

May 27, 2009

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# MODELLING AND SIMULATION OF LIQUID-VAPOR PHASE TRANSITION

A CONTRIBUTION TO THE STUDY OF THE BOILING CRISIS

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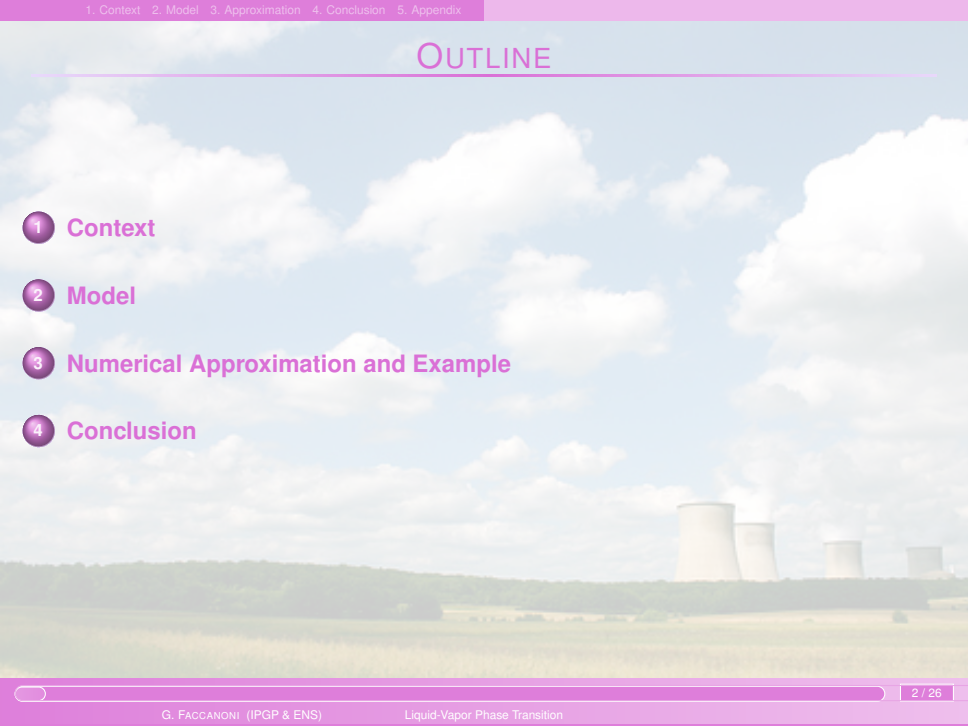
<sup>4</sup>DEN/DANS/DM2S/SFME/LETR – CEA Saclay (France)



# OUTLINE

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- 1 **Context**
- 2 **Model**
- 3 **Numerical Approximation and Example**
- 4 **Conclusion**



# OUTLINE

## 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

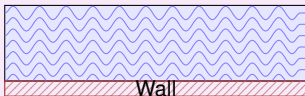
## 4 Conclusion

# BOILING CRISIS

## PHENOMENON

Liquid phase heated by a wall at a fixed temperature  $T^{\text{wall}}$ .

When  $T^{\text{wall}}$  increases, we switch from a **Nucleate Boiling** to a **Film Boiling**.

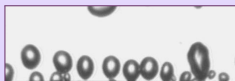
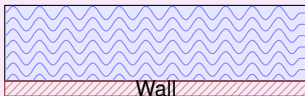


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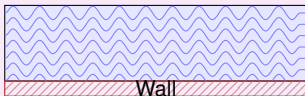
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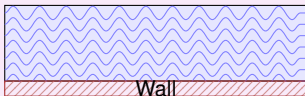
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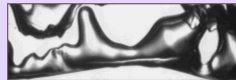
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## 2 Model

- Equation of State WITHOUT Phase Change
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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

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

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

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



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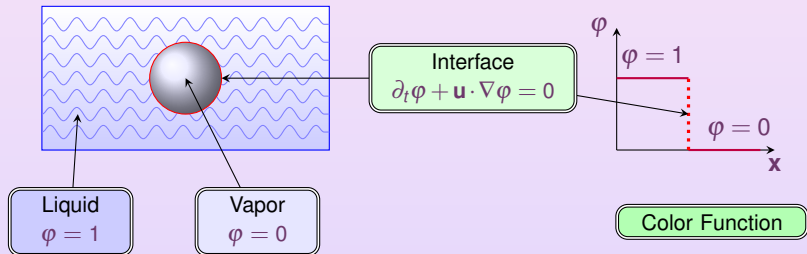
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- Equation of State **WITHOUT** Phase Change
- Equation of State **WITH** Phase Change
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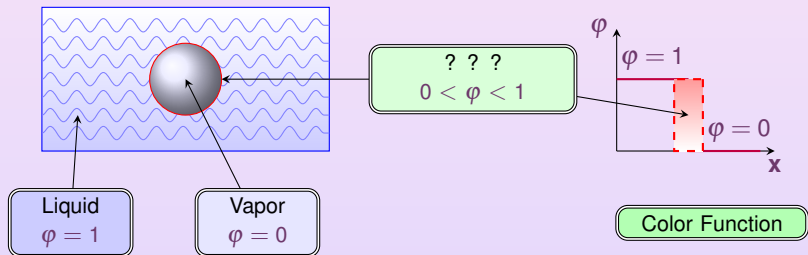
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## LIQUID-VAPOR INTERFACE



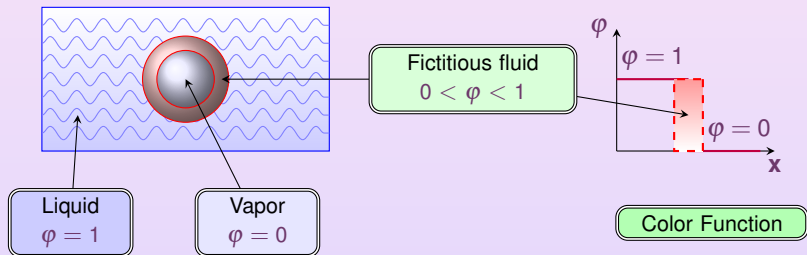
$$(\rho, \varepsilon) \mapsto P = \begin{cases} P^{\text{liq}} & \text{if } \varphi = 1; \\ P^{\text{vap}} & \text{if } \varphi = 0. \end{cases}$$

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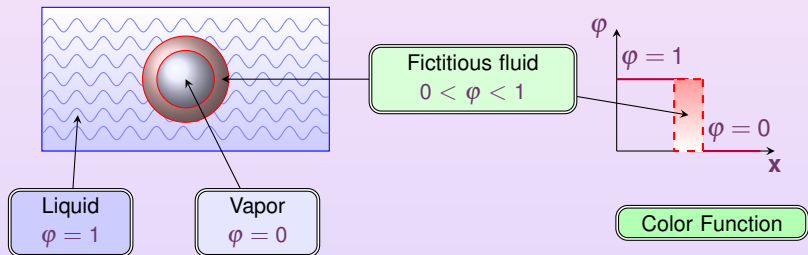
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## LIQUID-VAPOR INTERFACE



➡ 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.  $\nabla \varphi$ )
- coherence with classical thermodynamics [H. CALLEN]

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

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

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

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

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# EOS OF THE MIXTURE

- $\mathbf{w} \stackrel{\text{def}}{=} y\mathbf{w}_1 + (1 - y)\mathbf{w}_2$ ;
- $y$  mass fraction;
- $z$  volume fraction s.t.  $y\tau_1 = z\tau$ ;
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## EOS WITH PHASE CHANGE

**ENTROPY WITHOUT PH.CH.**

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

**ENTROPY AT EQUILIBRIUM**

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

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

Optimization Problem:

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

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:  $(z^*, y^*, \psi^*)$



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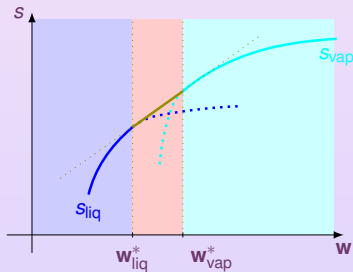
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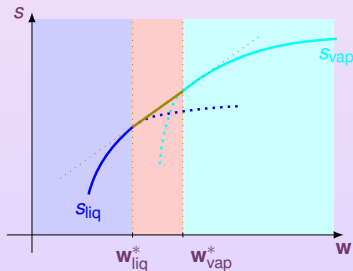
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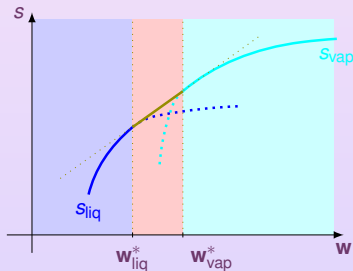
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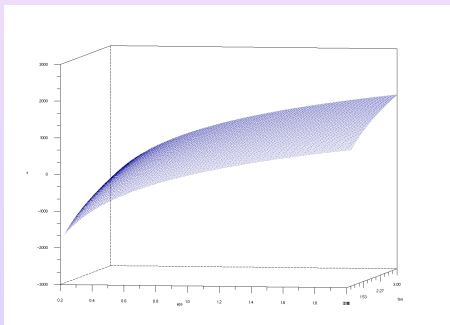
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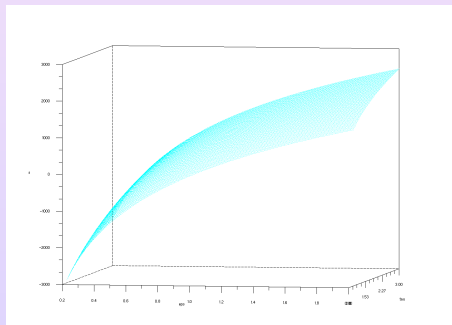
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# CONCAVE HULL WITH TWO PERFECT GASES

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

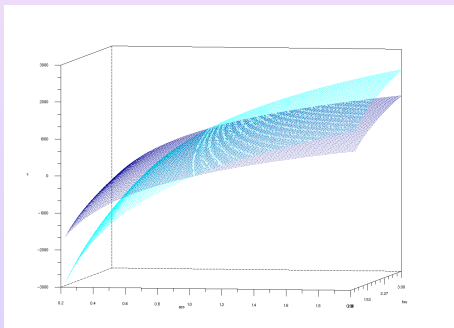


$$(\tau, \varepsilon) \mapsto s_{\text{vap}}$$



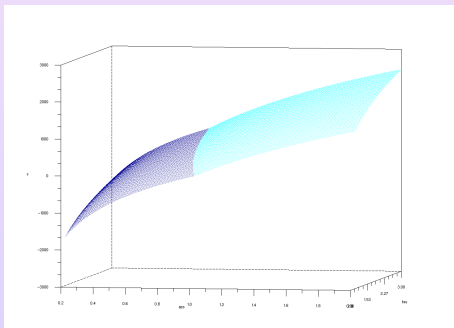
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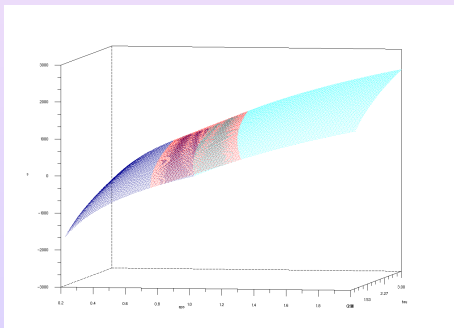
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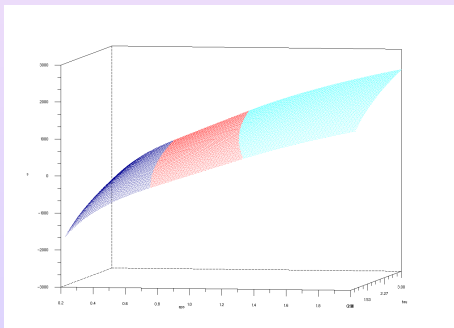
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# FROM $\mathbf{w} \mapsto \mathbf{s}^{\text{eq}}$ TO $\mathbf{w} \mapsto P^{\text{eq}}$

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

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

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

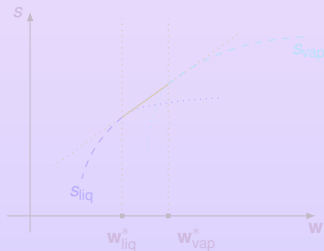
$$\mathbf{s}^{\text{eq}}(\tilde{\mathbf{w}}) = y^* \mathbf{s}_{\text{liq}}(\mathbf{w}_{\text{liq}}^*) + (1-y^*) \mathbf{s}_{\text{vap}}(\mathbf{w}_{\text{vap}}^*),$$

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

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

$$\mathbf{s}^{\text{eq}}(\tilde{\mathbf{w}}) = \max\{\mathbf{s}_{\text{liq}}(\tilde{\mathbf{w}}), \mathbf{s}_{\text{vap}}(\tilde{\mathbf{w}})\},$$

$$P^{\text{eq}}(\tilde{\mathbf{w}}) = P_{\text{liq}}(\tilde{\mathbf{w}})$$



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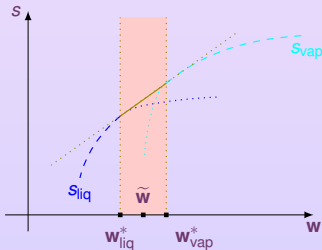
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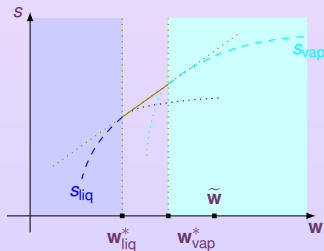
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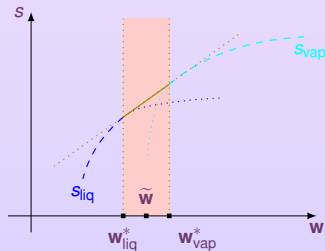
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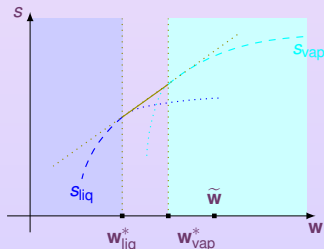
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## 2 Model

- Equation of State WITHOUT Phase Change
- Equation of State WITH Phase Change
- **The Phase Change Equation**
- Conservation Laws

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# SUMMARY OF THE MODEL

$$\mathbf{w} \mapsto S^{\text{eq}}$$

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

## Euler System

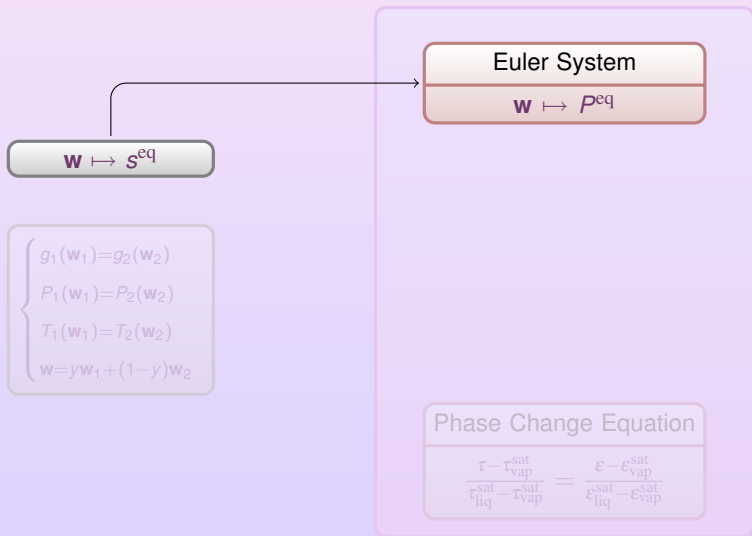
$$\mathbf{w} \mapsto P^{\text{eq}}$$

## Phase Change Equation

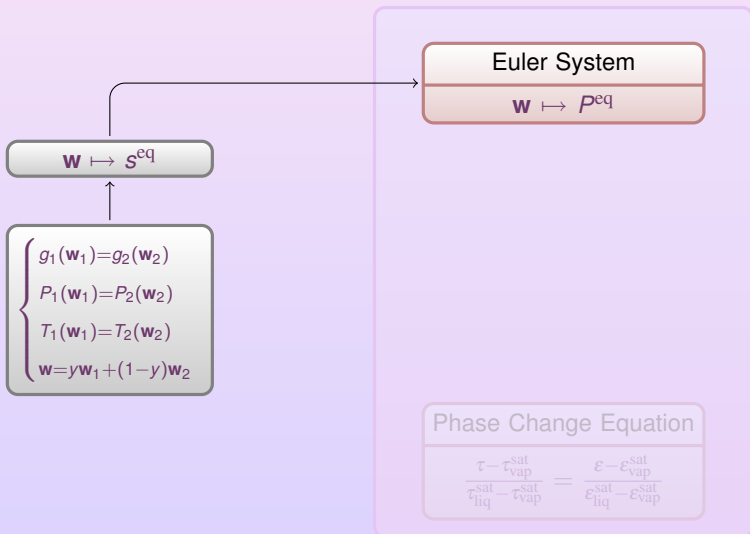
$$\frac{\tau - \tau_{\text{vap}}^{\text{sat}}}{\tau_{\text{liq}}^{\text{sat}} - \tau_{\text{vap}}^{\text{sat}}} = \frac{\varepsilon - \varepsilon_{\text{vap}}^{\text{sat}}}{\varepsilon_{\text{liq}}^{\text{sat}} - \varepsilon_{\text{vap}}^{\text{sat}}}$$



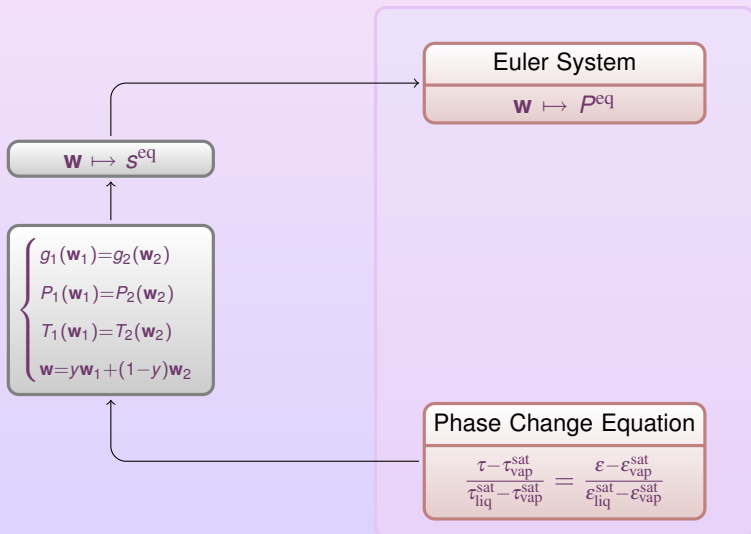
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 $(\tau, \varepsilon)$  fixed $(\tau_1, \varepsilon_1, \tau_2, \varepsilon_2, y)$  SOLUTION OF

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least square approximation

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# TABULATED EOS

$T$ (K)	$P^{\text{sat}}$ (MPa)	Volume ( $\text{m}^3/\text{kg}$ )		Internal Energy (kJ/kg)	
		$\tau_{\text{liq}}^{\text{sat}}$	$\tau_{\text{vap}}^{\text{sat}}$	$\epsilon_{\text{liq}}^{\text{sat}}$	$\epsilon_{\text{vap}}^{\text{sat}}$
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/>

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$(\tau, \varepsilon)$  fixed

## T SOLUTION OF

$$\frac{\tau - \tau_2^{\text{sat}}(T)}{\tau_1^{\text{sat}}(T) - \tau_2^{\text{sat}}(T)} = \frac{\varepsilon - \varepsilon_2^{\text{sat}}(T)}{\varepsilon_1^{\text{sat}}(T) - \varepsilon_2^{\text{sat}}(T)}$$

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$$\frac{\tau - \widehat{\tau}_2^{\text{sat}}(T)}{\widehat{\tau}_1^{\text{sat}}(T) - \widehat{\tau}_2^{\text{sat}}(T)} = \frac{\varepsilon - \widehat{\varepsilon}_2^{\text{sat}}(T)}{\widehat{\varepsilon}_1^{\text{sat}}(T) - \widehat{\varepsilon}_2^{\text{sat}}(T)}$$

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- Equation of State WITHOUT Phase Change
- Equation of State WITH Phase Change
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# 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

$$\textcircled{1} c(w) > 0, \quad \textcircled{2} s_{\tau\varepsilon}^{\text{eq}}(w) > 0$$

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

# DYNAMIC LIQUID-VAPOR PHASE CHANGE



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- 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

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# OUTLINE

## 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

# NUMERICAL SCHEME BASED ON RELAXATION APPROACH

$$\sigma(y, z, \psi, \tau, \varepsilon)$$

Optimization

$$s^{\text{eq}}(\tau, \varepsilon)$$

Off Equilibrium

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

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

$\mu_j \rightarrow \infty$

Equilibrium

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Two Steps:

- 1 Hydrodynamic (+ gravity, surface tension, heat diffusion, ...)
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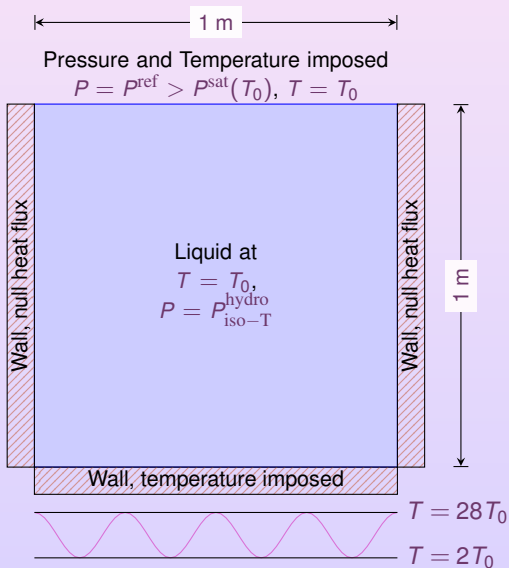
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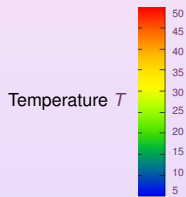
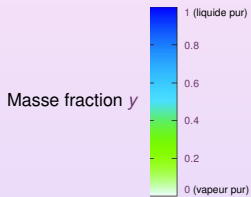
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# TRANSITION TO A FILM BOILING



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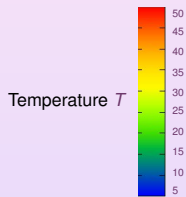
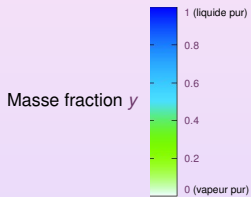
◀ Geometry

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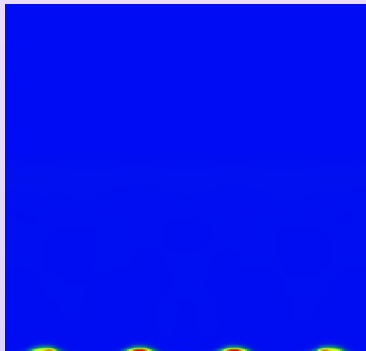
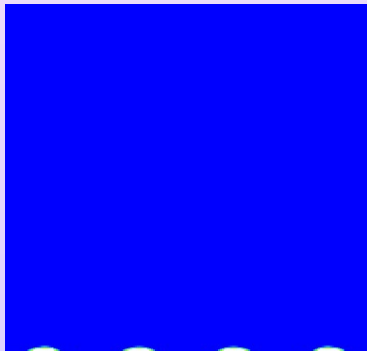
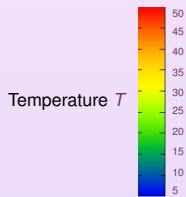
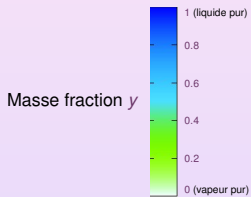


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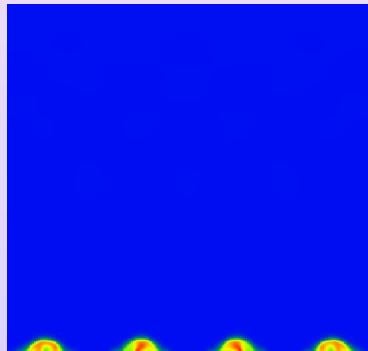
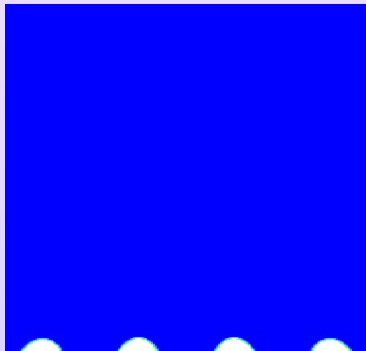
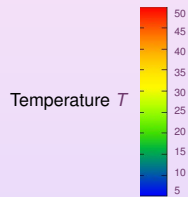
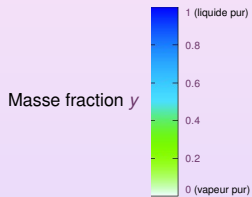


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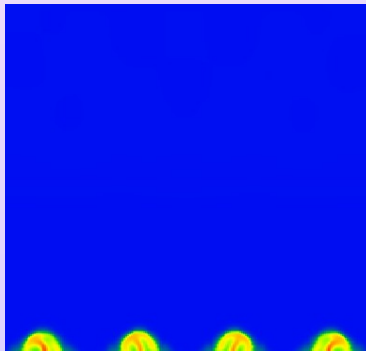
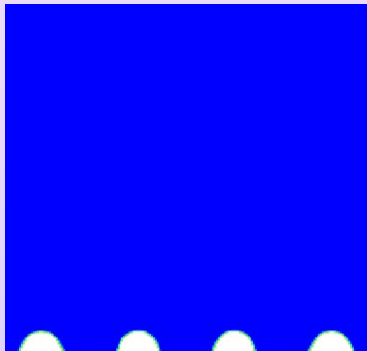
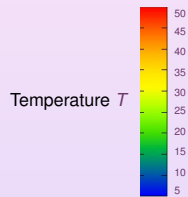
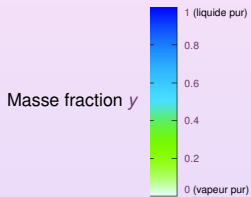


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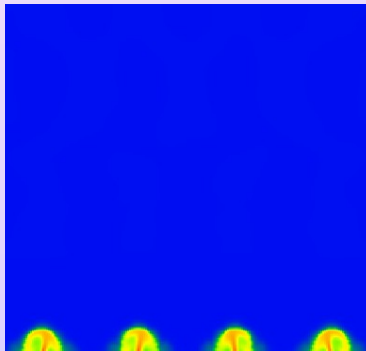
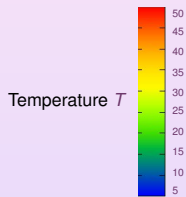
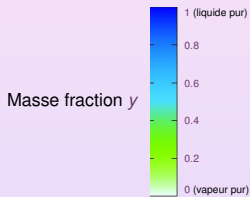


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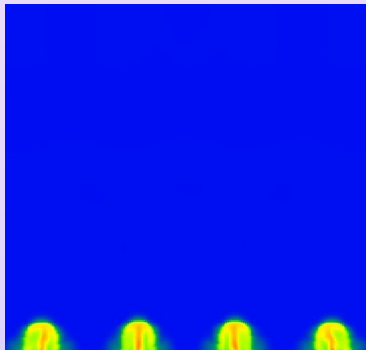
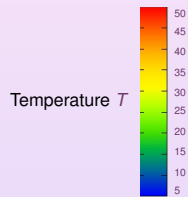
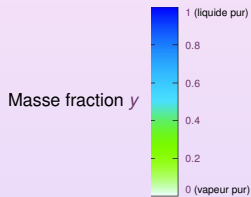


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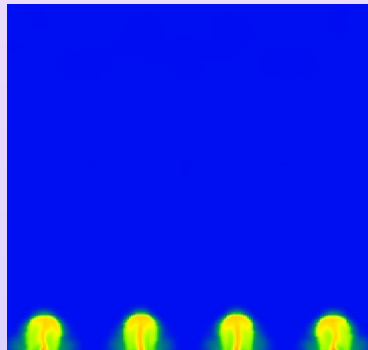
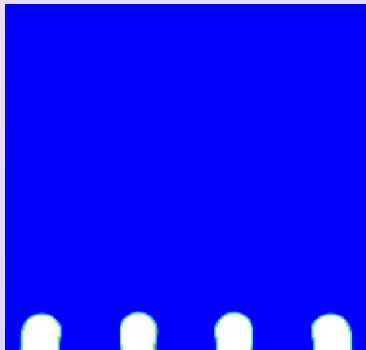
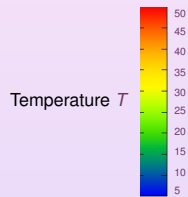
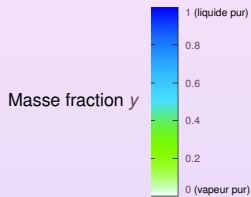


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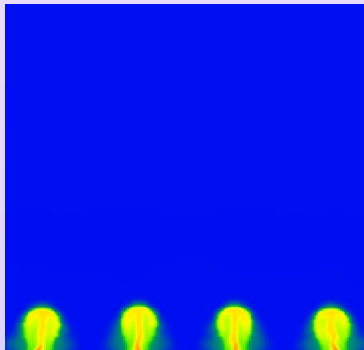
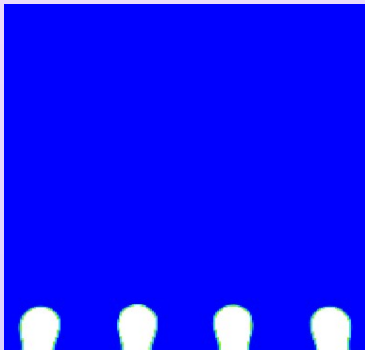
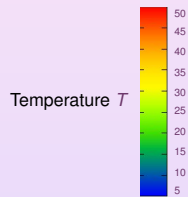
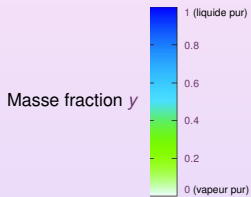


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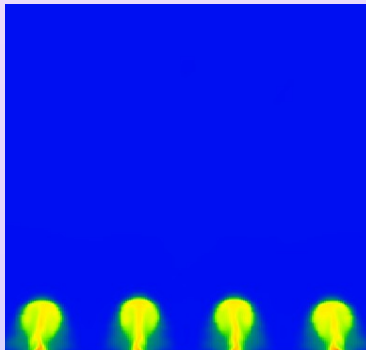
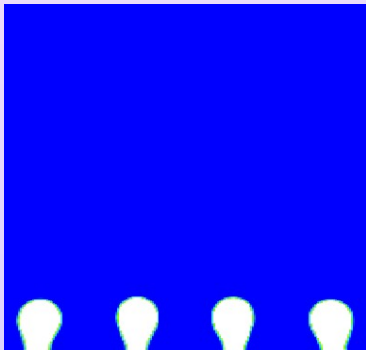
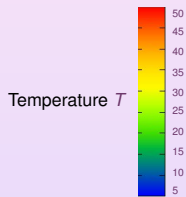
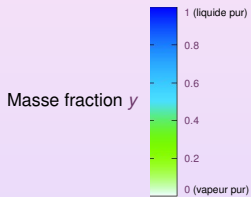
◀ Geometry

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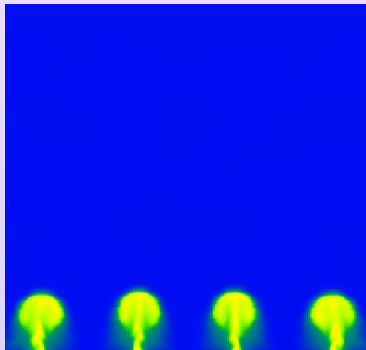
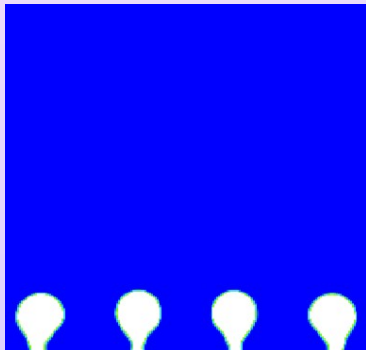
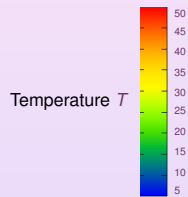
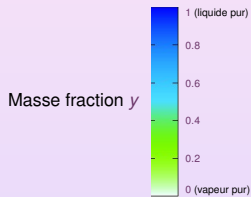


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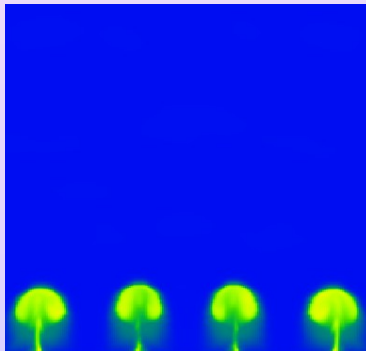
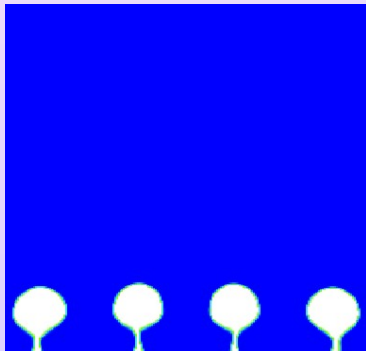
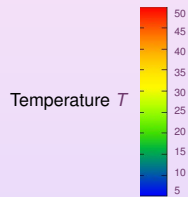
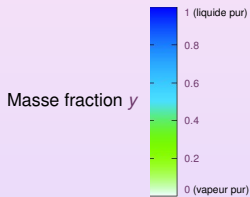


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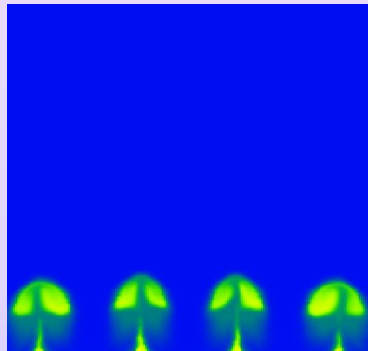
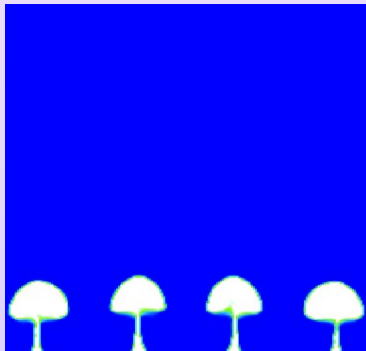
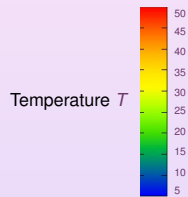
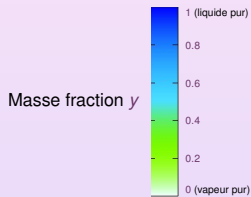


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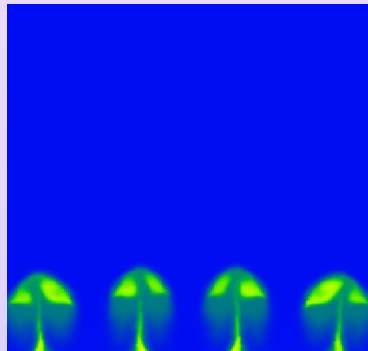
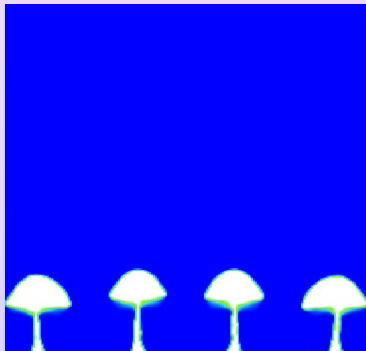
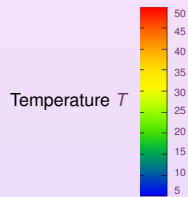
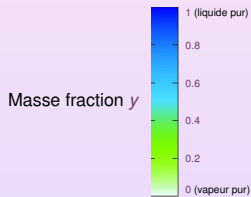


◀ Geometry

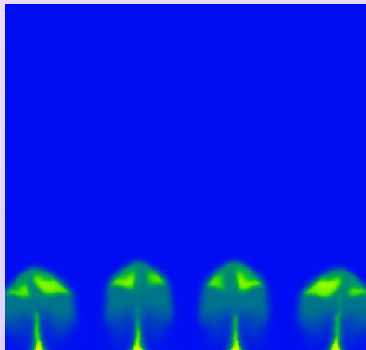
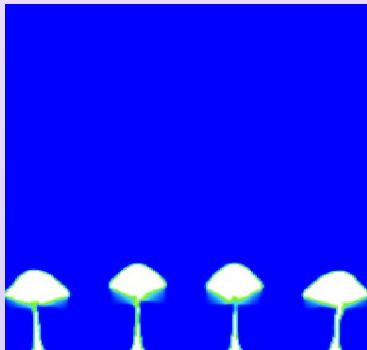
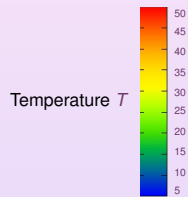
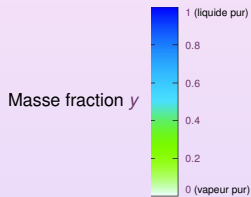
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# TRANSITION TO A FILM BOILING

[◀ Geometry](#)[▶ Play](#)[▶▶ Skip](#)

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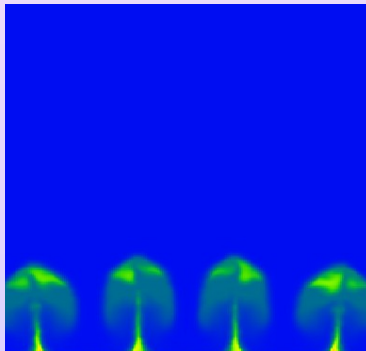
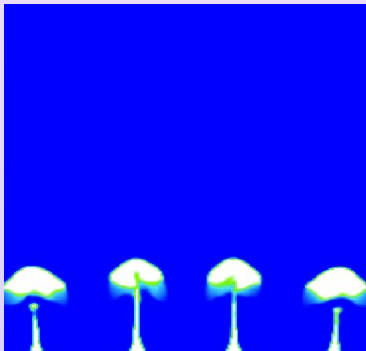
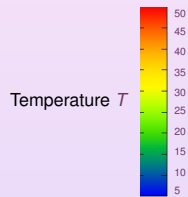
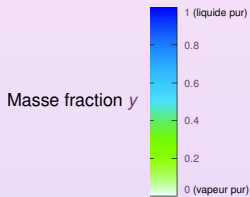


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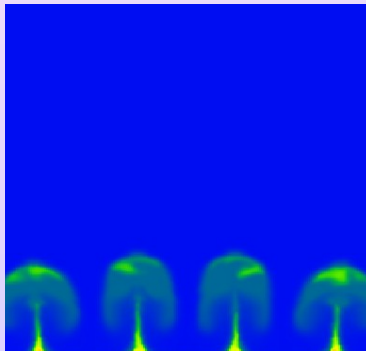
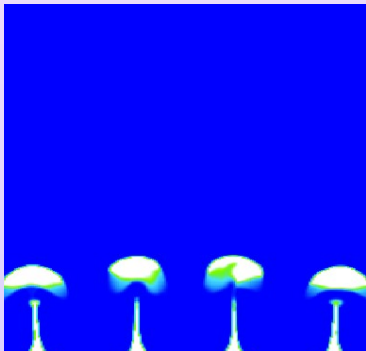
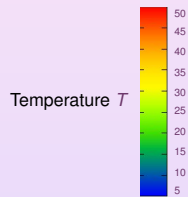
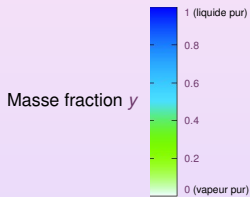


◀ Geometry

▶ Play

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# TRANSITION TO A FILM BOILING



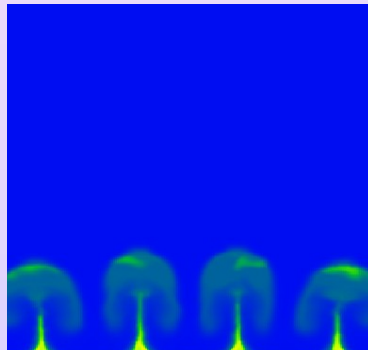
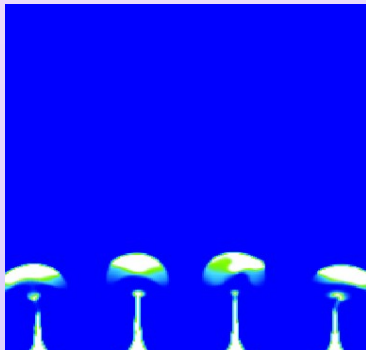
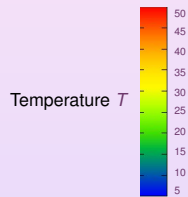
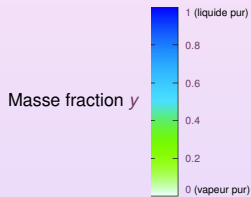
◀ Geometry

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# TRANSITION TO A FILM BOILING

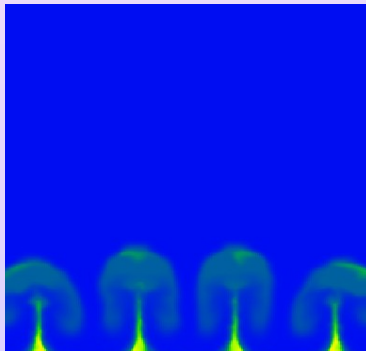
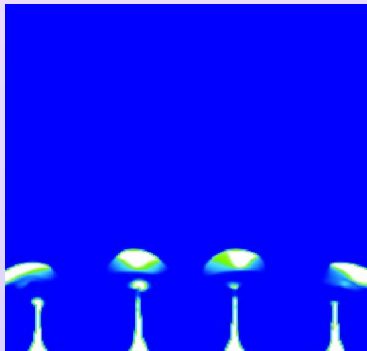
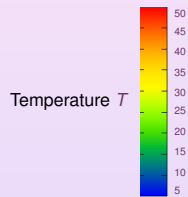
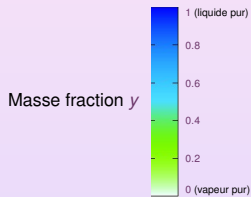


◀ Geometry

▶ Play

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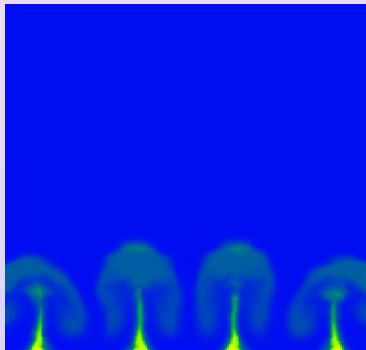
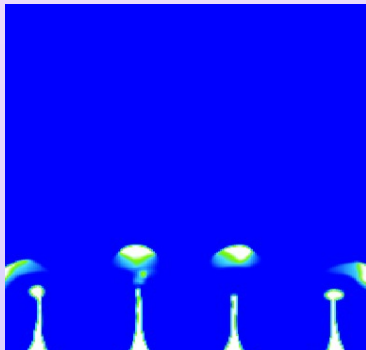
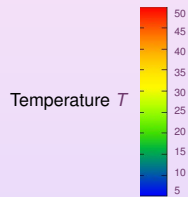
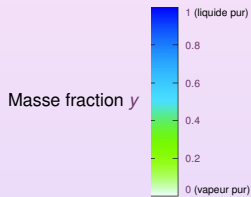


◀ Geometry

▶ Play

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# TRANSITION TO A FILM BOILING

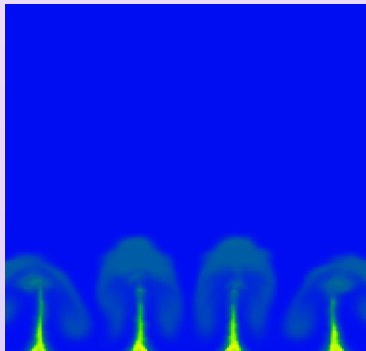
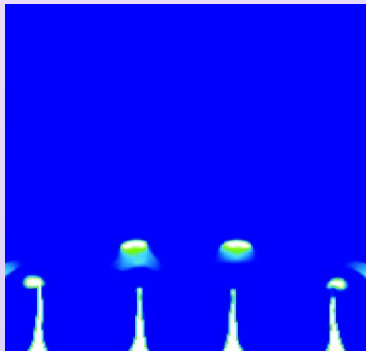
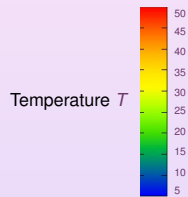
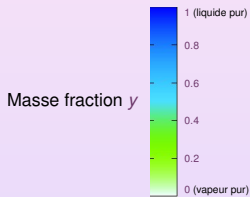


◀ Geometry

▶ Play

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# TRANSITION TO A FILM BOILING

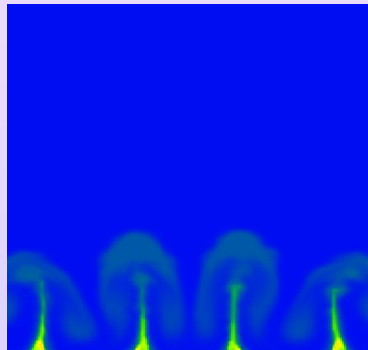
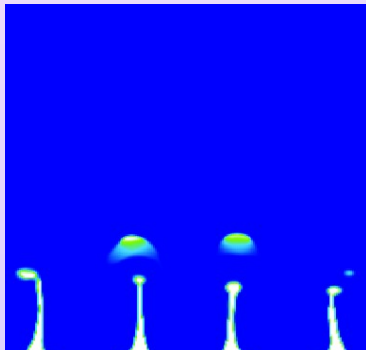
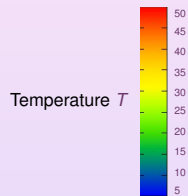
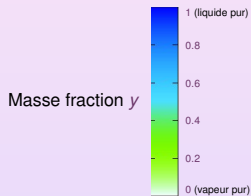


◀ Geometry

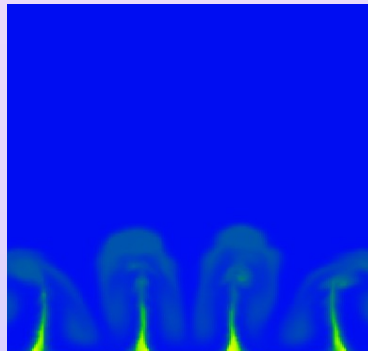
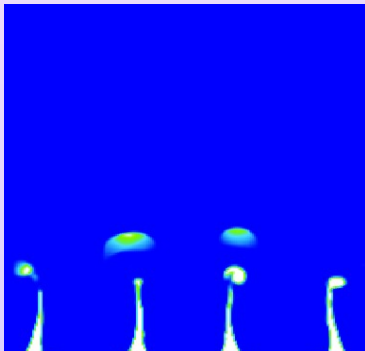
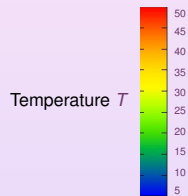
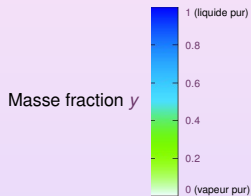
▶ Play

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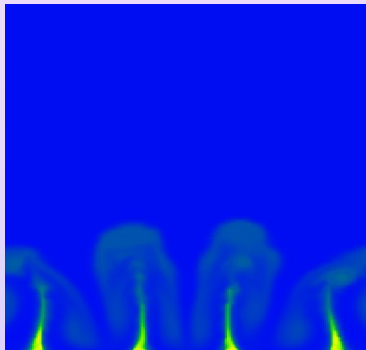
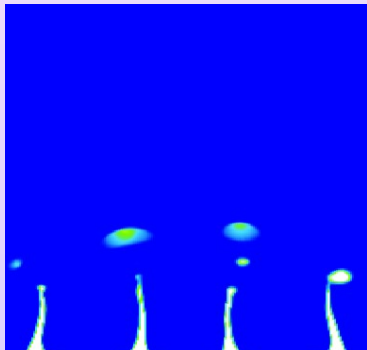
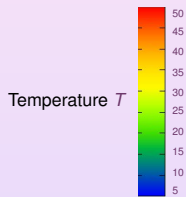
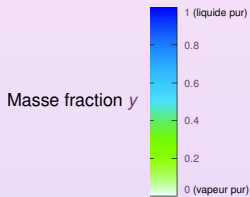
# TRANSITION TO A FILM BOILING

[◀ Geometry](#)[▶ Play](#)[▶▶ Skip](#)

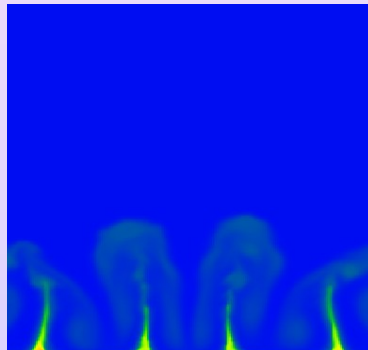
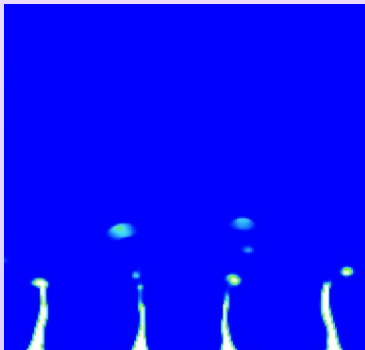
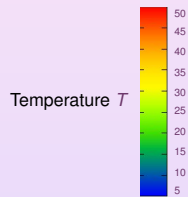
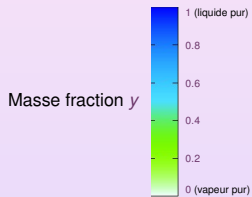
# TRANSITION TO A FILM BOILING

[◀ Geometry](#)[▶ Play](#)[▶▶ Skip](#)

# TRANSITION TO A FILM BOILING

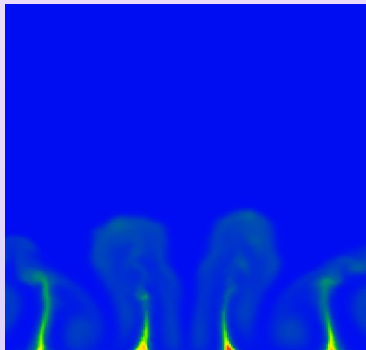
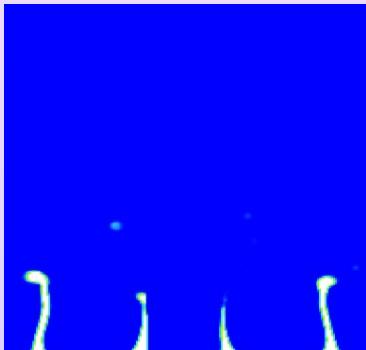
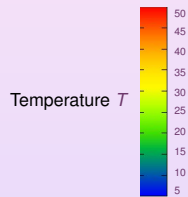
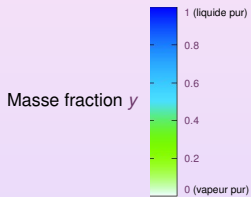
[◀ Geometry](#)[▶ Play](#)[▶▶ Skip](#)

# TRANSITION TO A FILM BOILING

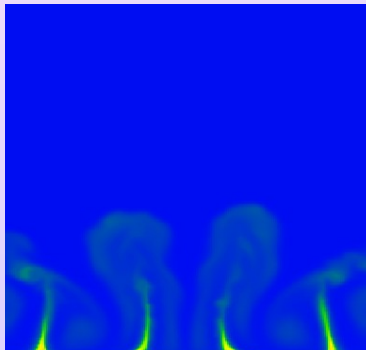
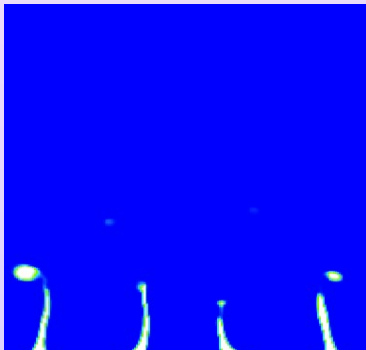
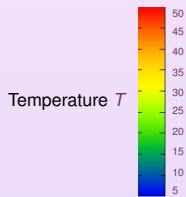
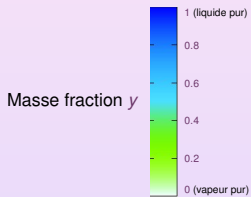
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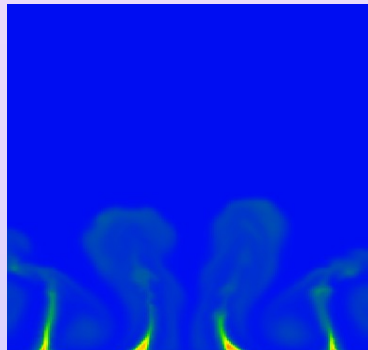
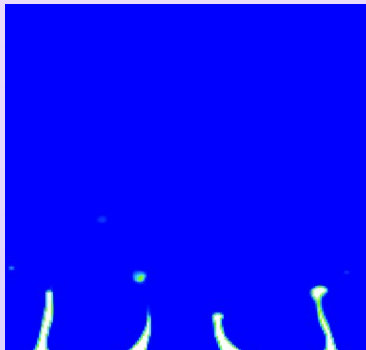
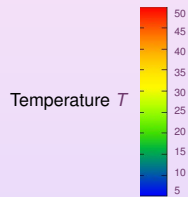
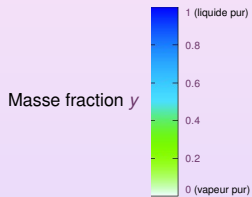
# TRANSITION TO A FILM BOILING

[◀ Geometry](#)[▶ Play](#)[▶▶ Skip](#)

# TRANSITION TO A FILM BOILING

[◀ Geometry](#)[▶ Play](#)[▶▶ Skip](#)

# TRANSITION TO A FILM BOILING

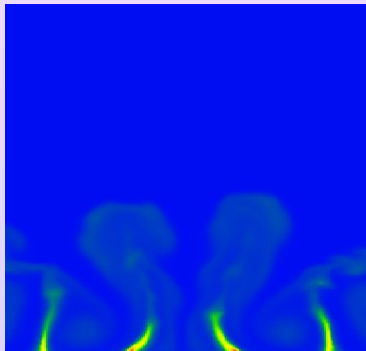
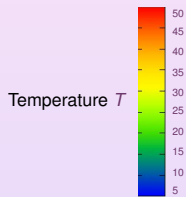
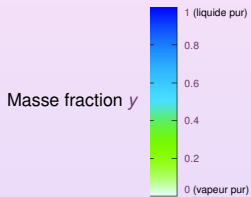


◀ Geometry

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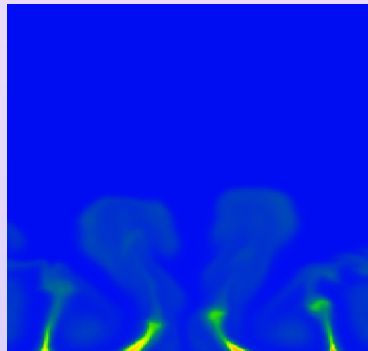
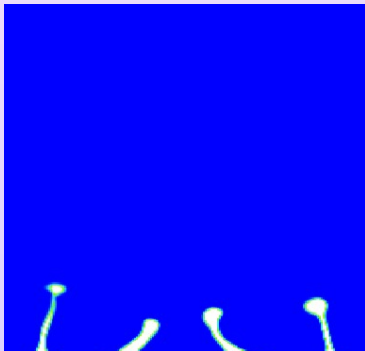
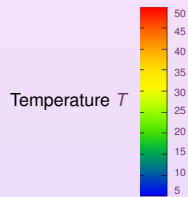
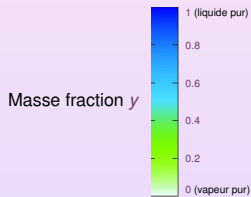


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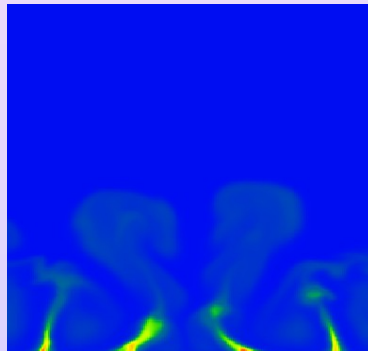
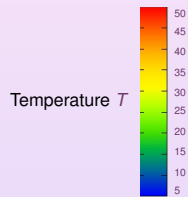
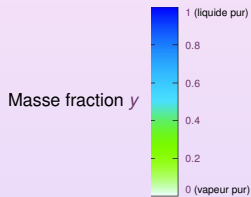
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# TRANSITION TO A FILM BOILING

[◀ Geometry](#)[▶ Play](#)[▶▶ Skip](#)

# TRANSITION TO A FILM BOILING

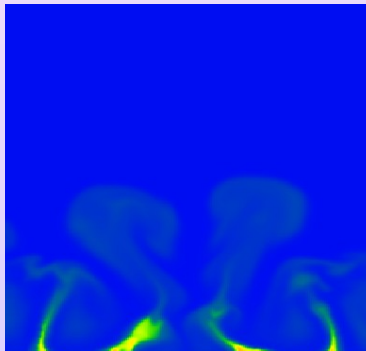
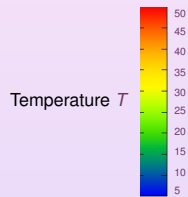
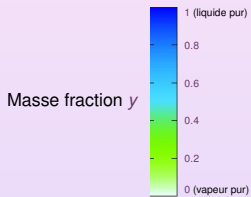


◀ Geometry

▶ Play

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# TRANSITION TO A FILM BOILING

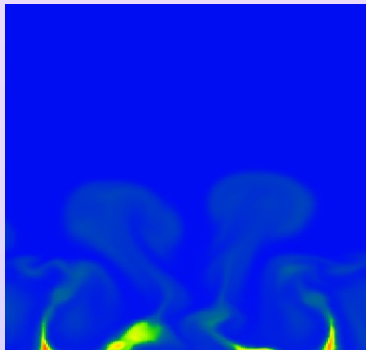
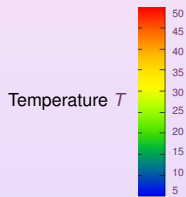
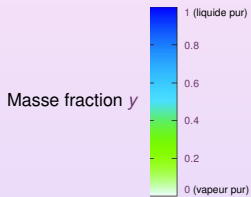


◀ Geometry

▶ Play

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# TRANSITION TO A FILM BOILING



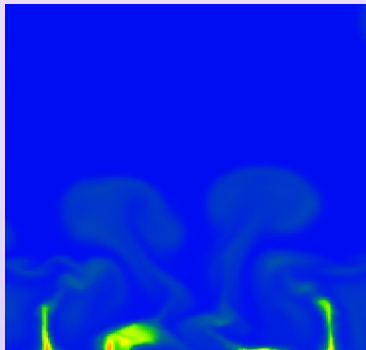
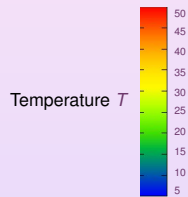
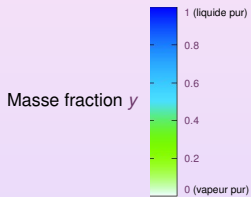
◀ Geometry

▶ Play

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# TRANSITION TO A FILM BOILING

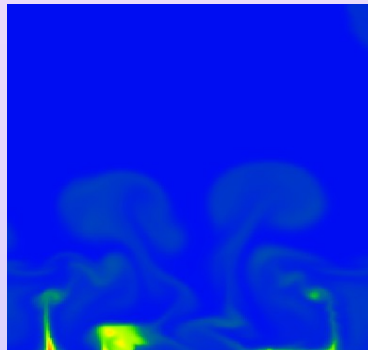
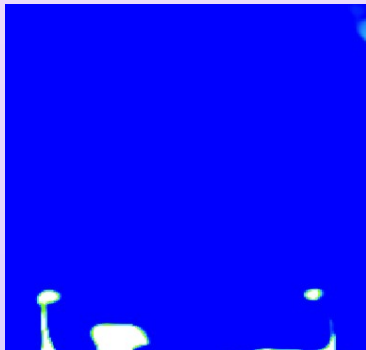
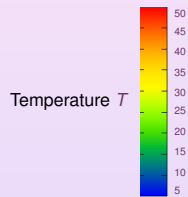
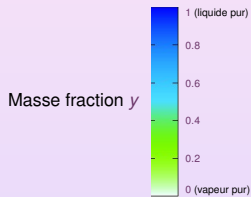


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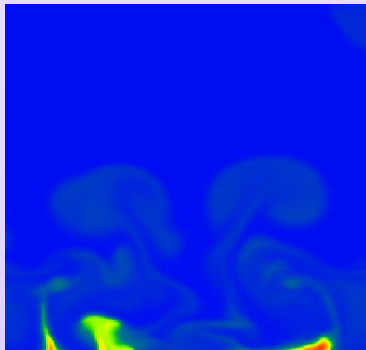
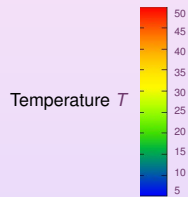
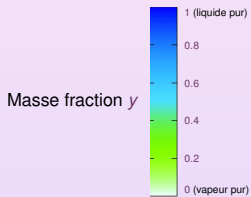
▶ Play

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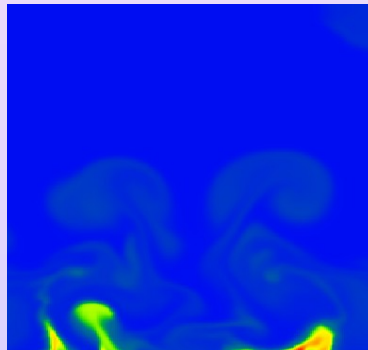
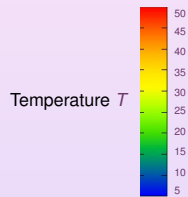
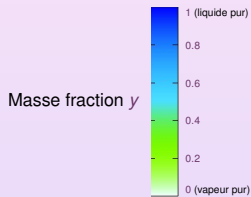
# TRANSITION TO A FILM BOILING

[◀ Geometry](#)[▶ Play](#)[▶▶ Skip](#)

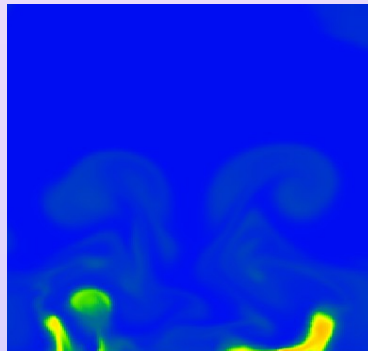
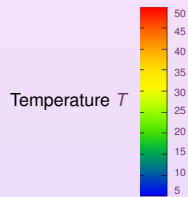
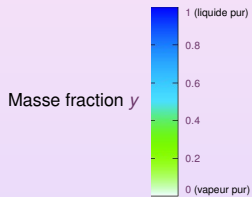
# TRANSITION TO A FILM BOILING

[◀ Geometry](#)[▶ Play](#)[▶▶ Skip](#)

# TRANSITION TO A FILM BOILING

[◀ Geometry](#)[▶ Play](#)[▶▶ Skip](#)

# TRANSITION TO A FILM BOILING

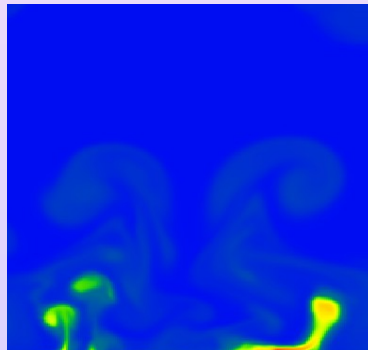
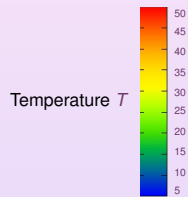
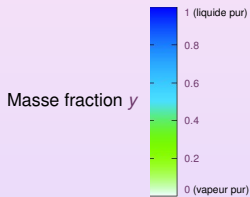


◀ Geometry

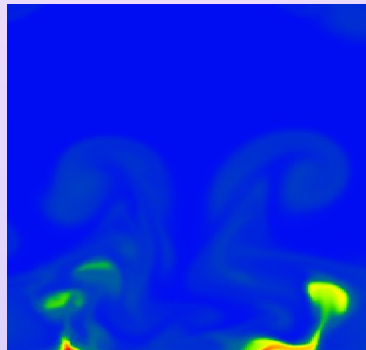
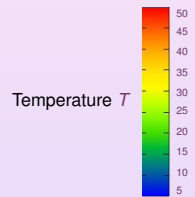
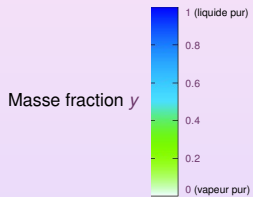
▶ Play

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# TRANSITION TO A FILM BOILING

[◀ Geometry](#)[▶ Play](#)[▶▶ Skip](#)

# TRANSITION TO A FILM BOILING

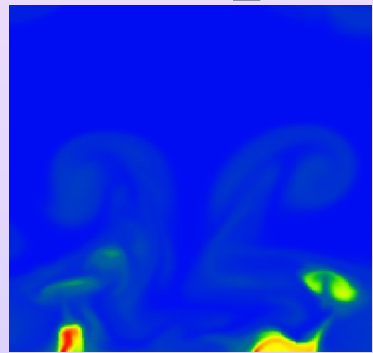
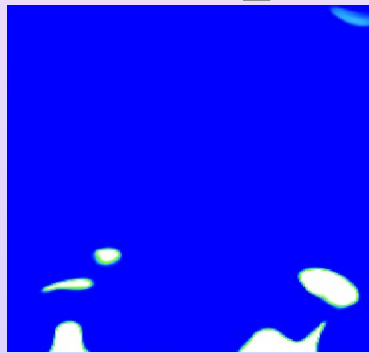
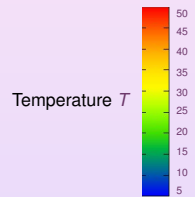
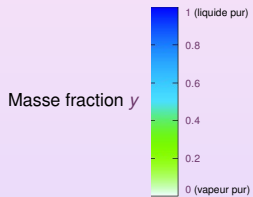


◀ Geometry

▶ Play

▶▶ Skip

# TRANSITION TO A FILM BOILING



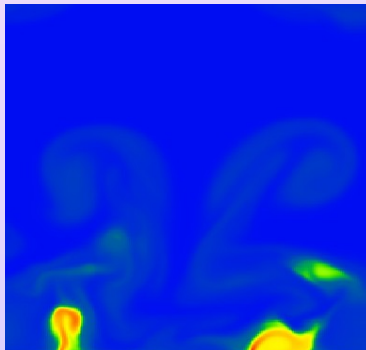
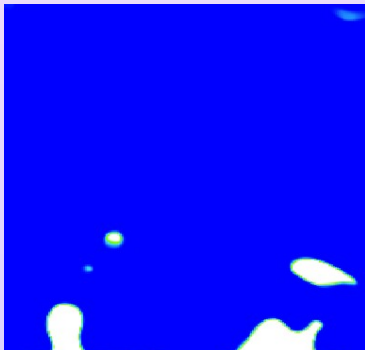
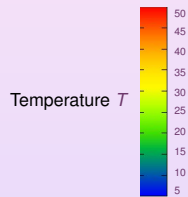
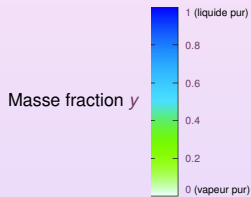
◀ Geometry

▶ Play

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# TRANSITION TO A FILM BOILING

[◀ Geometry](#)[▶ Play](#)[▶▶ Skip](#)

# OUTLINE

## 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

# 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,

- ✓ transtion: liquid phase  $\rightarrow$  nucleating boiling  $\rightarrow$  film boiling

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- Model
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# SUMMARY & PERSPECTIVES

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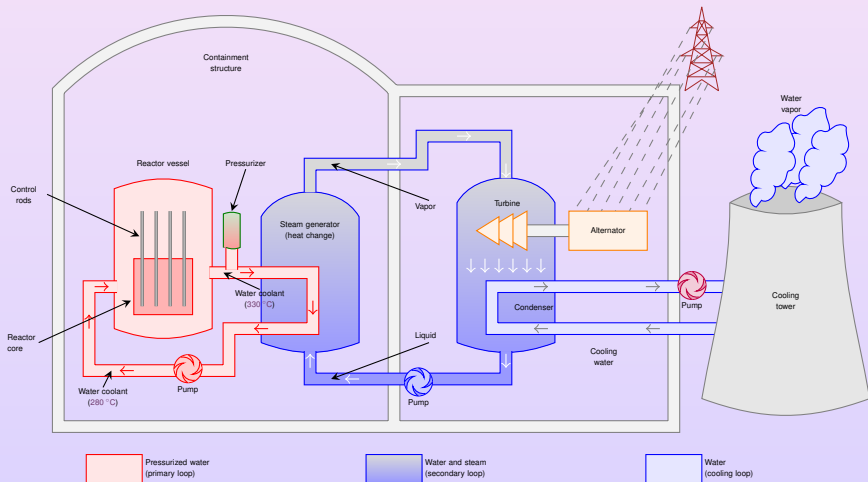
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- ✓ transtion: liquid phase  $\rightarrow$  nucleating boiling  $\rightarrow$  film boiling
- ✗ **quantitative simulations: implicit transport step (Low Mach) and 3D (parallelization).**

# APPENDIX

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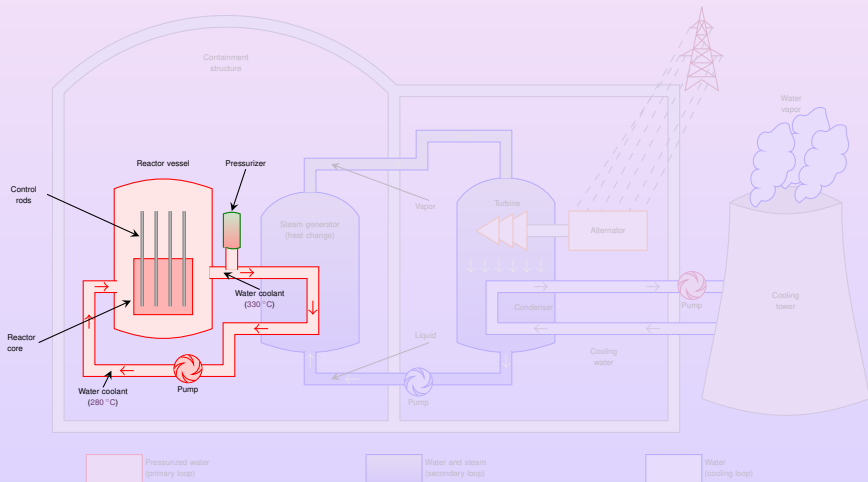
- ▶ PWR
- ▶ Stiffened Gas for Water
- ▶ Tabulated EOS for Water
- ▶ Speed of sound
- ▶ Isentropic curves
- ▶ Surface Tension
- ▶ Metastability
- ▶ Critical Point

# PRESSURIZED WATER REACTOR

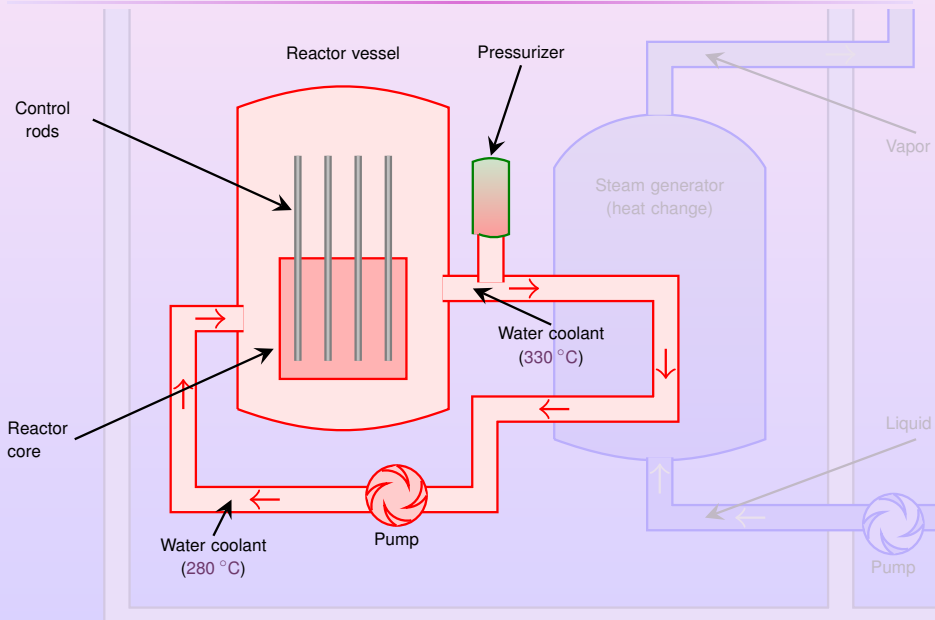




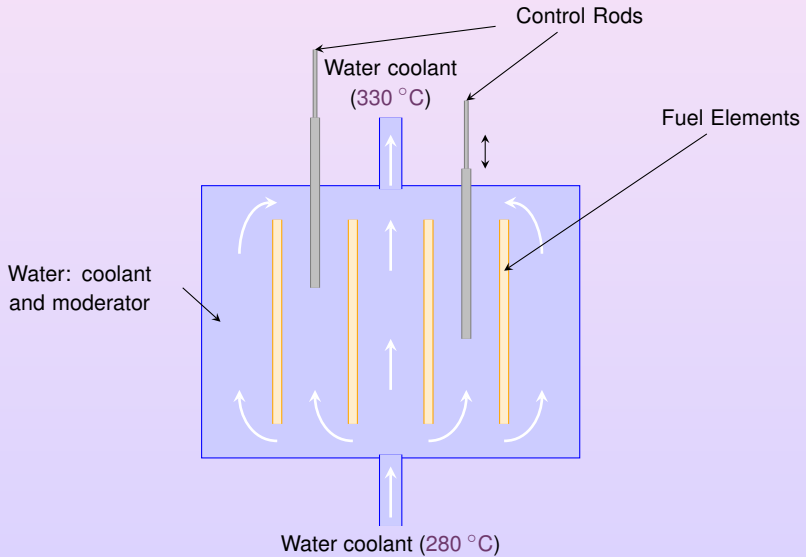
# PRESSURIZED WATER REACTOR



# PRESSURIZED WATER REACTOR



# CORE OF A PRESSURIZED WATER REACTOR



# STIFFENED GAS FOR WATER

Phase	$c_v$ [J/(kg·K)]	$\gamma$	$\pi$ [Pa]	$q$ [J/kg]	$m$ [J/(kg·K)]
Water	1816.2	2.35	$10^9$	$-1167.056 \times 10^3$	-32765.55596
Steam	1040.14	1.43	0	$2030.255 \times 10^3$	-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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# WATER TABULATED EOS

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

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

$$T \mapsto \epsilon_{\text{vap}}^{\text{sat}} \approx \widehat{\epsilon}_{\text{vap}}^{\text{sat}} \stackrel{\text{def}}{=} \frac{1}{\sum_{k=0}^6 a_k T^k}$$

$$T \mapsto \epsilon_{\text{liq}}^{\text{sat}} \approx \widehat{\epsilon}_{\text{liq}}^{\text{sat}} \stackrel{\text{def}}{=} \widehat{\epsilon}_{\text{vap}}^{\text{sat}}(T) \sum_{k=0}^6 b_k T^k$$

$$T \mapsto \tau_{\text{vap}}^{\text{sat}} \approx \widehat{\tau}_{\text{vap}}^{\text{sat}} \stackrel{\text{def}}{=} \frac{1}{\sum_{k=0}^8 c_k T^k}$$

$$T \mapsto \tau_{\text{liq}}^{\text{sat}} \approx \widehat{\tau}_{\text{liq}}^{\text{sat}} \stackrel{\text{def}}{=} \widehat{\tau}_{\text{vap}}^{\text{sat}}(T) \sum_{k=0}^9 d_k T^k$$



## SPEED OF SOUND

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

HESSIAN MATRIX OF  $\mathbf{w} \mapsto s^{\text{eq}}$ 

- for all  $\mathbf{w}$  pure phase state

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

- for all  $\mathbf{w}$  equilibrium mixture state

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

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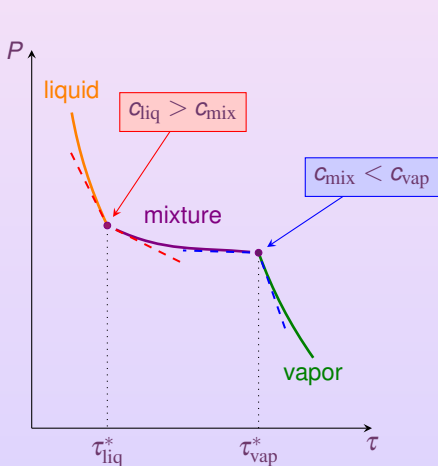
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## ISENTROPIC CURVES



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

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

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

- Pure Phases

- (H)  $\gamma > 0$
- (H)  $\Gamma > 0$
- (H)  $\mathcal{G} > 0$

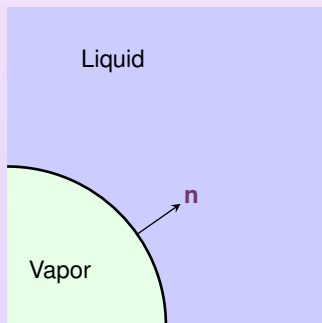
- Mixture

- (P)  $\gamma > 0$
- (P)  $\Gamma > 0$
- (H)  $\mathcal{G} > 0$

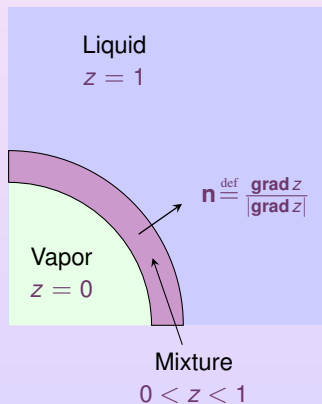
- Regularity: [J. CORREIA, P.G. LEFLOCH, M.D. THANH]
- Loss of convexity: [A. VOSS]

# CONTINUUM SURFACE FORCE (CSF) APPROACH

Physical Interface

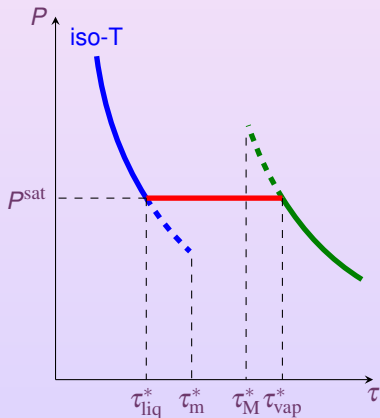


Diffuse Interface



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

## METASTABILITY

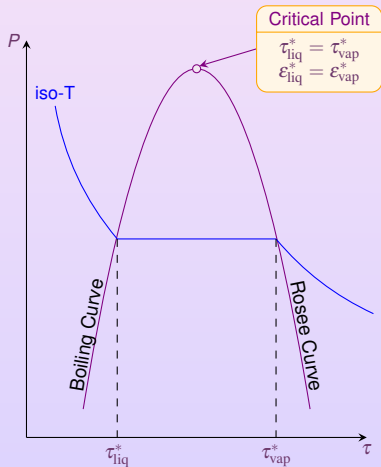


$$P^{\text{eq}} = \begin{cases} P_{\text{liq}}, & \text{if } \tau < \tau_{\text{liq}}^*, \\ P^{\text{sat}}, & \text{if } \tau_{\text{liq}}^* < \tau < \tau_{\text{vap}}^*, \\ P_{\text{vap}}, & \text{if } \tau_{\text{vap}}^* < \tau. \end{cases}$$

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



# CRITICAL POINT



## PHYSIC

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

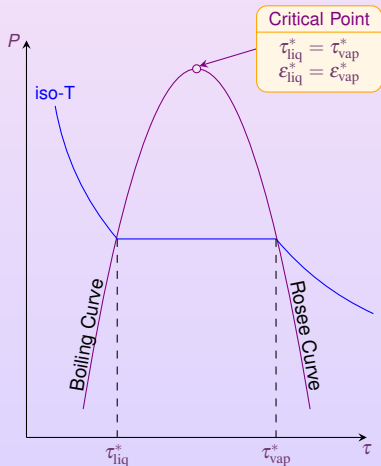
## EOS

**PG**  $\epsilon_{\text{liq}}^* = \epsilon_{\text{vap}}^* \Leftrightarrow c_{V\text{liq}} = c_{V\text{vap}}$  (indip. of  $T$ )

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

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- 2 Pure Phases EOS  $(\tau, \epsilon) \mapsto P_\alpha$
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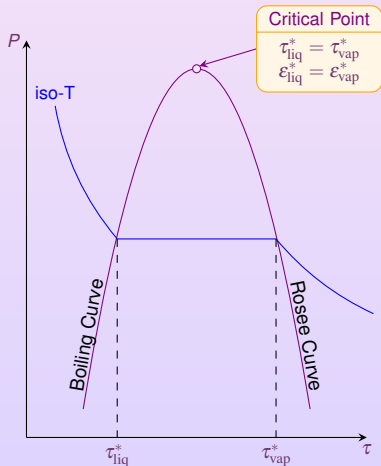
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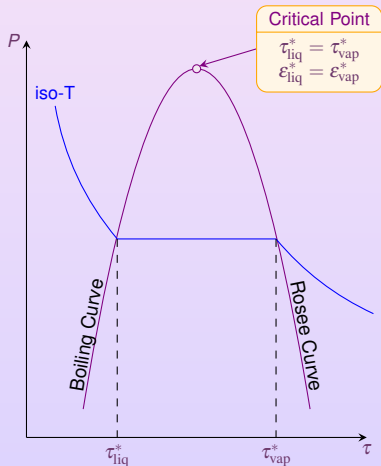
## EOS

**PG**  $\epsilon_{\text{liq}}^* = \epsilon_{\text{vap}}^* \Leftrightarrow c_{V\text{liq}} = c_{V\text{vap}}$  (indip. of  $T$ )

**SG**  $\{\tau_i, P_i^{\text{sat},e}\}_i \rightsquigarrow (\tau, \epsilon) \mapsto P_\alpha \rightsquigarrow \tau \mapsto P^{\text{sat}}$   
 $\tau_{\text{liq}}^* = \tau_{\text{vap}}^*$  but  $\epsilon_{\text{liq}}^* \neq \epsilon_{\text{vap}}^*$

**TAB**  $\{\tau_i, P_i^{\text{sat},e}\}_i \rightsquigarrow \tau \mapsto P^{\text{sat}}$   
 $\{(\tau_i, \epsilon_i), (P_\alpha^c)_i\}_i \rightsquigarrow (\tau, \epsilon) \mapsto P_\alpha$

# CRITICAL POINT



## PHYSIC

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

## EOS

**PG**  $\epsilon_{\text{liq}}^* = \epsilon_{\text{vap}}^* \Leftrightarrow c_{V\text{liq}} = c_{V\text{vap}}$  (indip. of  $T$ )

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