mathbf{w}_1) = g_2(\mathbf{w}_2) \\ P_1(\mathbf{w}_1) = P_2(\mathbf{w}_2) \\ T_1(\mathbf{w}_1) = T_2(\mathbf{w}_2) \\ \mathbf{w} = y\mathbf{w}_1 + (1-y)\mathbf{w}_2 \end{cases}$$

Phase Change Equation

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

SUMMARY OF THE MODEL

Euler System

$$\mathbf{w} \longmapsto P^{\text{eq}}$$

$$\mathbf{w} \longmapsto s^{\text{eq}}$$

$$\begin{cases} g_1(\mathbf{w}_1) = g_2(\mathbf{w}_2) \\ P_1(\mathbf{w}_1) = P_2(\mathbf{w}_2) \\ T_1(\mathbf{w}_1) = T_2(\mathbf{w}_2) \\ \mathbf{w} = y\mathbf{w}_1 + (1-y)\mathbf{w}_2 \end{cases}$$

Phase Change Equation

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

Summary of the Model

Euler System

$$\mathbf{w} \longmapsto P^{\mathrm{eq}}$$

$$\mathbf{w} \longmapsto s^{\mathrm{eq}}$$

$$\begin{cases} g_1(\mathbf{w}_1) = g_2(\mathbf{w}_2) \\ P_1(\mathbf{w}_1) = P_2(\mathbf{w}_2) \\ T_1(\mathbf{w}_1) = T_2(\mathbf{w}_2) \\ \mathbf{w} = y\mathbf{w}_1 + (1-y)\mathbf{w}_2 \end{cases}$$

Phase Change Equation

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

SUMMARY OF THE MODEL

$\mathbf{w} \longmapsto s^{\text{eq}}$

$$\begin{cases} g_1(\mathbf{w}_1) = g_2(\mathbf{w}_2) \\ P_1(\mathbf{w}_1) = P_2(\mathbf{w}_2) \\ T_1(\mathbf{w}_1) = T_2(\mathbf{w}_2) \\ \mathbf{w} = y\mathbf{w}_1 + (1-y)\mathbf{w}_2 \end{cases}$$

Euler System

$\mathbf{w} \longmapsto P^{\text{eq}}$

Phase Change Equation

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

ANALYTICAL EOS

(τ, ε) fixed

$(\tau_1, \varepsilon_1, \tau_2, \varepsilon_2, y)$ SOLUTION OF

$$\begin{cases} g_1(\tau_1,\varepsilon_1) = g_2(\tau_2,\varepsilon_2) \\ P_1(\tau_1,\varepsilon_1) = P_2(\tau_2,\varepsilon_2) \\ T_1(\tau_1,\varepsilon_1) = T_2(\tau_2,\varepsilon_2) \\ \tau = y\tau_1 + (1-y)\tau_2 \\ \varepsilon = y\varepsilon_1 + (1-y)\varepsilon_2 \end{cases}$$

(P, T) SOLUTION OF

$$\begin{cases} g_1(P,T) = g_2(P,T) \\ \dfrac{\tau - \tau_2(P,T)}{\tau_1(P,T) - \tau_2(P,T)} = \dfrac{\varepsilon - \varepsilon_2(P,T)}{\varepsilon_1(P,T) - \varepsilon_2(P,T)} \end{cases}$$

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

T SOLUTION OF

$$\frac{\tau - \tau_2^{\text{sat}}(T)}{\tau_1^{\text{sat}}(T) - \tau_2^{\text{sat}}(T)} = \frac{\varepsilon - \varepsilon_2^{\text{sat}}(T)}{\varepsilon_1^{\text{sat}}(T) - \varepsilon_2^{\text{sat}}(T)} \quad \text{where} \quad \begin{pmatrix}\tau \\ \varepsilon\end{pmatrix}_\alpha^{\text{sat}}(T) \stackrel{\text{def}}{=} \begin{pmatrix}\tau \\ \varepsilon\end{pmatrix}_\alpha (P^{\text{sat}}(T), T)$$

Analytical EOS

(τ, ε) fixed

$(\tau_1, \varepsilon_1, \tau_2, \varepsilon_2, y)$ SOLUTION OF

$$\begin{cases} g_1(\tau_1, \varepsilon_1) = g_2(\tau_2, \varepsilon_2) \\ P_1(\tau_1, \varepsilon_1) = P_2(\tau_2, \varepsilon_2) \\ T_1(\tau_1, \varepsilon_1) = T_2(\tau_2, \varepsilon_2) \\ \tau = y\tau_1 + (1-y)\tau_2 \\ \varepsilon = y\varepsilon_1 + (1-y)\varepsilon_2 \end{cases}$$

(P, T) SOLUTION OF

$$\begin{cases} g_1(P,T) = g_2(P,T) \\ \dfrac{\tau - \tau_2(P,T)}{\tau_1(P,T) - \tau_2(P,T)} = \dfrac{\varepsilon - \varepsilon_2(P,T)}{\varepsilon_1(P,T) - \varepsilon_2(P,T)} \end{cases}$$

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

T SOLUTION OF

$$\frac{\tau - \tau_2^{\text{sat}}(T)}{\tau_1^{\text{sat}}(T) - \tau_2^{\text{sat}}(T)} = \frac{\varepsilon - \varepsilon_2^{\text{sat}}(T)}{\varepsilon_1^{\text{sat}}(T) - \varepsilon_2^{\text{sat}}(T)} \quad \text{where} \quad \begin{pmatrix} \tau \\ \varepsilon \end{pmatrix}_\alpha^{\text{sat}}(T) \stackrel{\text{def}}{=} \begin{pmatrix} \tau \\ \varepsilon \end{pmatrix}_\alpha (P^{\text{sat}}(T), T)$$

Analytical EOS

(τ,ε) fixed

$(\tau_1,\varepsilon_1,\tau_2,\varepsilon_2,y)$ solution of

$$\begin{cases} g_1(\tau_1,\varepsilon_1)=g_2(\tau_2,\varepsilon_2)\\ P_1(\tau_1,\varepsilon_1)=P_2(\tau_2,\varepsilon_2)\\ T_1(\tau_1,\varepsilon_1)=T_2(\tau_2,\varepsilon_2)\\ \tau=y\tau_1+(1-y)\tau_2\\ \varepsilon=y\varepsilon_1+(1-y)\varepsilon_2 \end{cases}$$

(P,T) solution of

$$\begin{cases} g_1(P,T)=g_2(P,T)\\ \dfrac{\tau-\tau_2(P,T)}{\tau_1(P,T)-\tau_2(P,T)}=\dfrac{\varepsilon-\varepsilon_2(P,T)}{\varepsilon_1(P,T)-\varepsilon_2(P,T)} \end{cases}$$

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

T solution of

$$\frac{\tau-\tau_2^{\text{sat}}(T)}{\tau_1^{\text{sat}}(T)-\tau_2^{\text{sat}}(T)}=\frac{\varepsilon-\varepsilon_2^{\text{sat}}(T)}{\varepsilon_1^{\text{sat}}(T)-\varepsilon_2^{\text{sat}}(T)}\quad\text{where}\quad\begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_\alpha^{\text{sat}}(T)\stackrel{\text{def}}{=}\begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_\alpha(P^{\text{sat}}(T),T)$$

Analytical EOS

(τ, ε) fixed

$(\tau_1, \varepsilon_1, \tau_2, \varepsilon_2, y)$ SOLUTION OF

$$\begin{cases} g_1(\tau_1, \varepsilon_1) = g_2(\tau_2, \varepsilon_2) \\ P_1(\tau_1, \varepsilon_1) = P_2(\tau_2, \varepsilon_2) \\ T_1(\tau_1, \varepsilon_1) = T_2(\tau_2, \varepsilon_2) \\ \tau = y\tau_1 + (1-y)\tau_2 \\ \varepsilon = y\varepsilon_1 + (1-y)\varepsilon_2 \end{cases}$$

(P, T) SOLUTION OF

$$\begin{cases} g_1(P, T) = g_2(P, T) \\ \dfrac{\tau - \tau_2(P,T)}{\tau_1(P,T) - \tau_2(P,T)} = \dfrac{\varepsilon - \varepsilon_2(P,T)}{\varepsilon_1(P,T) - \varepsilon_2(P,T)} \end{cases}$$

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T SOLUTION OF

$$\frac{\tau - \tau_2^{\text{sat}}(T)}{\tau_1^{\text{sat}}(T) - \tau_2^{\text{sat}}(T)} = \frac{\varepsilon - \varepsilon_2^{\text{sat}}(T)}{\varepsilon_1^{\text{sat}}(T) - \varepsilon_2^{\text{sat}}(T)} \quad \text{where} \quad \begin{pmatrix} \tau \\ \varepsilon \end{pmatrix}_\alpha^{\text{sat}}(T) \stackrel{\text{def}}{=} \begin{pmatrix} \tau \\ \varepsilon \end{pmatrix}_\alpha (P^{\text{sat}}(T), T)$$

ANALYTICAL EOS

(τ,ε) fixed

$(\tau_1,\varepsilon_1,\tau_2,\varepsilon_2,y)$ SOLUTION OF

$$\begin{cases} g_1(\tau_1,\varepsilon_1)=g_2(\tau_2,\varepsilon_2)\\ P_1(\tau_1,\varepsilon_1)=P_2(\tau_2,\varepsilon_2)\\ T_1(\tau_1,\varepsilon_1)=T_2(\tau_2,\varepsilon_2)\\ \tau=y\tau_1+(1-y)\tau_2\\ \varepsilon=y\varepsilon_1+(1-y)\varepsilon_2 \end{cases}$$

(P,T) SOLUTION OF

$$\begin{cases} g_1(P,T)=g_2(P,T)\\ \dfrac{\tau-\tau_2(P,T)}{\tau_1(P,T)-\tau_2(P,T)}=\dfrac{\varepsilon-\varepsilon_2(P,T)}{\varepsilon_1(P,T)-\varepsilon_2(P,T)} \end{cases}$$

least square approximation

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

T SOLUTION OF

$$\frac{\tau-\tau_2^{\text{sat}}(T)}{\tau_1^{\text{sat}}(T)-\tau_2^{\text{sat}}(T)}=\frac{\varepsilon-\varepsilon_2^{\text{sat}}(T)}{\varepsilon_1^{\text{sat}}(T)-\varepsilon_2^{\text{sat}}(T)}\quad\text{where}\quad\begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_\alpha^{\text{sat}}(T)\stackrel{\text{def}}{=}\begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_\alpha(\widehat{P}^{\text{sat}}(T),T)$$

TABULATED EOS

		Volume (m^3/kg)		Internal Energy (kJ/kg)	
T (K)	P^{sat} (MPa)	$\tau^{\text{sat}}_{\text{liq}}$	$\tau^{\text{sat}}_{\text{vap}}$	$\varepsilon^{\text{sat}}_{\text{liq}}$	$\varepsilon^{\text{sat}}_{\text{vap}}$
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/`

TABULATED EOS

(τ, ε) fixed

T SOLUTION OF

$$\frac{\tau - \tau_2^{\text{sat}}(T)}{\tau_1^{\text{sat}}(T) - \tau_2^{\text{sat}}(T)} = \frac{\varepsilon - \varepsilon_2^{\text{sat}}(T)}{\varepsilon_1^{\text{sat}}(T) - \varepsilon_2^{\text{sat}}(T)} \quad \text{with} \quad \begin{pmatrix}\tau \\ \varepsilon\end{pmatrix}_\alpha^{\text{sat}}(T) \quad \text{tabulated}$$

$$\wr$$

$$\frac{\tau - \widehat{\tau}_2^{\text{sat}}(T)}{\widehat{\tau}_1^{\text{sat}}(T) - \widehat{\tau}_2^{\text{sat}}(T)} = \frac{\varepsilon - \widehat{\varepsilon}_2^{\text{sat}}(T)}{\widehat{\varepsilon}_1^{\text{sat}}(T) - \widehat{\varepsilon}_2^{\text{sat}}(T)} \quad \text{with} \quad \begin{pmatrix}\widehat{\tau} \\ \widehat{\varepsilon}\end{pmatrix}_\alpha^{\text{sat}}(T)$$

TABULATED EOS

(τ, ε) fixed

T SOLUTION OF

$$\frac{\tau - \tau_2^{\text{sat}}(T)}{\tau_1^{\text{sat}}(T) - \tau_2^{\text{sat}}(T)} = \frac{\varepsilon - \varepsilon_2^{\text{sat}}(T)}{\varepsilon_1^{\text{sat}}(T) - \varepsilon_2^{\text{sat}}(T)}$$ with $\begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_\alpha^{\text{sat}}(T)$ tabulated

$\wr\wr$

$$\frac{\tau - \widehat{\tau}_2^{\text{sat}}(T)}{\widehat{\tau}_1^{\text{sat}}(T) - \widehat{\tau}_2^{\text{sat}}(T)} = \frac{\varepsilon - \widehat{\varepsilon}_2^{\text{sat}}(T)}{\widehat{\varepsilon}_1^{\text{sat}}(T) - \widehat{\varepsilon}_2^{\text{sat}}(T)}$$ with $\begin{pmatrix}\widehat{\tau}\\ \widehat{\varepsilon}\end{pmatrix}_\alpha^{\text{sat}}(T)$

least square approximations

TABULATED EOS

(τ, ε) fixed

T SOLUTION OF

$$\frac{\tau-\tau_2^{\text{sat}}(T)}{\tau_1^{\text{sat}}(T)-\tau_2^{\text{sat}}(T)}=\frac{\varepsilon-\varepsilon_2^{\text{sat}}(T)}{\varepsilon_1^{\text{sat}}(T)-\varepsilon_2^{\text{sat}}(T)} \quad \text{with} \quad \begin{pmatrix}\tau\\ \varepsilon\end{pmatrix}_\alpha^{\text{sat}}(T) \quad \text{tabulated}$$

$$\wr\wr$$

$$\frac{\tau-\widehat{\tau}_2^{\text{sat}}(T)}{\widehat{\tau}_1^{\text{sat}}(T)-\widehat{\tau}_2^{\text{sat}}(T)}=\frac{\varepsilon-\widehat{\varepsilon}_2^{\text{sat}}(T)}{\widehat{\varepsilon}_1^{\text{sat}}(T)-\widehat{\varepsilon}_2^{\text{sat}}(T)} \quad \text{with} \quad \begin{pmatrix}\widehat{\tau}\\ \widehat{\varepsilon}\end{pmatrix}_\alpha^{\text{sat}}(T)$$

least square approximations

OUTLINE

Dynamic Liquid-Vapor Phase Change

Euler System

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

Mathematical Properties

If $\tau_1^* \neq \tau_2^*$ and $\varepsilon_1^* \neq \varepsilon_2^*$ (first order phase transition) then

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

Dynamic Liquid-Vapor Phase Change

Euler System

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

Mathematical Properties

If $\tau_1^* \neq \tau_2^*$ and $\varepsilon_1^* \neq \varepsilon_2^*$ (first order phase transition) then

❶ $c(\mathbf{w}) > 0$, ❷ $s_{\tau\varepsilon}^{\text{eq}}(\mathbf{w}) > 0$

❶ Euler system: strict hyperbolicity ($\neq$ p-system),

❷ Riemann problem: multitude of entropy (Lax) solutions [R. Menikoff, B. J. Plohr], uniqueness of Liu solution.

DYNAMIC LIQUID-VAPOR PHASE CHANGE

EULER SYSTEM

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

MATHEMATICAL PROPERTIES

If $\tau_1^* \neq \tau_2^*$ and $\varepsilon_1^* \neq \varepsilon_2^*$ (first order phase transition) then

❶ $c(\mathbf{w}) > 0$, ❷ $s_{\tau\varepsilon}^{\mathrm{eq}}(\mathbf{w}) > 0$

❶ Euler system: strict hyperbolicity ($\neq$ p-system),

❷ Riemann problem: multitude of entropy (Lax) solutions [R. MENIKOFF, B. J. PLOHR], uniqueness of Liu solution.

OUTLINE

Numerical Scheme based on Relaxation Approach

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

Off Equilibrium

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

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

Equilibrium

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

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

Two Steps:

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

Numerical Scheme based on Relaxation Approach

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

Off Equilibrium

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

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

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

Equilibrium

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

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Numerical Scheme based on Relaxation Approach

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

Off Equilibrium

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

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

Equilibrium

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

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

Two Steps:

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

Numerical Scheme based on Relaxation Approach

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

Off Equilibrium

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

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Equilibrium

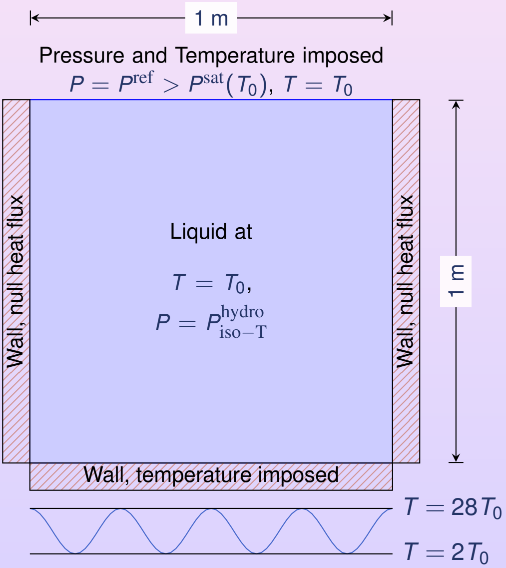
$$\begin{cases}\partial_t\rho+\operatorname{div}(\rho\mathbf{u})=0\\ \partial_t(\rho\mathbf{u})+\operatorname{div}(\rho\mathbf{u}\otimes\mathbf{u}+P^{\text{eq}}\mathbb{I})=0\\ \partial_t(\rho e)+\operatorname{div}((\rho e+P^{\text{eq}})\mathbf{u})=0\end{cases}$$

$$P^{\text{eq}}(\rho,\varepsilon)=\frac{s_\tau^{\text{eq}}}{s_\varepsilon^{\text{eq}}}$$

Two Steps:

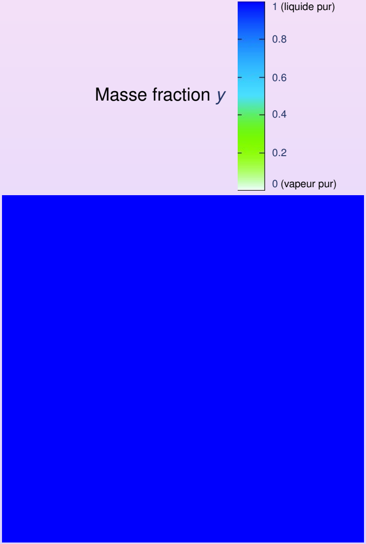
1. Hydrodynamic (+ gravity, surface tension, heat diffusion, ...)
2. Projection by solving the Phase-Change Equation

Transition to a Film Boiling

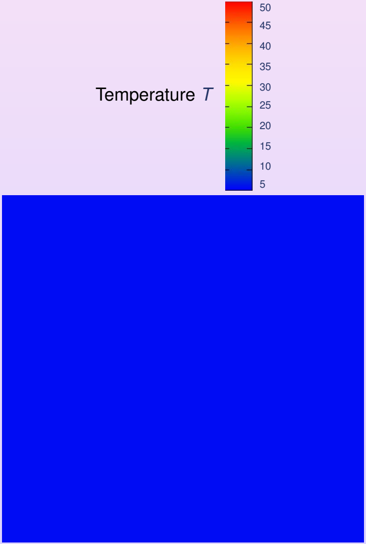


Transition to a Film Boiling

Masse fraction y



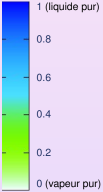
Temperature T



Geometry Play Skip

TRANSITION TO A FILM BOILING

Masse fraction y



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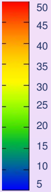
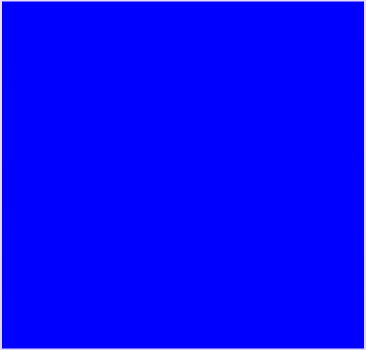
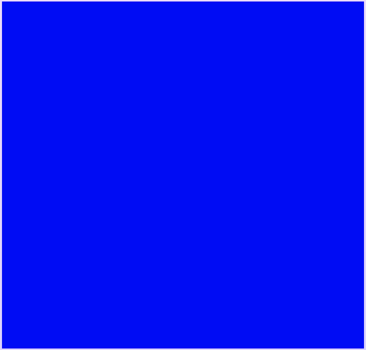
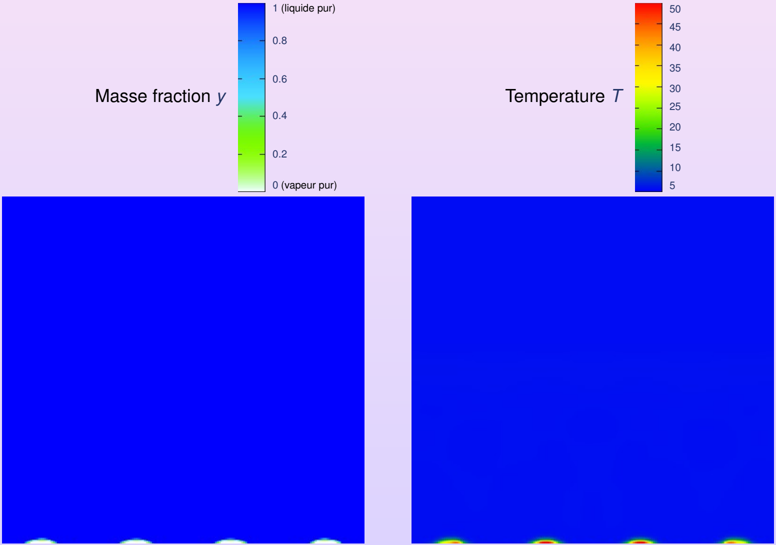






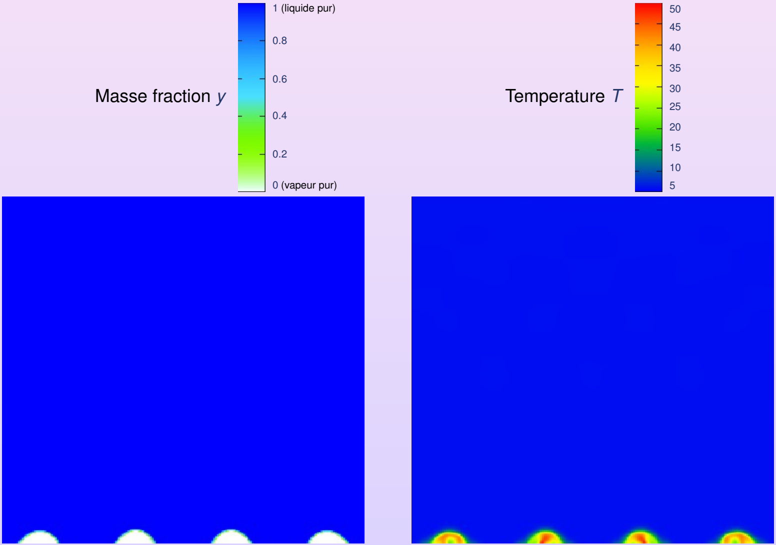
◀ Geometry ▶ Play ⏩ Skip

Transition to a Film Boiling



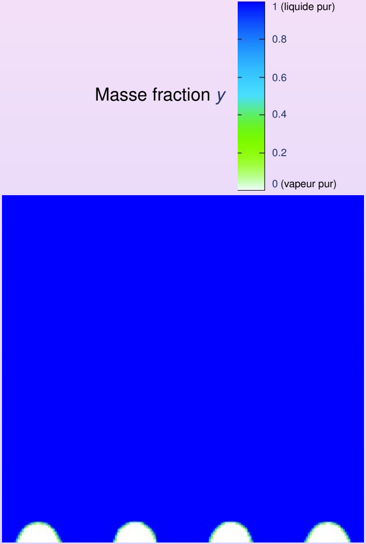
Geometry Play Skip

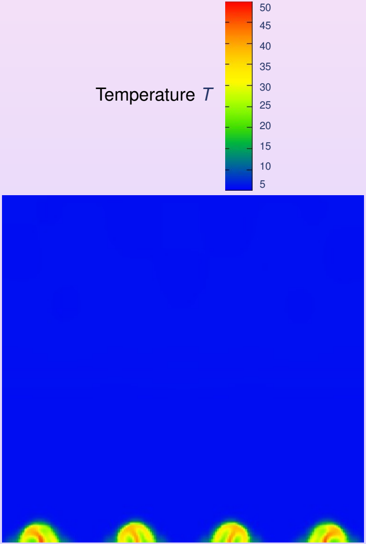
Transition to a Film Boiling



Geometry Play Skip

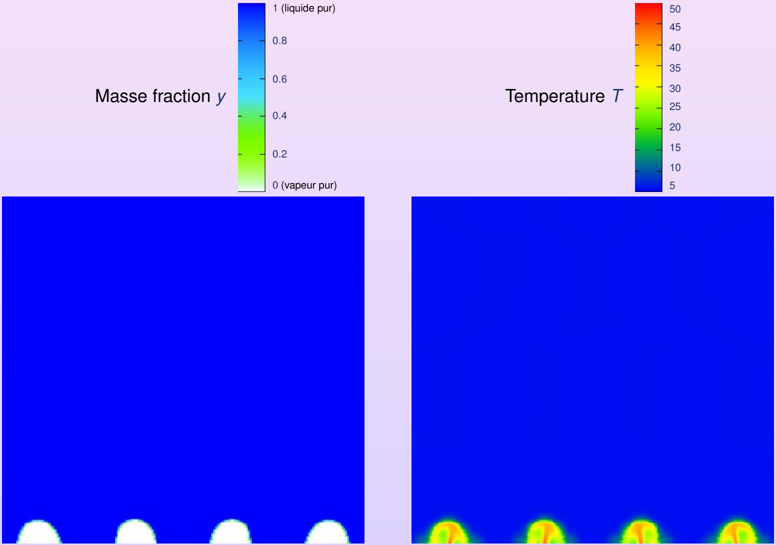
Transition to a Film Boiling



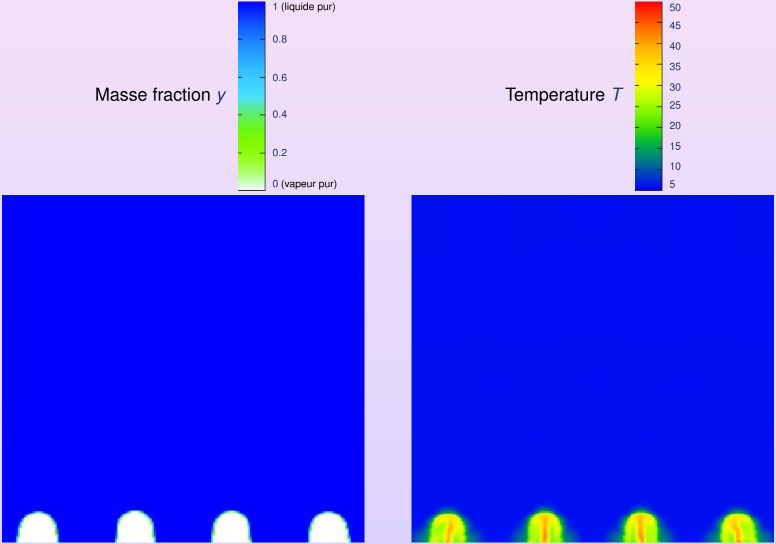


◂ Geometry ▸ Play ▸▸ Skip

TRANSITION TO A FILM BOILING

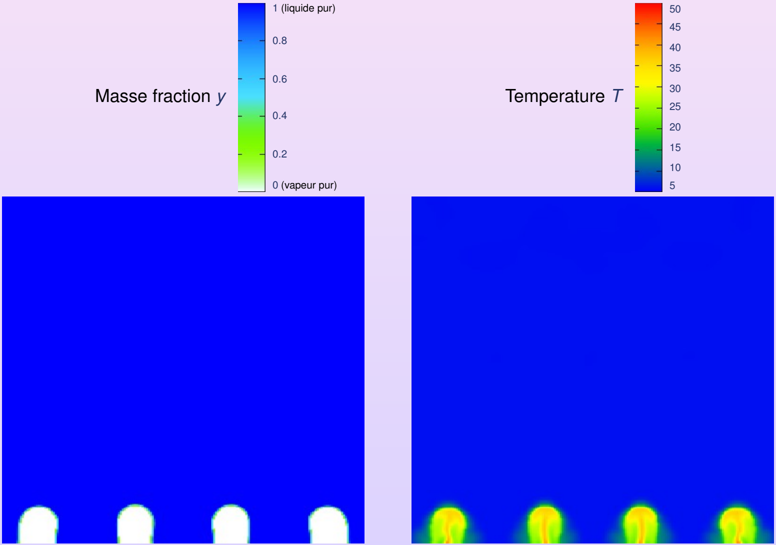


Transition to a Film Boiling



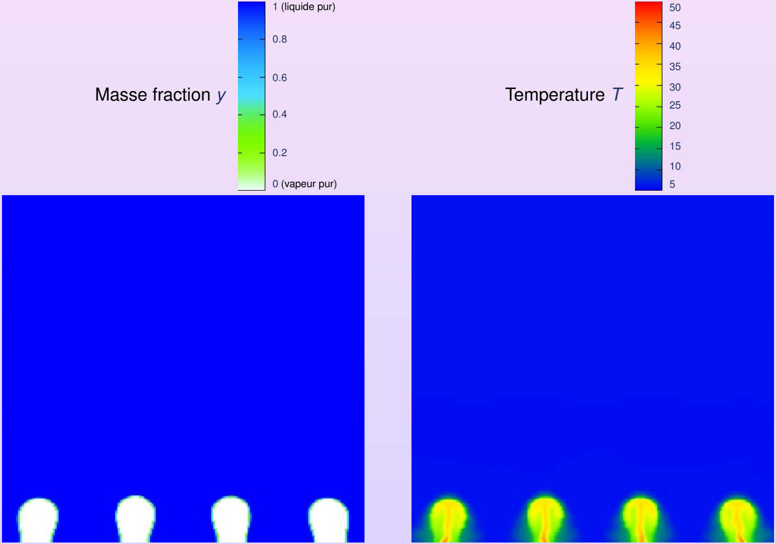
◂ Geometry ▸ Play ▸▸ Skip

Transition to a Film Boiling



Geometry Play Skip

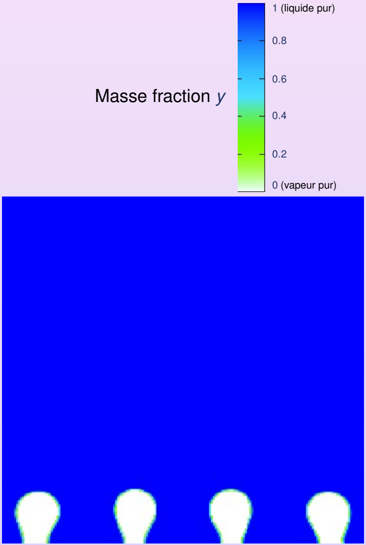
Transition to a Film Boiling



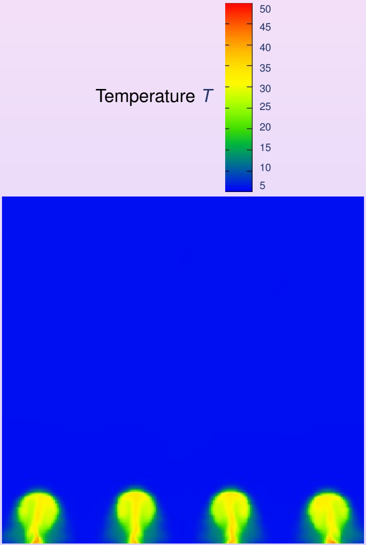
Geometry Play Skip

Transition to a Film Boiling

Masse fraction y

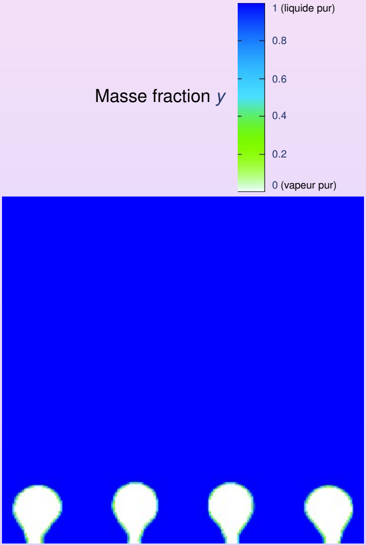


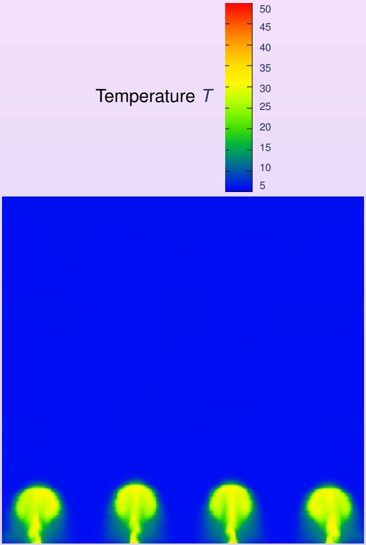
Temperature T



◂ Geometry ▸ Play ▸▸ Skip

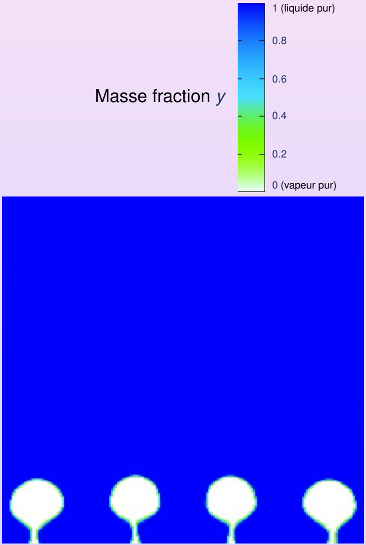
TRANSITION TO A FILM BOILING

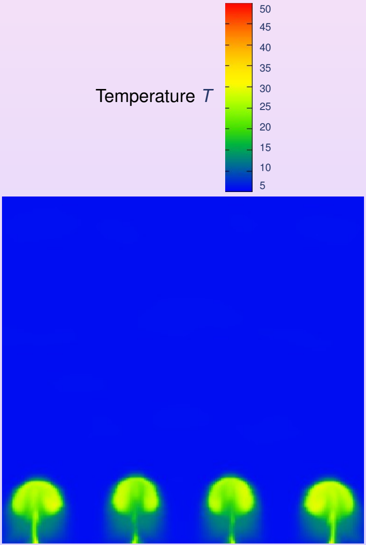




◀ Geometry ▶ Play ▶▶ Skip

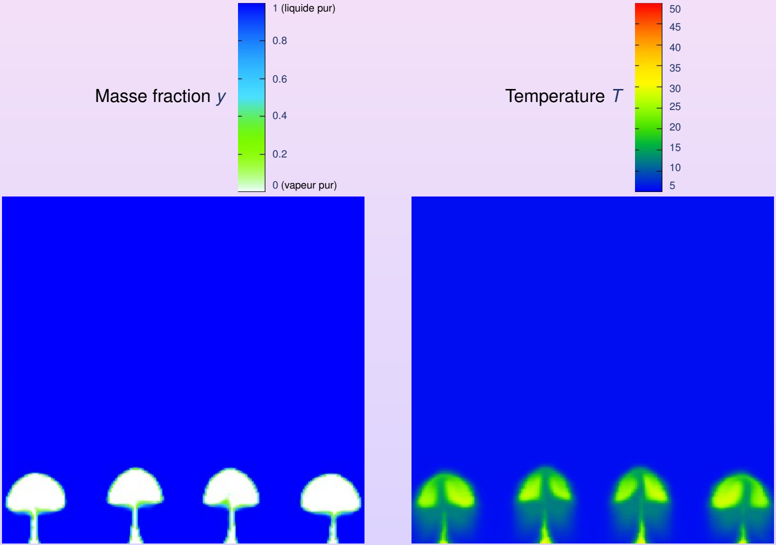
TRANSITION TO A FILM BOILING





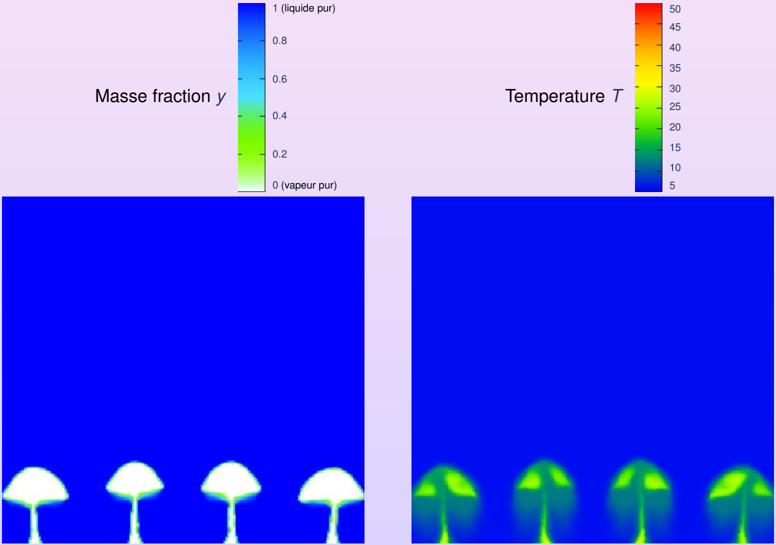
Geometry Play Skip

Transition to a Film Boiling



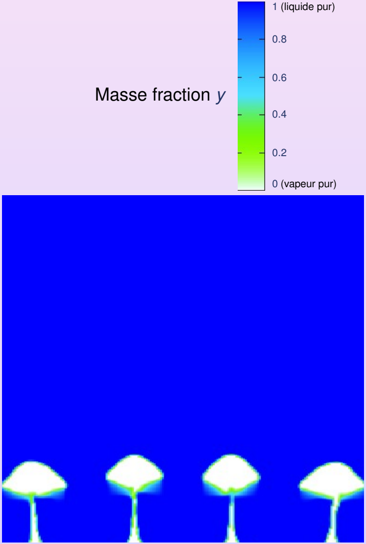
Geometry Play Skip

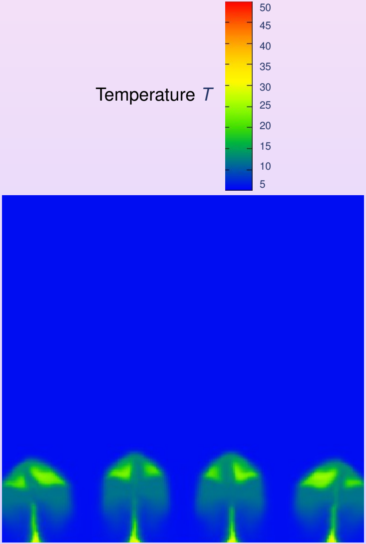
TRANSITION TO A FILM BOILING



Geometry Play Skip

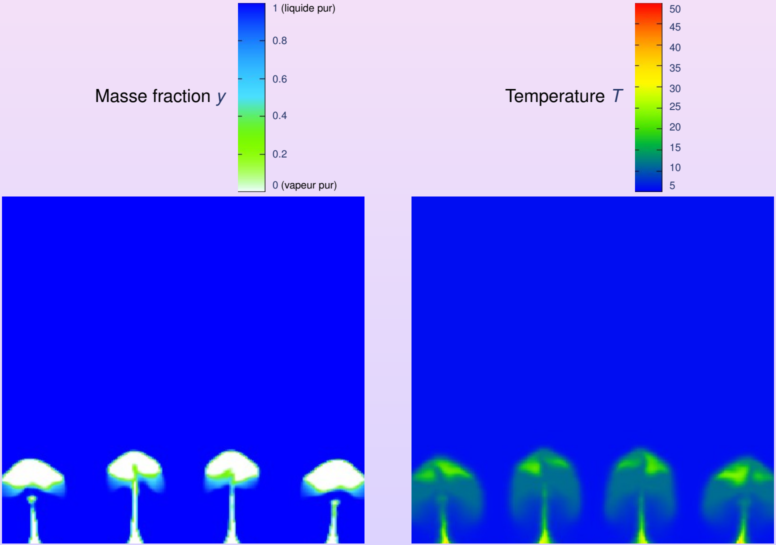
Transition to a Film Boiling





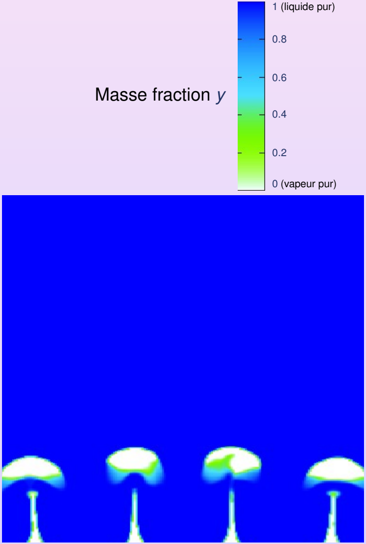
Geometry Play Skip

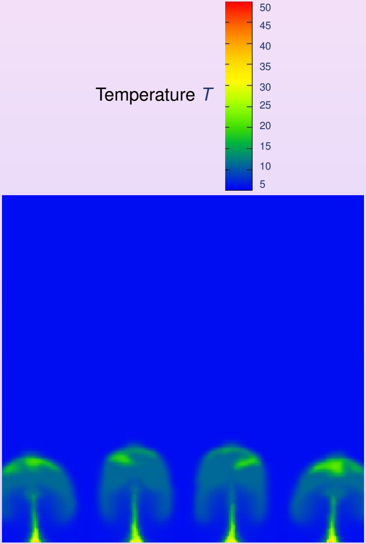
TRANSITION TO A FILM BOILING



Geometry Play Skip

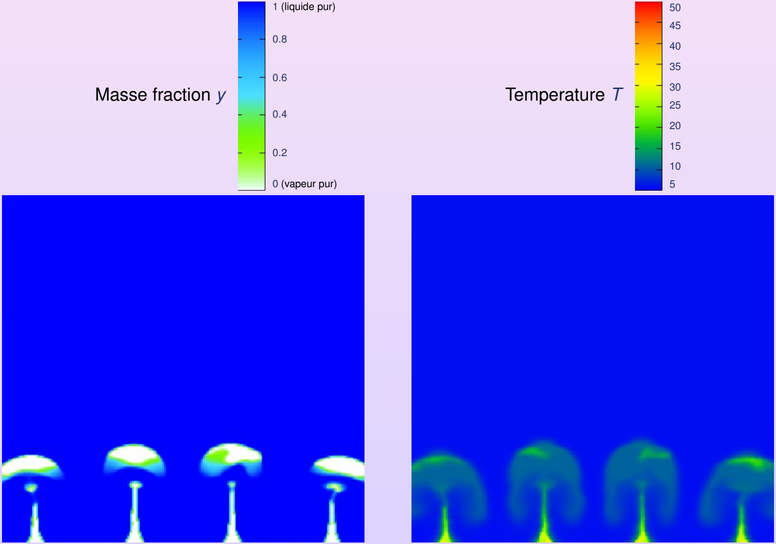
TRANSITION TO A FILM BOILING





◂ Geometry ▸ Play ▸▸ Skip

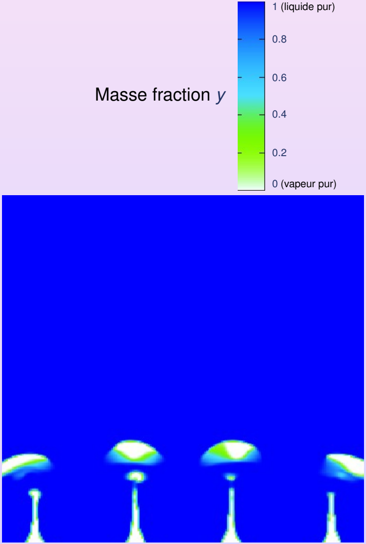
Transition to a Film Boiling



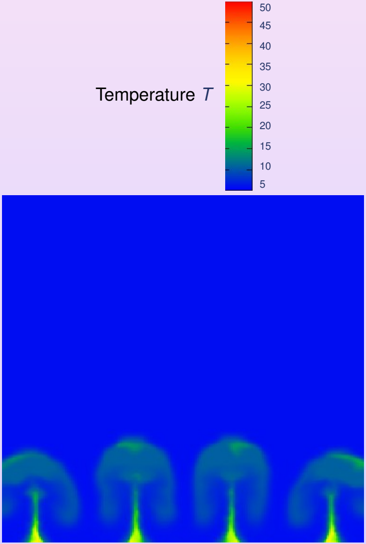
Geometry Play Skip

Transition to a Film Boiling

Masse fraction y

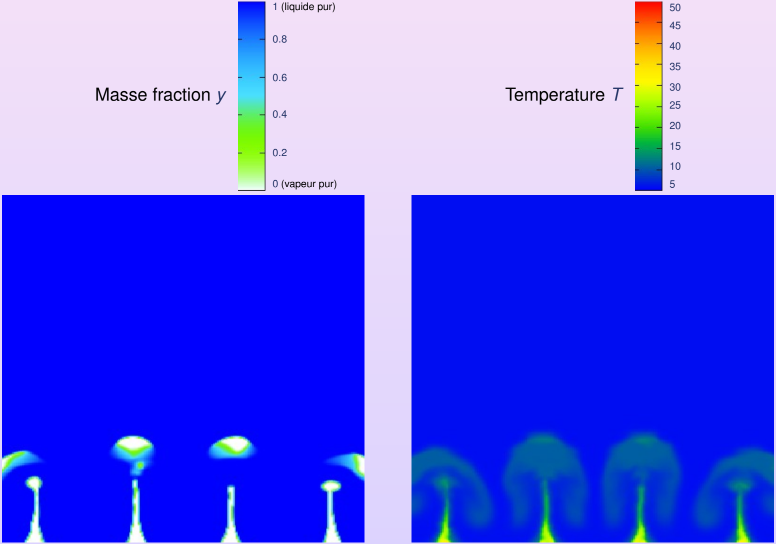


Temperature T



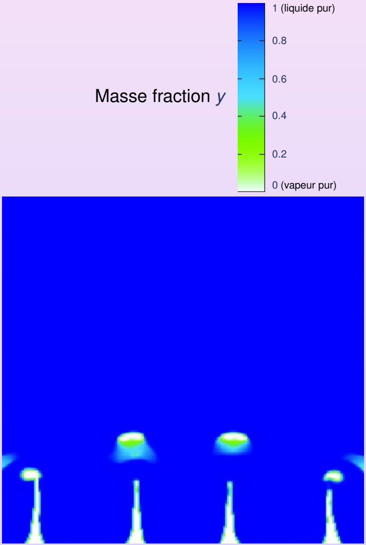
◂ Geometry ▸ Play ▸▸ Skip

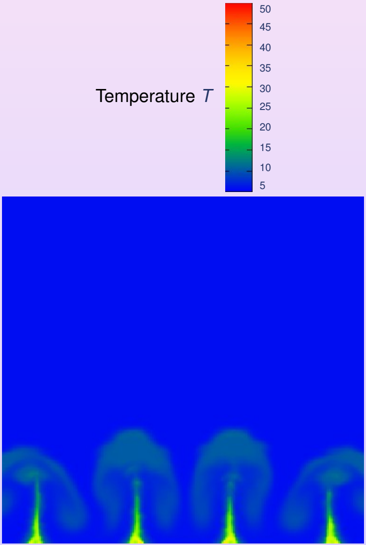
Transition to a Film Boiling



Geometry Play Skip

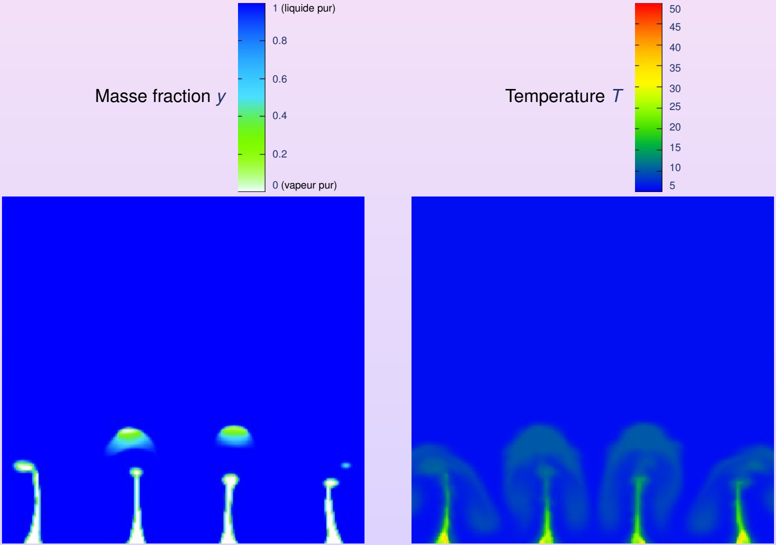
Transition to a Film Boiling





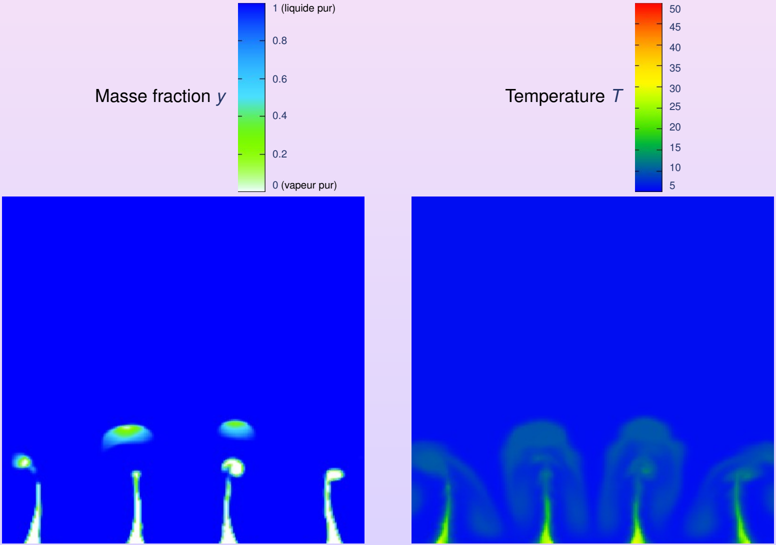
◂ Geometry ▸ Play ▸▸ Skip

Transition to a Film Boiling



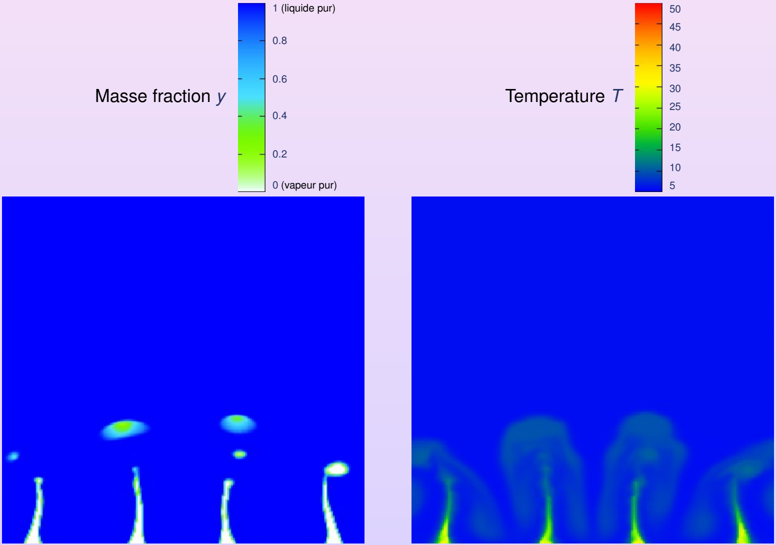
Geometry Play Skip

Transition to a Film Boiling



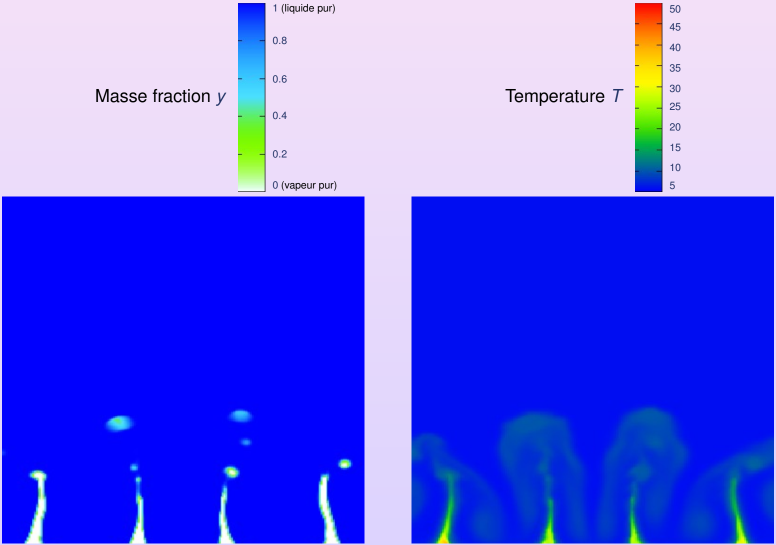
Geometry Play Skip

TRANSITION TO A FILM BOILING



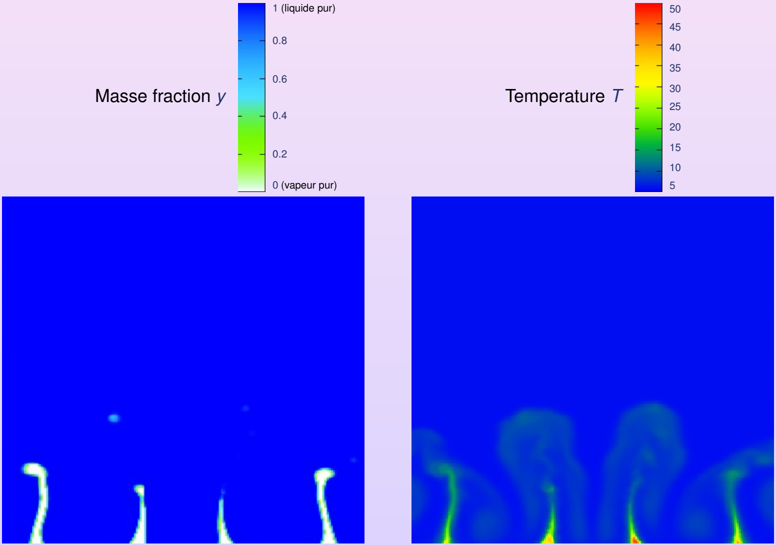
Geometry Play Skip

TRANSITION TO A FILM BOILING



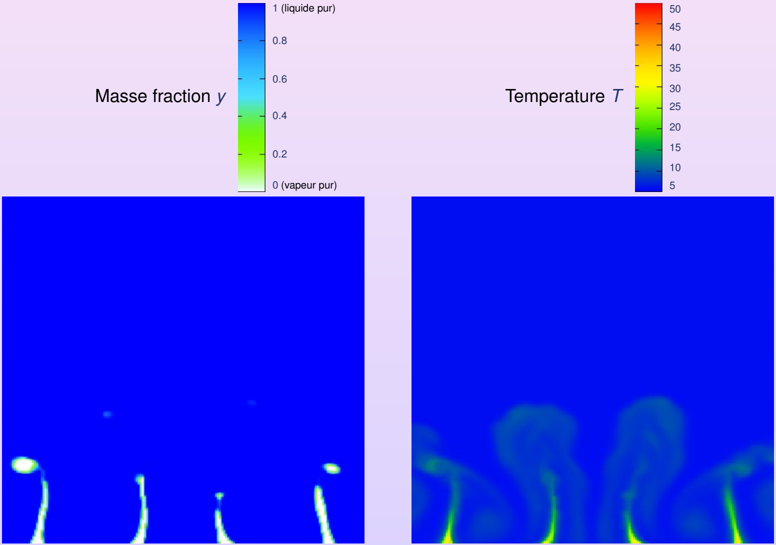
Geometry Play Skip

Transition to a Film Boiling



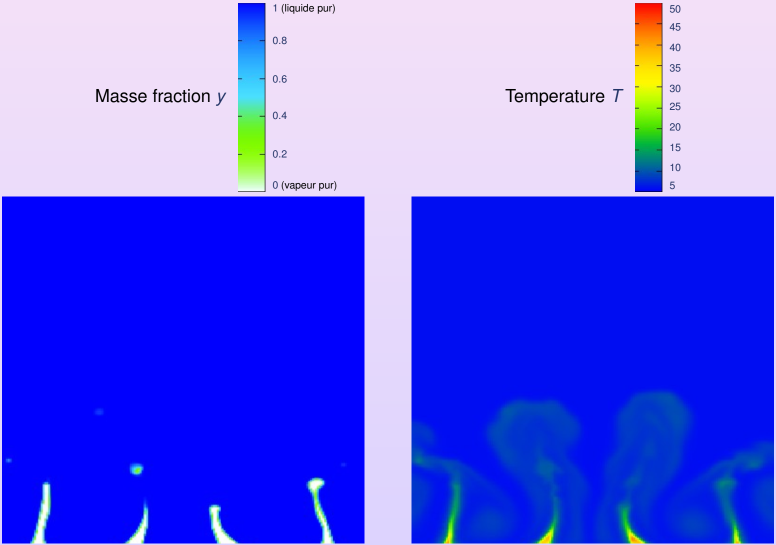
Geometry Play Skip

Transition to a Film Boiling



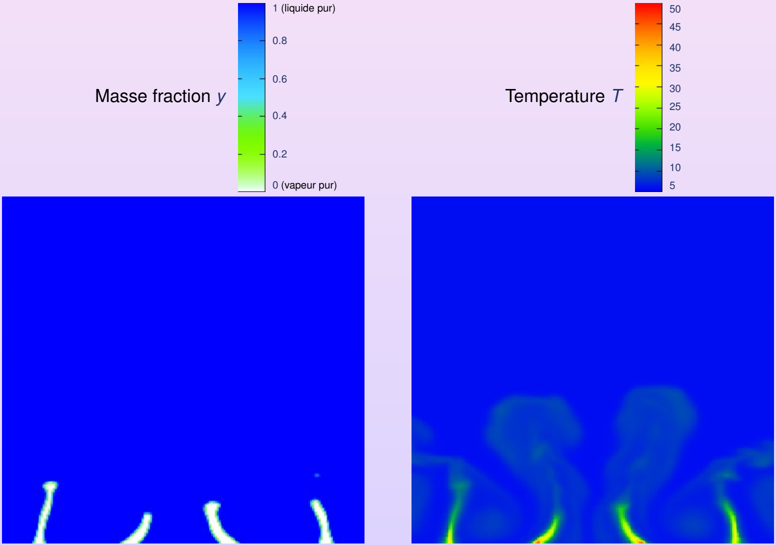
Geometry Play Skip

Transition to a Film Boiling



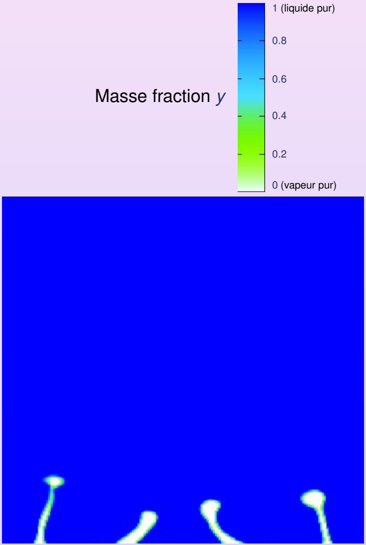
◀ Geometry ▶ Play ▶▶ Skip

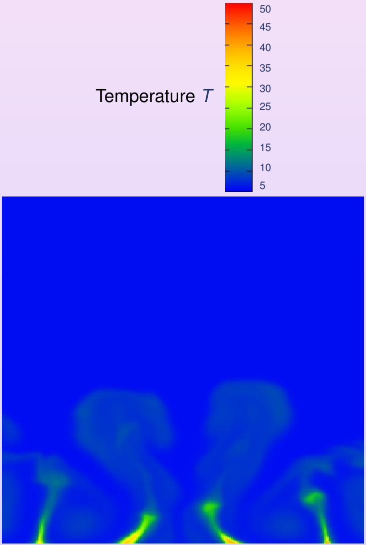
TRANSITION TO A FILM BOILING



Geometry Play Skip

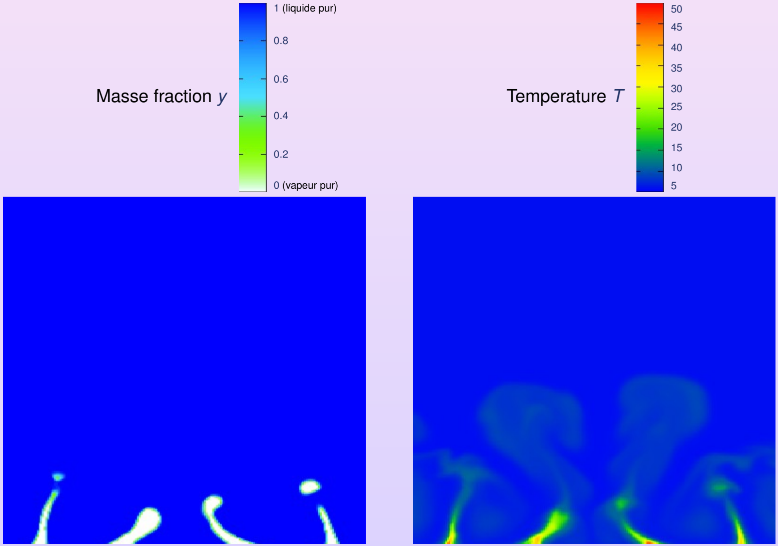
TRANSITION TO A FILM BOILING





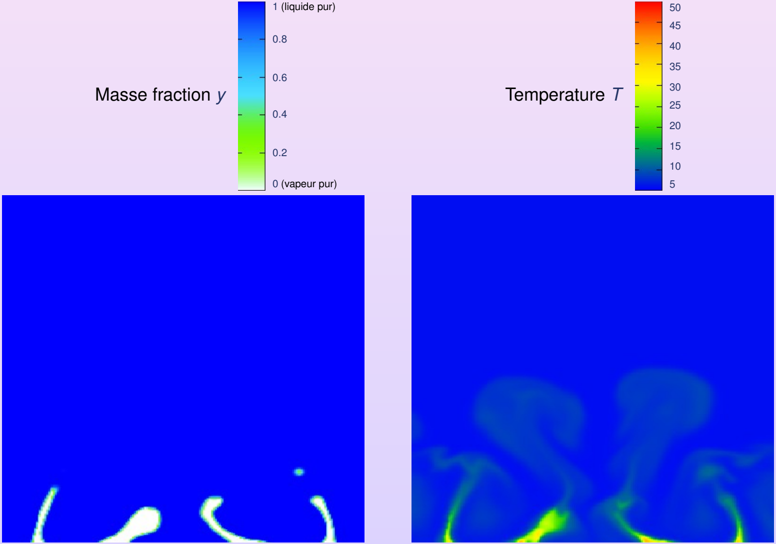
◂ Geometry ▸ Play ▸▸ Skip

Transition to a Film Boiling



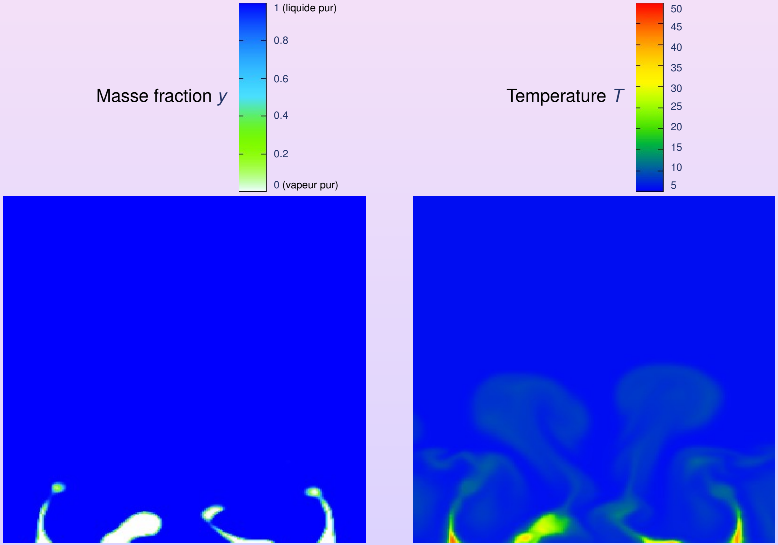
Geometry Play Skip

Transition to a Film Boiling



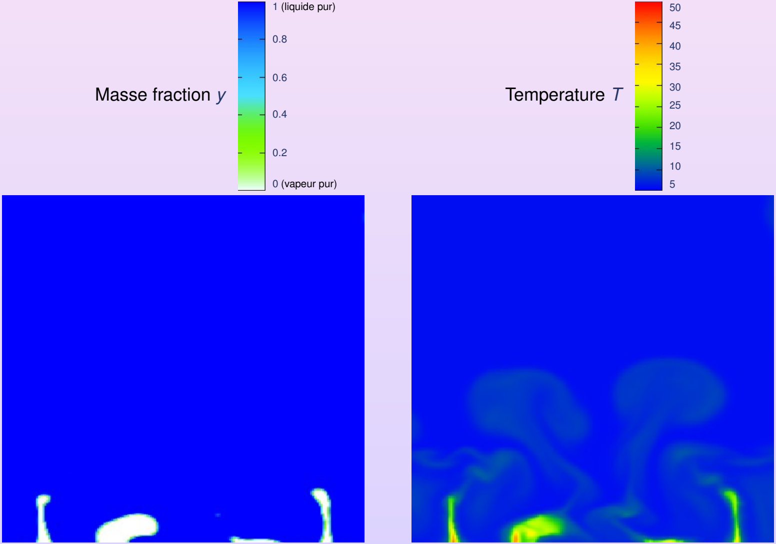
Geometry Play Skip

Transition to a Film Boiling



Geometry Play Skip

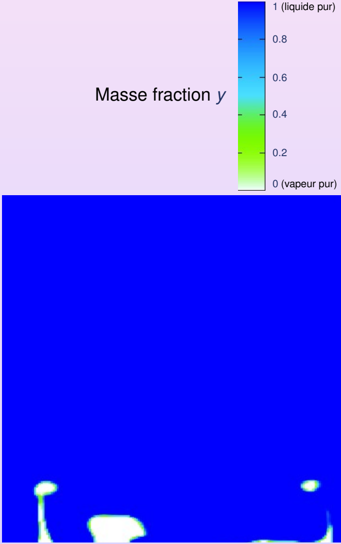
Transition to a Film Boiling



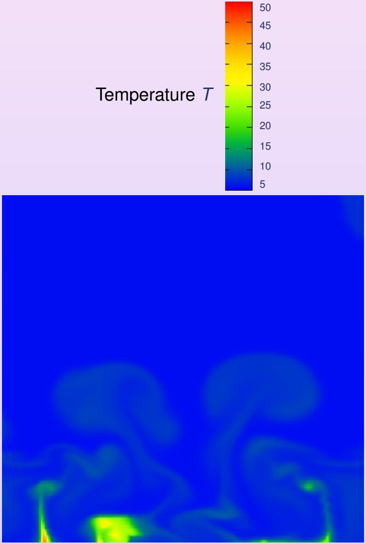
Geometry Play Skip

Transition to a Film Boiling

Masse fraction y

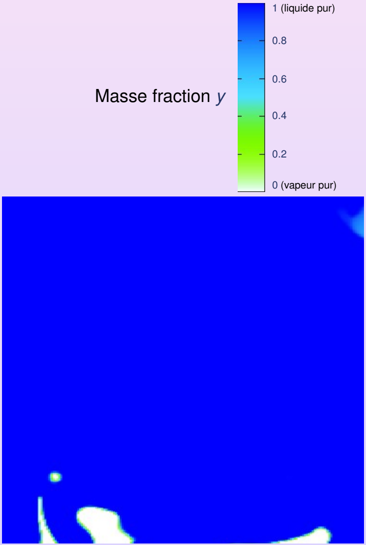


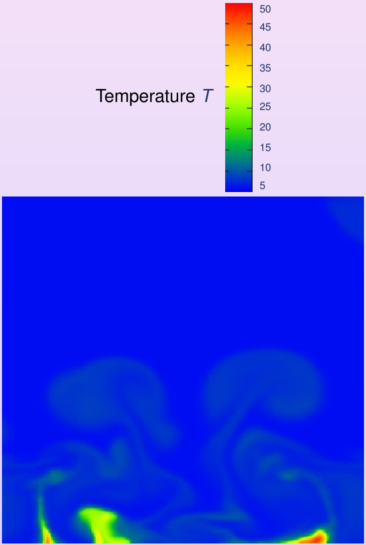
Temperature T



Geometry Play Skip

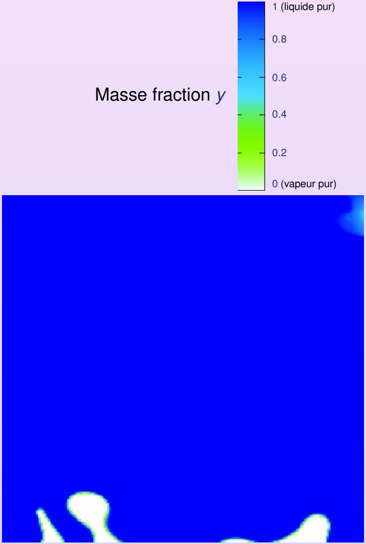
Transition to a Film Boiling

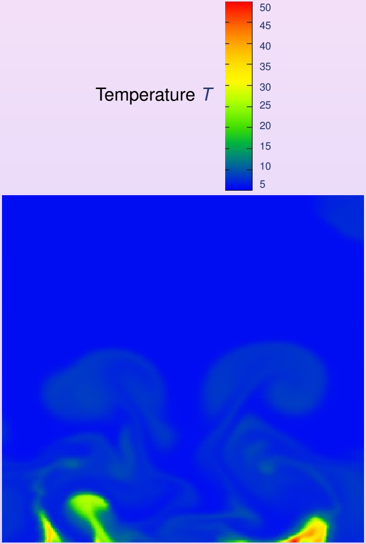




Geometry Play Skip

TRANSITION TO A FILM BOILING

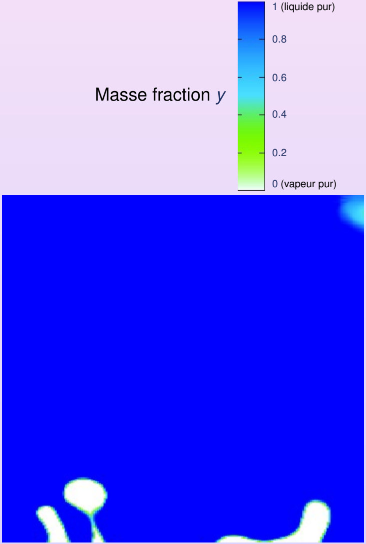




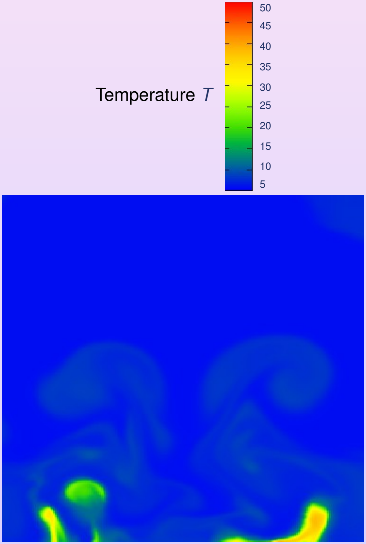
Geometry Play Skip

TRANSITION TO A FILM BOILING

Masse fraction y



Temperature T



Geometry Play Skip

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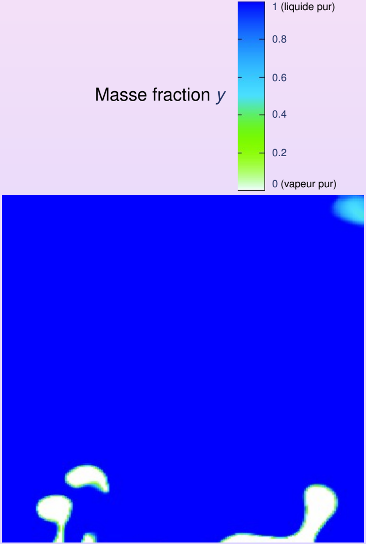

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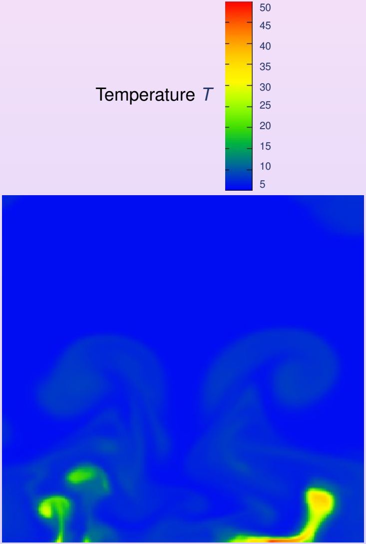

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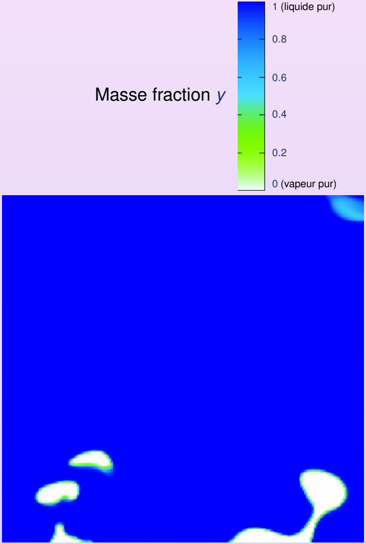

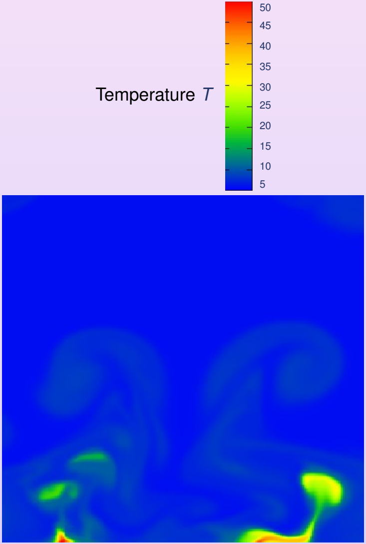

Geometry Play Skip

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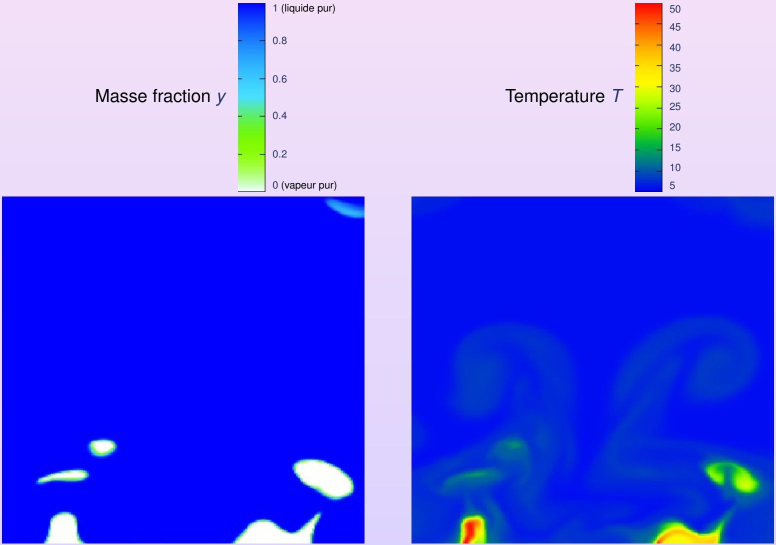

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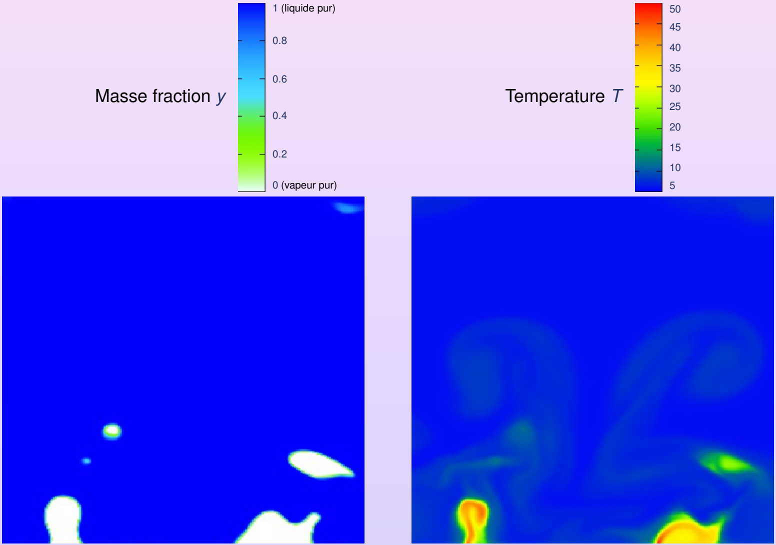

Geometry Play Skip

OUTLINE

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 system 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,
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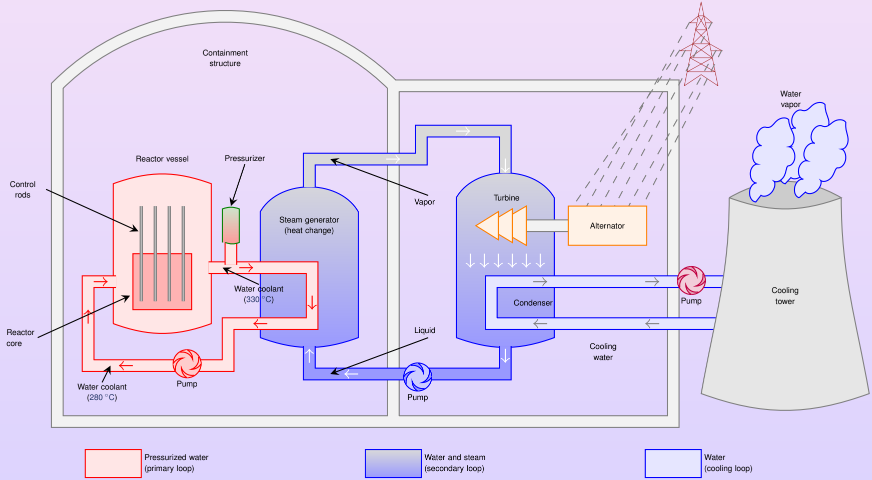
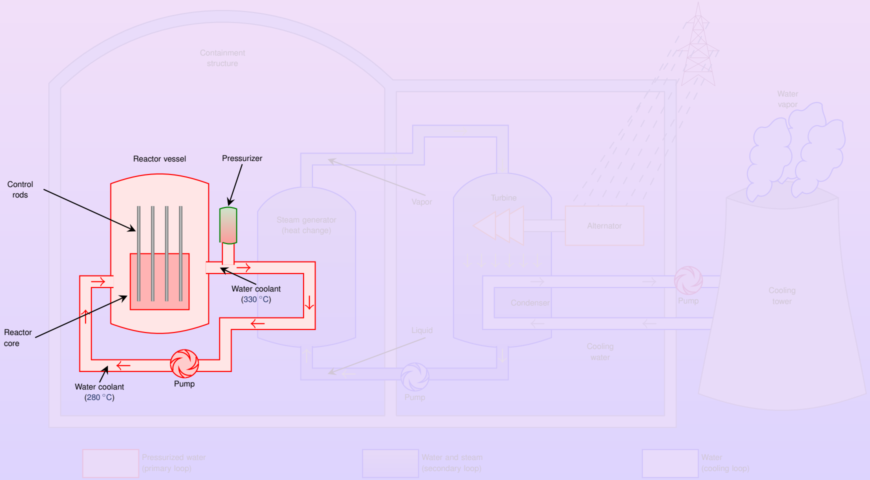
  - ✗ quantitative simulations: implicit transport step (Low Mach) and 3D (parallelization).

APPENDIX

Pressurized Water Reactor



Pressurized Water Reactor



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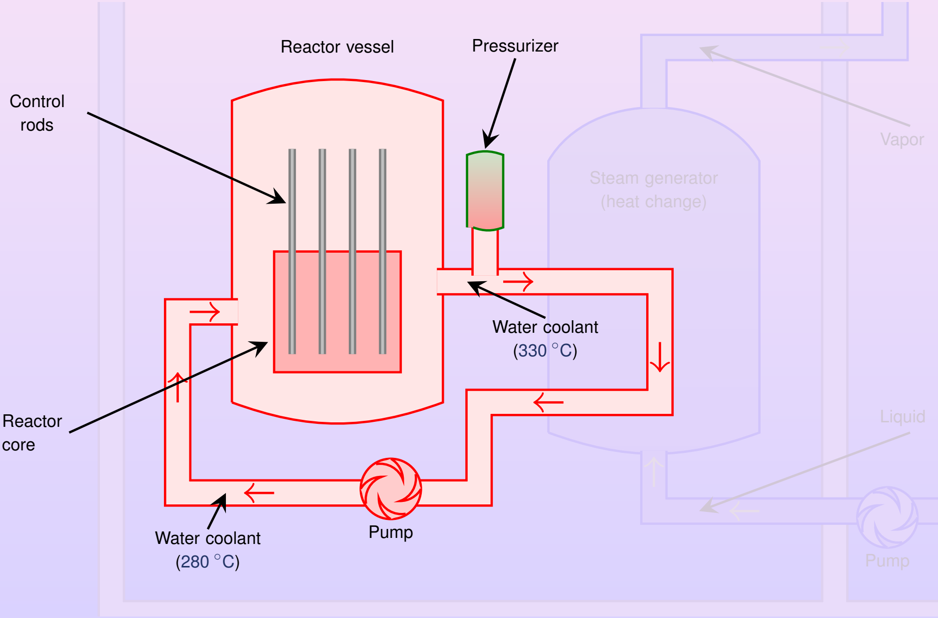
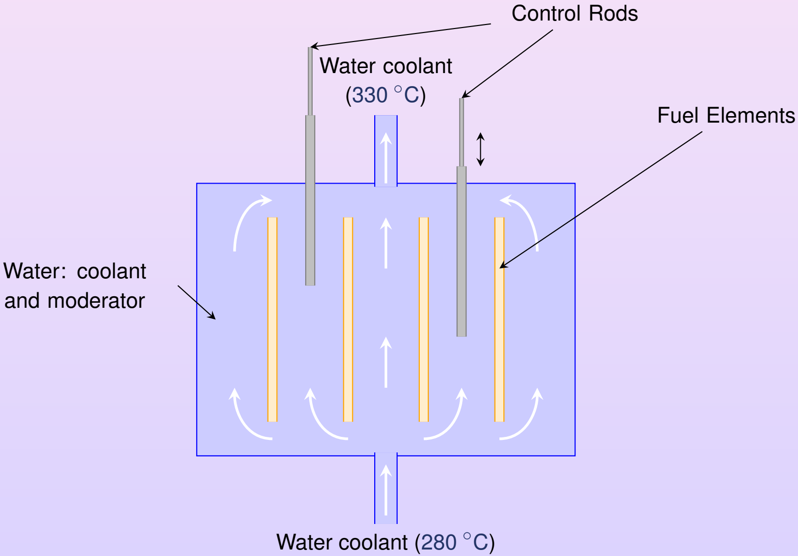


Core of a Pressurized Water Reactor



Stiffened Gas for Water

Phase	c_v [J/(kg·K)]	γ	π [Pa]	q [J/kg]	m [J/(kg·K)]
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.

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

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$$\left.\begin{array}{l} T^i = 278\text{K}\ldots 610\text{K}, \\ g_1(P,T^i) = g_2(P,T^i) \Rightarrow P^{\text{sat}}(T^i) \end{array}\right\} \Rightarrow \mathfrak{A} = \left\{\left(T^i, P^{\text{sat}}(T^i)\right)\right\}_{i=0}^{83}$$

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WATER TABULATED EOS

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

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

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

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SPEED OF SOUND

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

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

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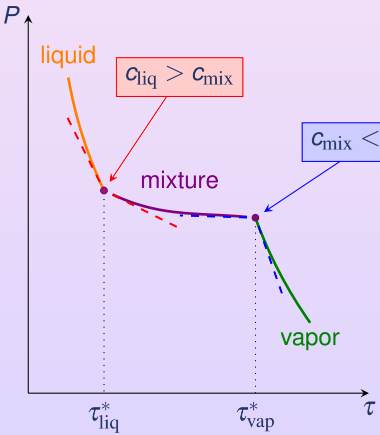
Isentropic curves



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

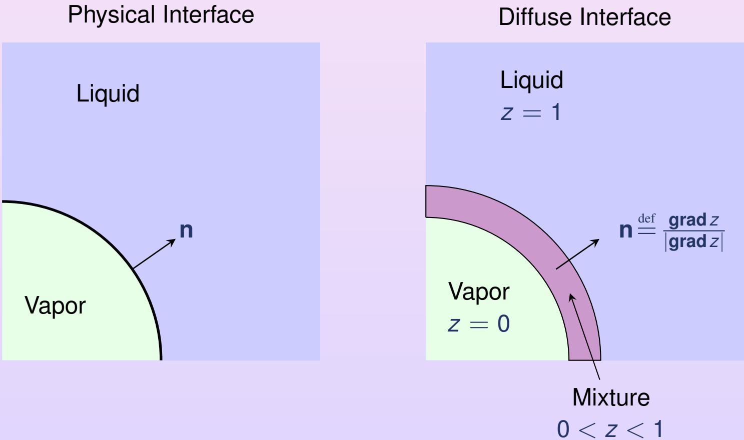
$$\Gamma \stackrel{\rm def}{=} \tau \left.\frac{\partial P}{\partial \varepsilon}\right|_\tau$$

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

- 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]

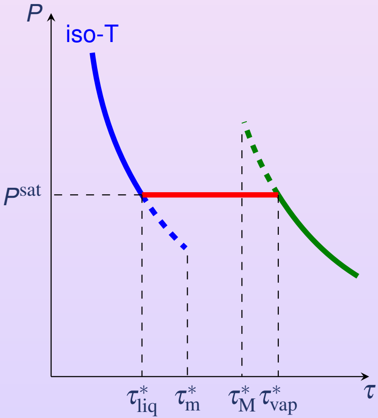
Continuum Surface Force (CSF) Approach



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

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

METASTABILITY



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

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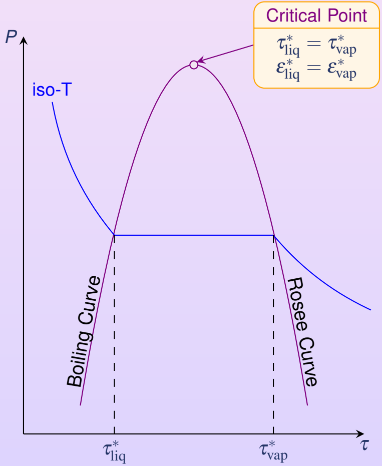
Critical Point



Physic

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Eq

EOS

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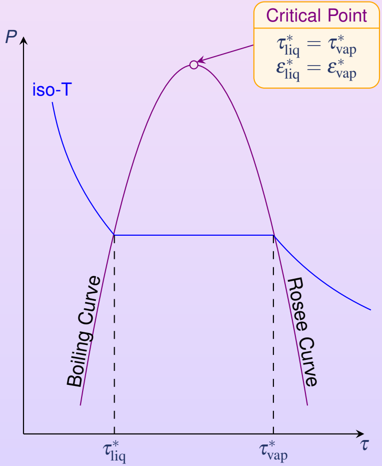
TAB $\left\{\tau_i, P_i^{\mathrm{sat,e}}\right\}_i \rightsquigarrow \tau \mapsto P^{\mathrm{sat}}$
$\left\{(\tau_i, \varepsilon_i), (P_\alpha^i)\right\}_i \rightsquigarrow (\tau, \varepsilon) \mapsto P_\alpha$

Critical Point



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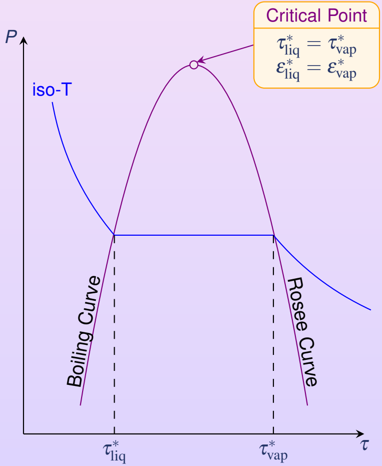

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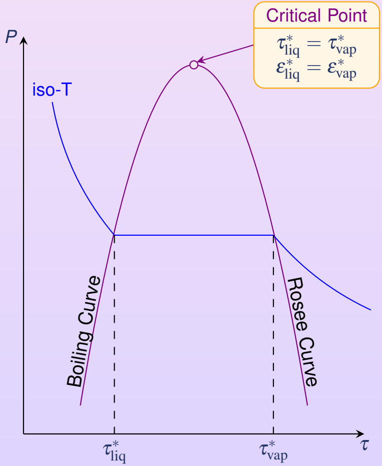
TAB $\left\{\tau_i, P_i^{\text{sat,e}}\right\}_i \rightsquigarrow \tau \mapsto P^{\text{sat}}$
$\left\{(\tau_i, \varepsilon_i), (P^{\text{e}}_\alpha)_i\right\}_i \rightsquigarrow (\tau, \varepsilon) \mapsto P_\alpha$

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 $\left\{\tau_i, P_i^{\text{sat,e}}\right\}_i \rightsquigarrow \tau \mapsto P^{\text{sat}}$

$\{(\tau_i, \varepsilon_i), (P^{\text{e}}_\alpha)_i\}_i \rightsquigarrow (\tau, \varepsilon) \mapsto P_\alpha$