

Grenoble, March 17, 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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Outline

1 Context

2 Model

3 Numerical Approximation

4 Numerical Examples

5 Conclusion

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2 Model

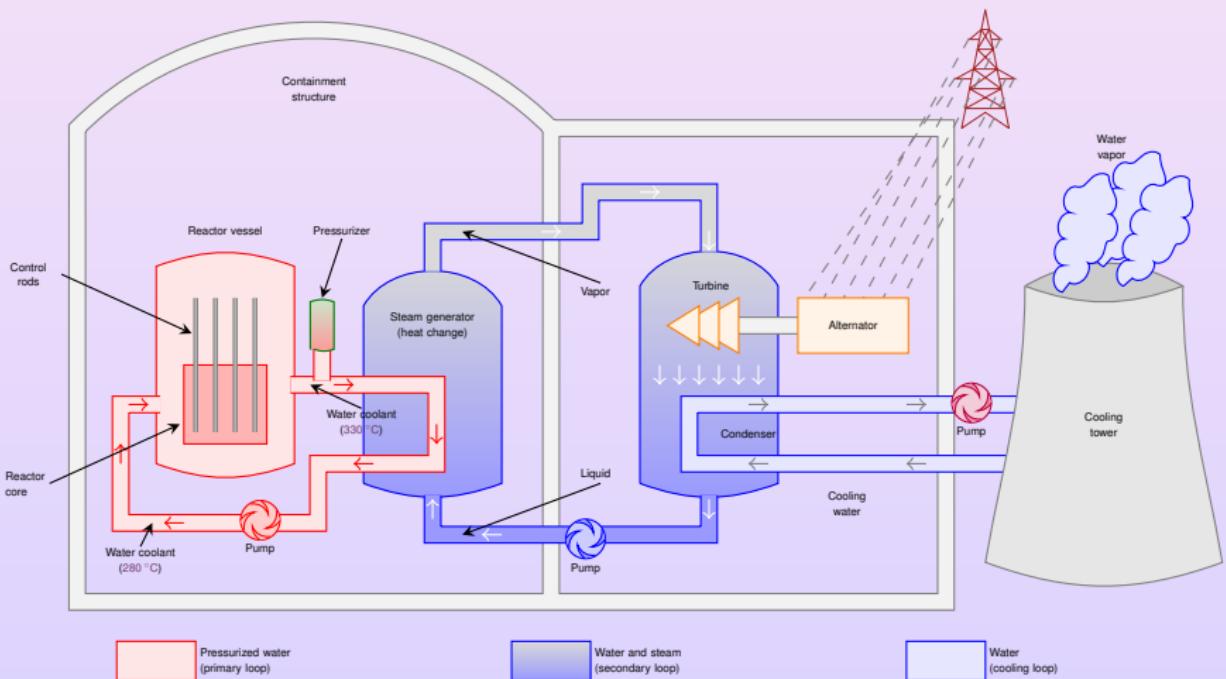
- Equation of State WITHOUT Phase Change
- Equation of State WITH Phase Change
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3 Numerical Approximation

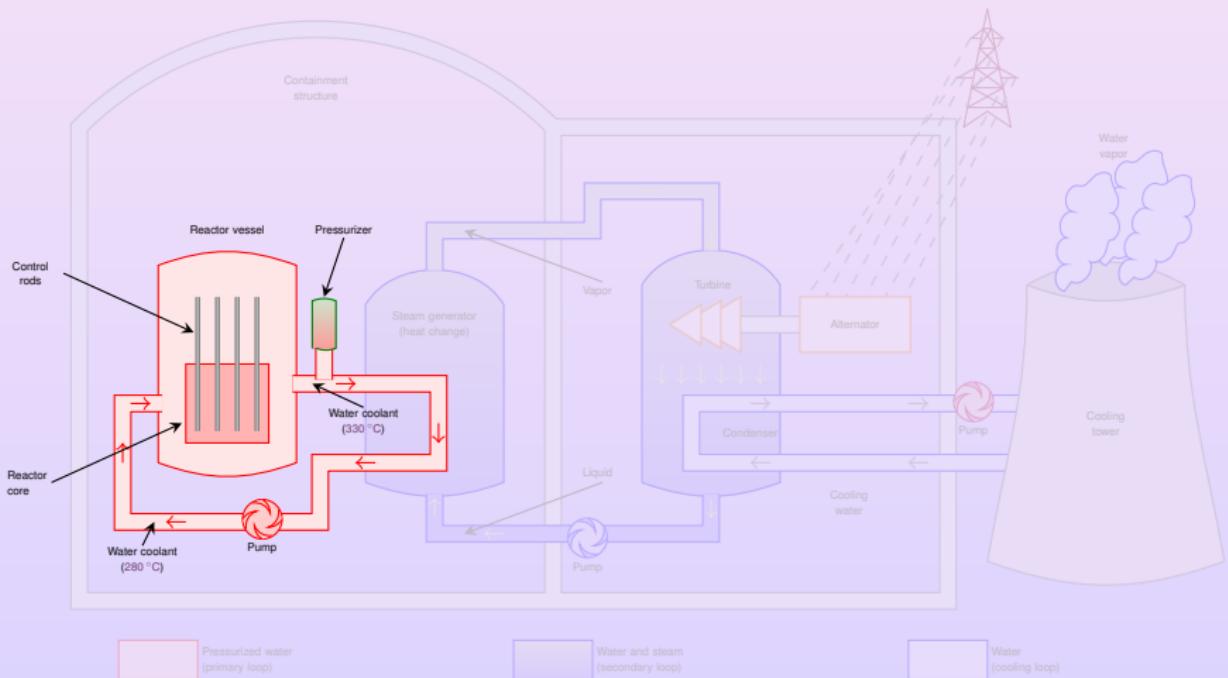
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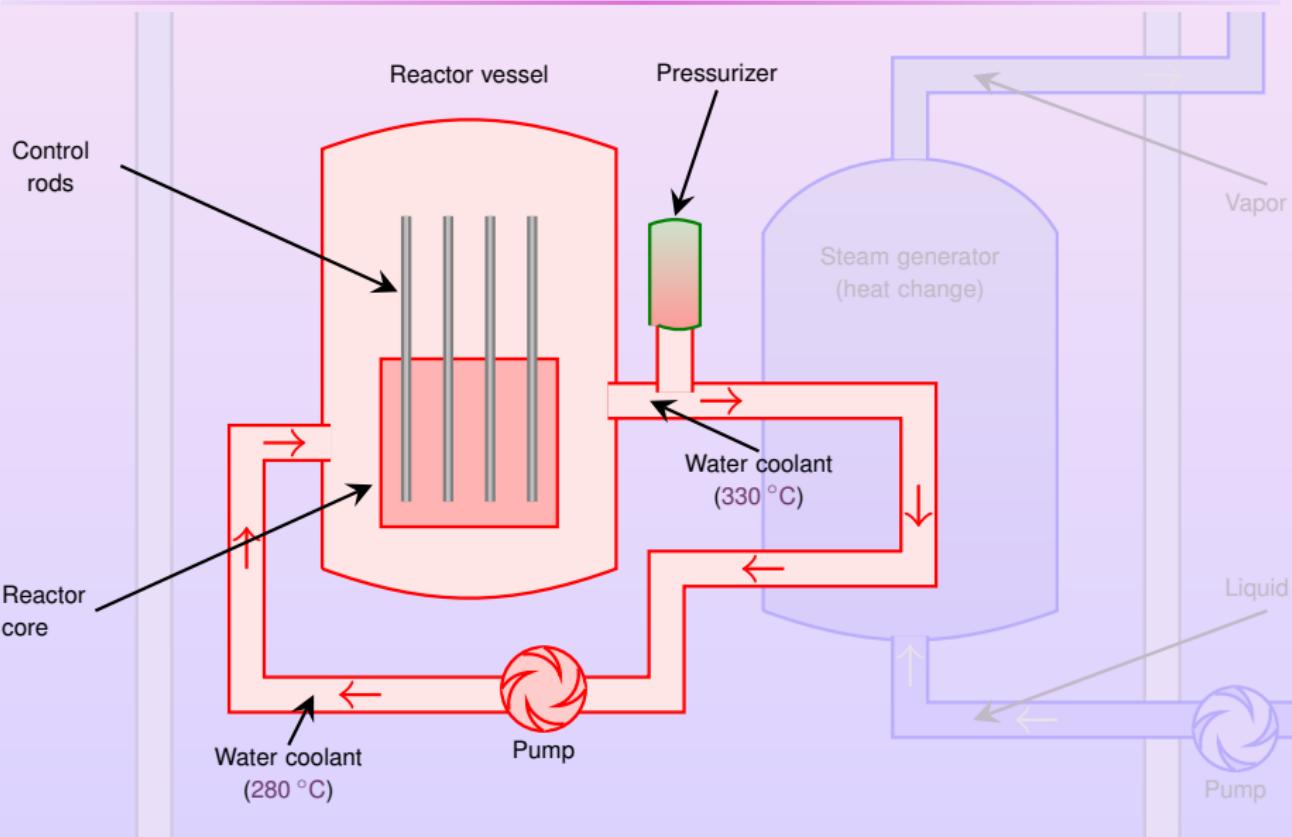
Pressurized Water Reactor



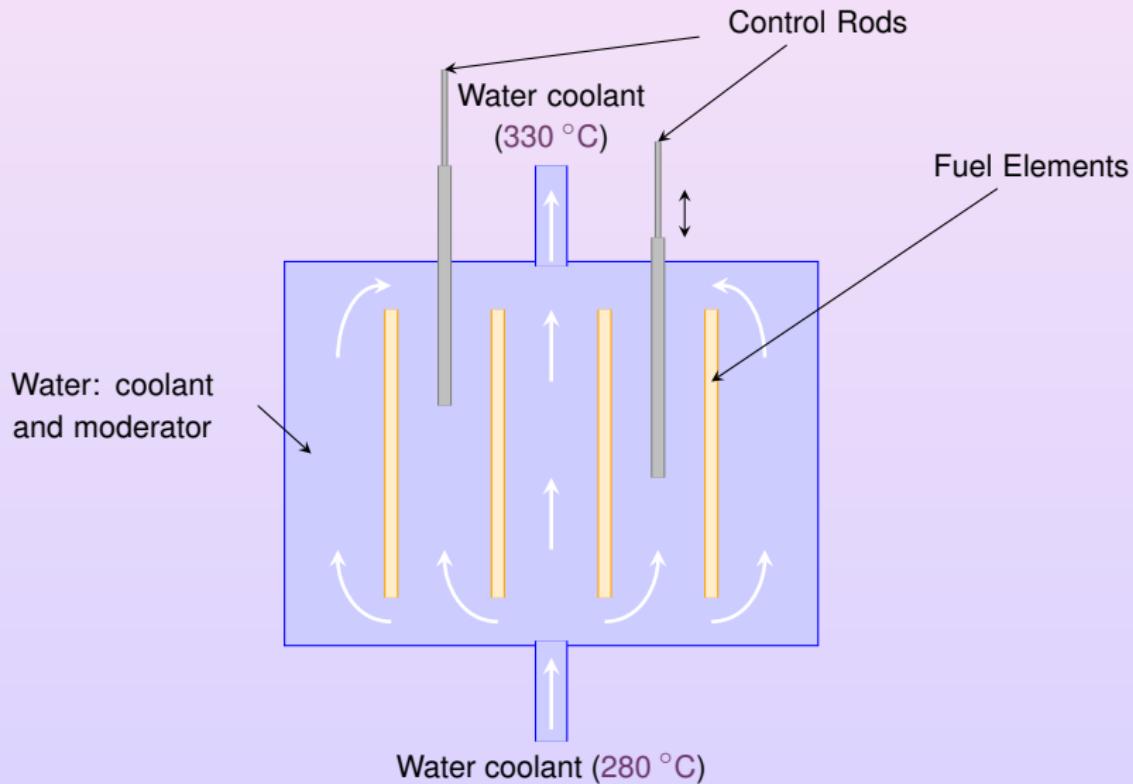
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Core of a Pressurized Water Reactor

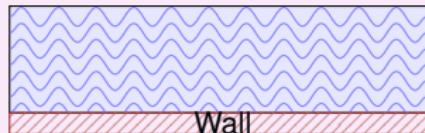


Boiling Crisis

PHENOMENON

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

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

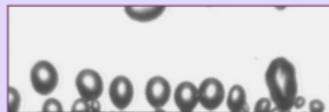
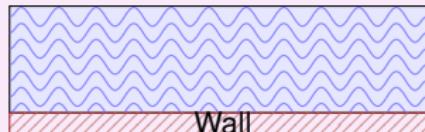


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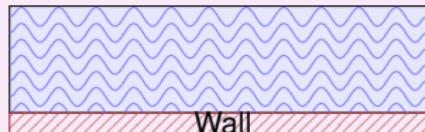
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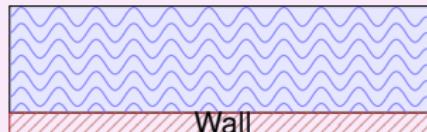
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OMEGA - CEA Grenoble



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“Ingredients” of the Model

✓ Simulating all bubbles,

- System of PDEs for the fluid flow (monophasic or diphasic),
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- 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,
- $(\rho, \varepsilon) \mapsto \mathfrak{S}_{\text{sf}}$ surface forces,
- $(\rho, \varepsilon) \mapsto \operatorname{div}(q)$ heat transfer.

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

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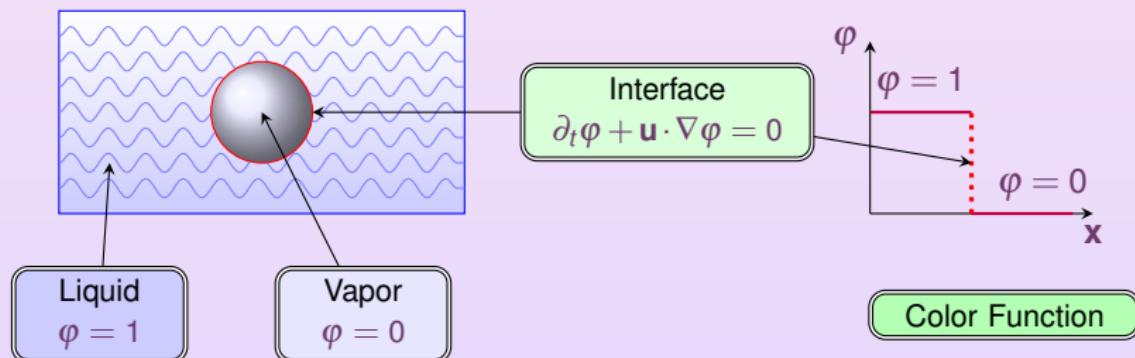
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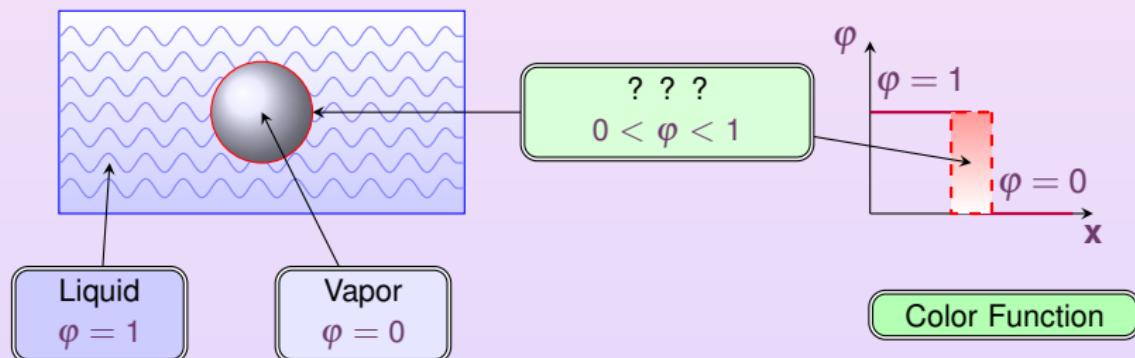
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Liquid-Vapor Interface



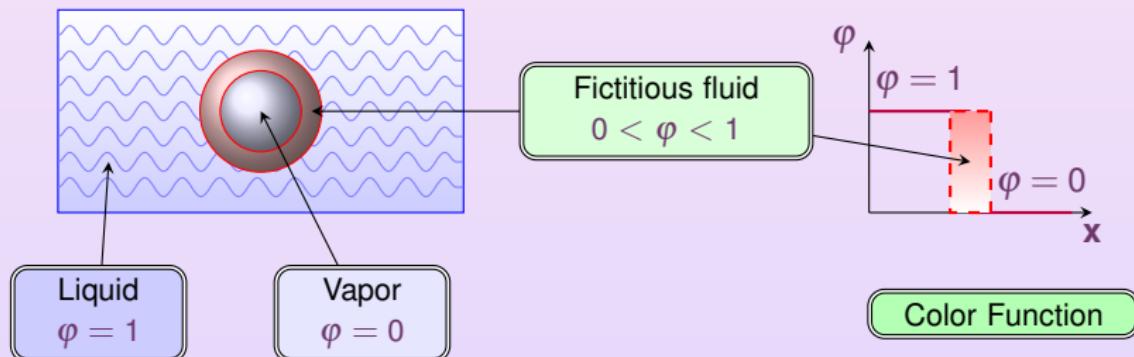
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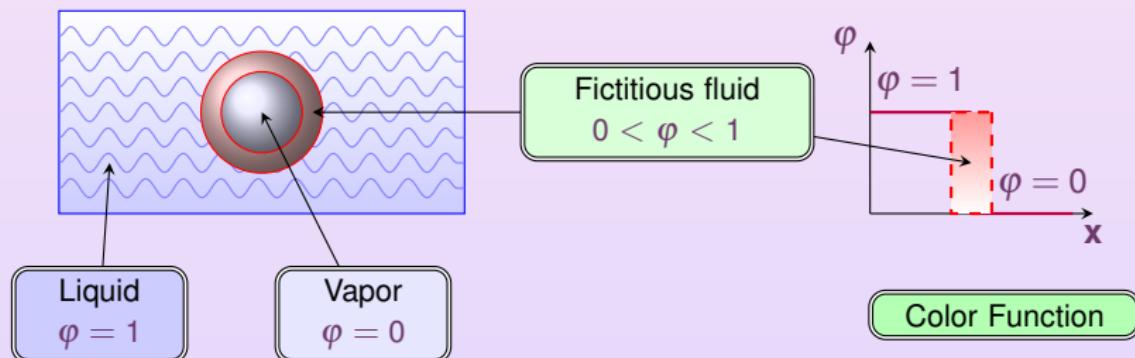
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Liquid-Vapor Interface



➡ 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. $\cancel{\varphi}$)
- 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.);


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

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- $\mathbf{w} \stackrel{\text{def}}{=} y\mathbf{w}_1 + (1 - y)\mathbf{w}_2;$
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EOS with Phase Change

ENTROPY WITHOUT PH.CH.

$$(w, z, y, \psi) \mapsto \sigma$$



ENTROPY AT EQUILIBRIUM

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

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

Optimization Problem:

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

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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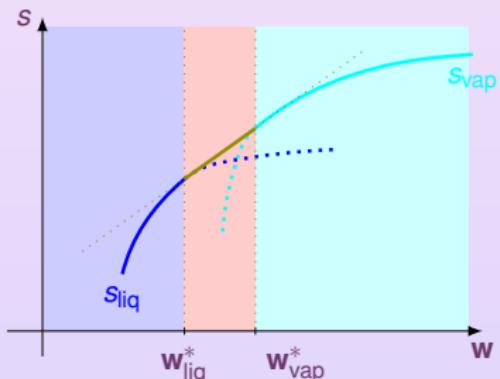
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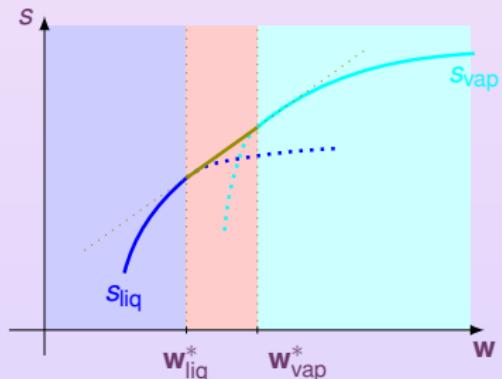
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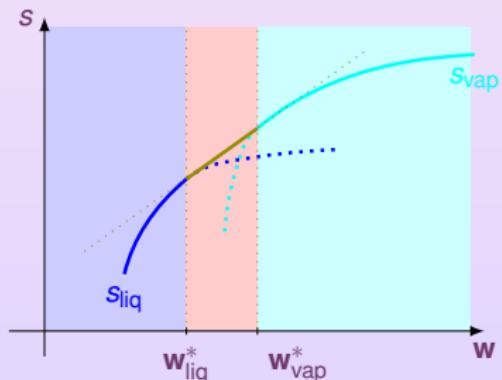
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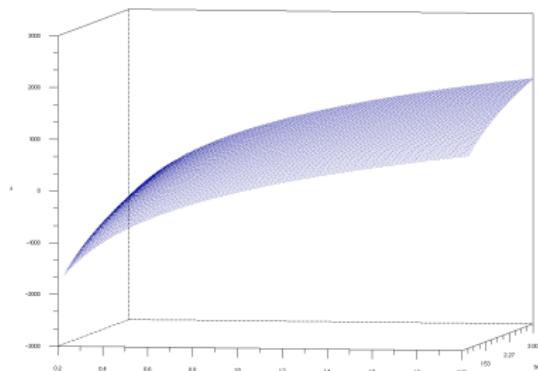
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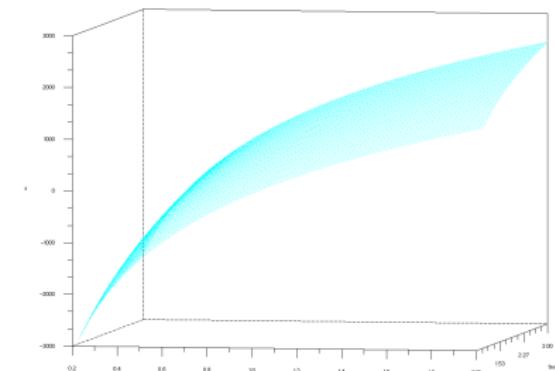
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Concave Hull with two Perfect Gases

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

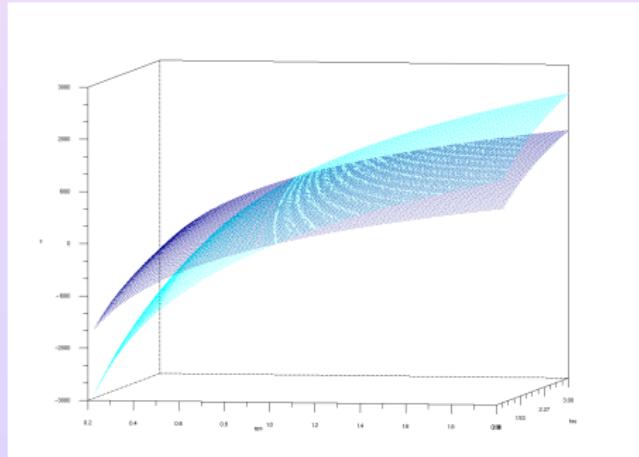


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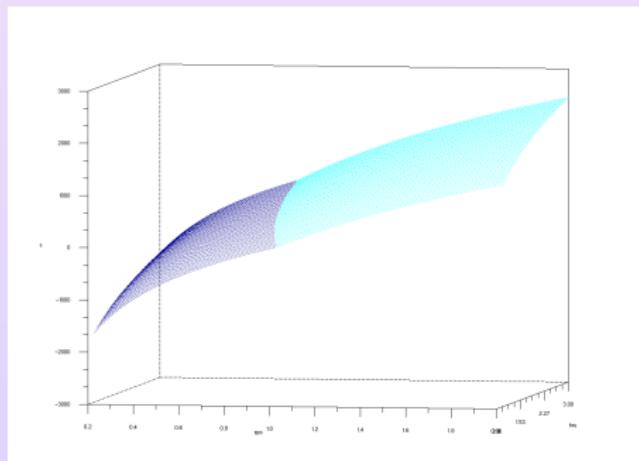
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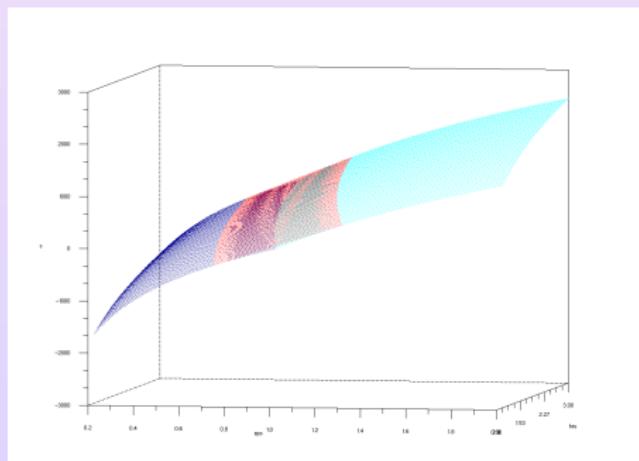
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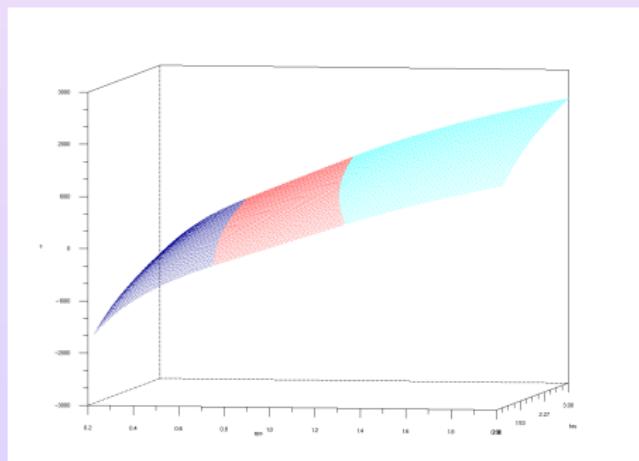
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From $\mathbf{w} \mapsto s^{\text{eq}}$ to $\mathbf{w} \mapsto P^{\text{eq}}$

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**

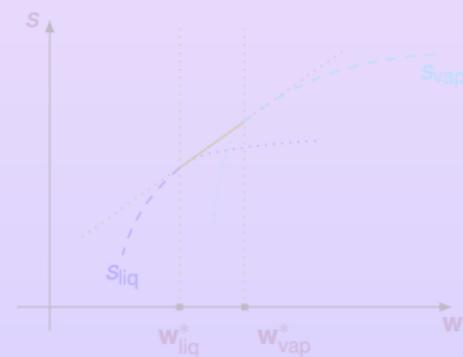
$$s^{\text{eq}}(\tilde{\mathbf{w}}) = y^* s_{\text{liq}}(\mathbf{w}_{\text{liq}}^*) + (1 - y^*) s_{\text{vap}}(\mathbf{w}_{\text{vap}}^*),$$

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

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

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

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



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

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

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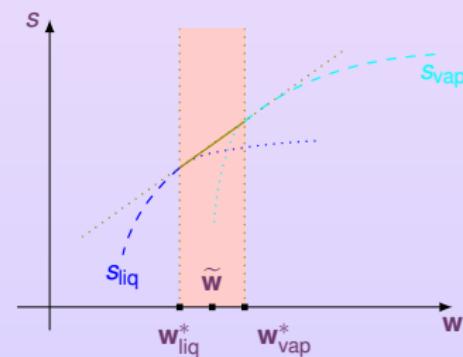
$$s^{\text{eq}}(\tilde{\mathbf{w}}) = y^* s_{\text{liq}}(\mathbf{w}_{\text{liq}}^*) + (1 - y^*) s_{\text{vap}}(\mathbf{w}_{\text{vap}}^*),$$

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

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

$$\left(\begin{array}{l} \text{if } s_{\text{liq}} > s_{\text{vap}} \\ \text{if } s_{\text{liq}} < s_{\text{vap}} \end{array} \right)$$



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

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

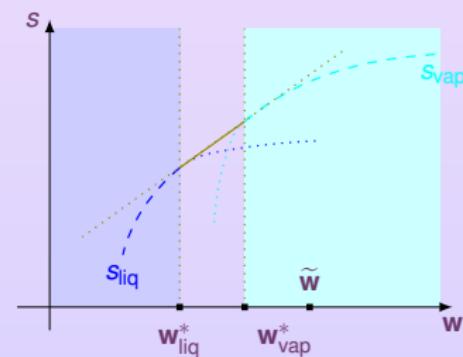
$$s^{\text{eq}}(\tilde{\mathbf{w}}) = y^* s_{\text{liq}}(\mathbf{w}_{\text{liq}}^*) + (1 - y^*) s_{\text{vap}}(\mathbf{w}_{\text{vap}}^*),$$

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

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

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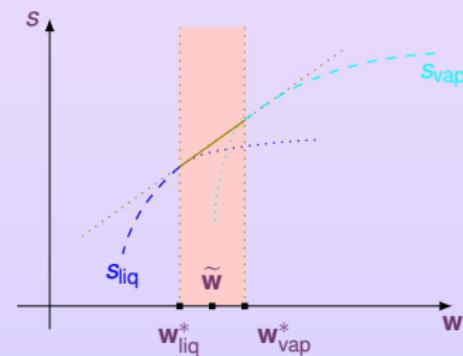
$$s^{\text{eq}}(\tilde{\mathbf{w}}) = y^* s_{\text{liq}}(\mathbf{w}_{\text{liq}}^*) + (1 - y^*) s_{\text{vap}}(\mathbf{w}_{\text{vap}}^*),$$

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

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

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

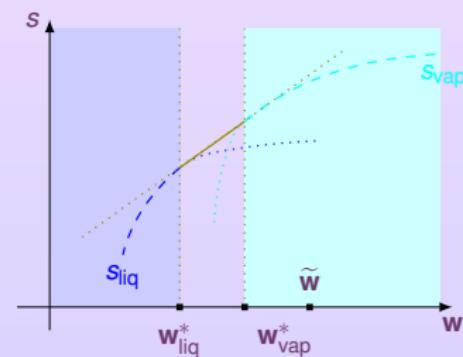
$$s^{\text{eq}}(\tilde{\mathbf{w}}) = y^* s_{\text{liq}}(\mathbf{w}_{\text{liq}}^*) + (1 - y^*) s_{\text{vap}}(\mathbf{w}_{\text{vap}}^*),$$

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

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

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

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Summary of the Model

Euler System

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

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

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

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

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

$$\begin{cases} g_1(w_1) = g_2(w_2) \\ P_1(w_1) = P_2(w_2) \\ T_1(w_1) = T_2(w_2) \\ w = yw_1 + (1-y)w_2 \end{cases}$$

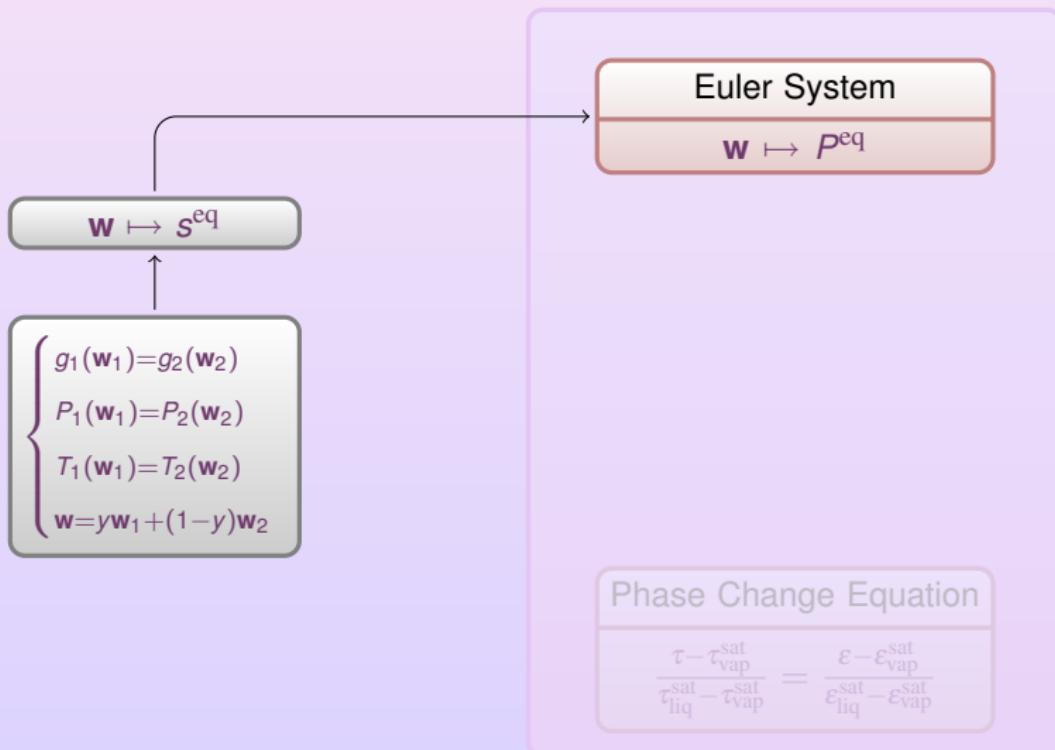
Euler System

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

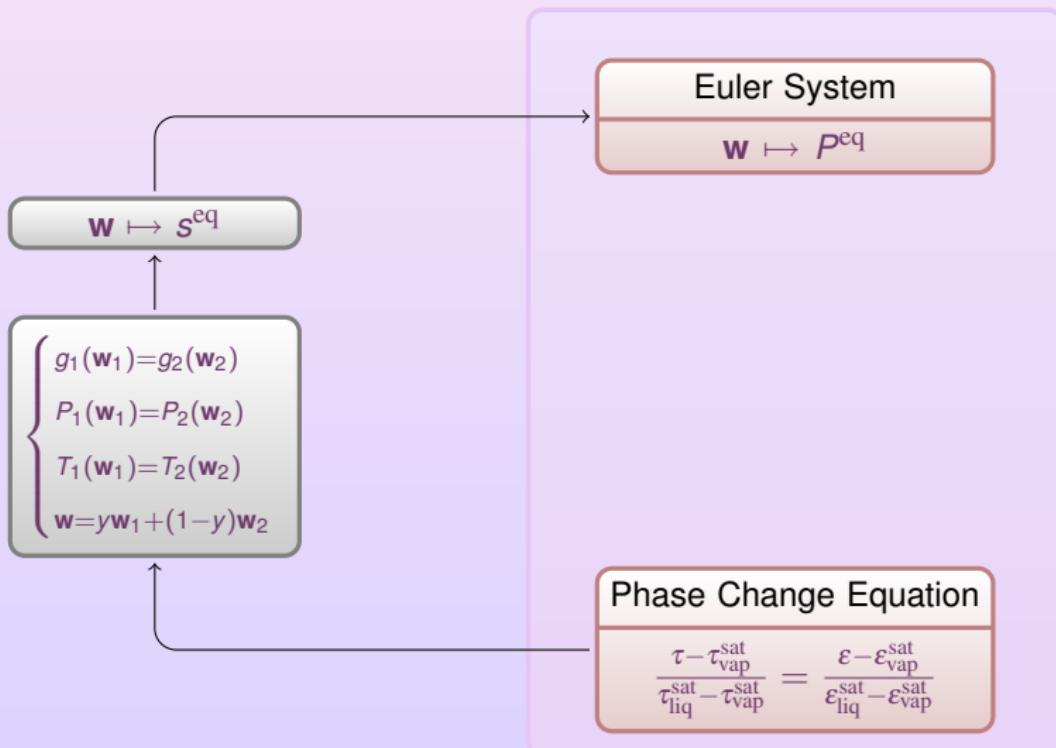
Phase Change Equation

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

Summary of the Model



Summary of the Model



Summary of the Model

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

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

Euler System

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

Phase Change Equation

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

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

4 Numerical Examples

5 Conclusion

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

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

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

T SOLUTION OF

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

Analytical EOS

(τ, ε) fixed

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

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

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

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Analytical EOS

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

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

Analytical EOS

(τ, ε) fixed

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

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

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

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least square
approximation

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

T SOLUTION OF

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

Tabulated EOS

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

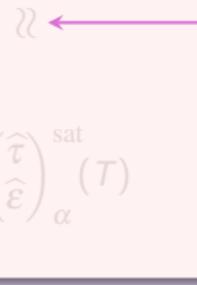
Source: <http://webbook.nist.gov/chemistry/fluid/>

Tabulated EOS

(τ, ε) fixed

T SOLUTION OF

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



$$\left(\begin{matrix} \hat{\tau} \\ \hat{\varepsilon} \end{matrix}\right)_\alpha^{\text{sat}}(T)$$

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

least square
approximations

Tabulated EOS

(τ, ε) fixed

T SOLUTION OF

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

|| ←

$$\frac{\tau - \hat{\tau}_2^{\text{sat}}(T)}{\hat{\tau}_1^{\text{sat}}(T) - \hat{\tau}_2^{\text{sat}}(T)} = \frac{\varepsilon - \hat{\varepsilon}_2^{\text{sat}}(T)}{\hat{\varepsilon}_1^{\text{sat}}(T) - \hat{\varepsilon}_2^{\text{sat}}(T)} \quad \text{with} \quad \left(\begin{matrix} \hat{\tau} \\ \hat{\varepsilon} \end{matrix}\right)_\alpha^{\text{sat}}(T)$$

least square
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Tabulated EOS

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T SOLUTION OF

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

|| ←

$$\frac{\tau - \hat{\tau}_2^{\text{sat}}(T)}{\hat{\tau}_1^{\text{sat}}(T) - \hat{\tau}_2^{\text{sat}}(T)} = \frac{\varepsilon - \hat{\varepsilon}_2^{\text{sat}}(T)}{\hat{\varepsilon}_1^{\text{sat}}(T) - \hat{\varepsilon}_2^{\text{sat}}(T)} \quad \text{with} \quad \left(\begin{matrix} \hat{\tau} \\ \hat{\varepsilon} \end{matrix}\right)_\alpha^{\text{sat}}(T)$$

least square
approximations

Phase Change Equation: Summary

PHASE CHANGE EQUATION

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

with

$$T \mapsto \left(\frac{\tau}{\varepsilon} \right)_{\alpha}^{\text{sat}} (T) = \left(\frac{\tau}{\varepsilon} \right)_{\alpha} (T, P^{\text{sat}}(T))$$

or

$$P \mapsto \left(\frac{\tau}{\varepsilon} \right)_{\alpha}^{\text{sat}} (P) = \left(\frac{\tau}{\varepsilon} \right)_{\alpha} (T^{\text{sat}}(P), P)$$

Phase Change Equation: Summary

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

- **Analytical EOS:** we compute the saturation functions τ_α^{sat} and $\varepsilon_\alpha^{\text{sat}}$ by the Coexistence Curve:

- Exact: $T \mapsto P^{\text{sat}}(T)$ or $P \mapsto T^{\text{sat}}(P)$

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

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

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

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

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

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

4 Numerical Examples

5 Conclusion

Dynamic Liquid-Vapor Phase Change

EULER SYSTEM

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

PROPERTIES

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

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

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

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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

4 Numerical Examples

5 Conclusion

Relaxation Approach

$$\partial_t \mathbf{U} + \operatorname{div} \mathbf{F}(\mathbf{U}) = \mathbf{0}$$

Relaxation Approach

$$\partial_t \mathbf{V} + \operatorname{div} \mathbf{G}(\mathbf{V}) = \frac{1}{\mu} \mathbf{R}(\mathbf{V}) \quad \xrightarrow[\mu \rightarrow 0]{\text{Formally}} \quad \partial_t \mathbf{U} + \operatorname{div} \mathbf{F}(\mathbf{U}) = \mathbf{0}$$

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$$P^{\text{eq}}(\rho, \varepsilon) = \frac{s_{\tau}^{\text{eq}}}{s_{\varepsilon}^{\text{eq}}}, \quad e \stackrel{\text{def}}{=} \frac{|\mathbf{u}|^2}{2} + \varepsilon$$

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HOW TO BUILD THE AUGMENTED SYSTEM

1 Lagrangian:

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

Action:

$$\mathcal{A}(v) \stackrel{\text{def}}{=} \int_{t_1}^{t_2} \int_{\widehat{\Omega}(t; v)} \mathcal{L}(\widehat{\rho}, \widehat{\rho \mathbf{u}}, \widehat{s}, \widehat{y}, \widehat{z}, \widehat{\psi})(\widehat{\mathbf{x}}, t; v) d\widehat{\mathbf{x}} dt$$

Minimization of the Action: $\frac{d\mathcal{A}}{dv}(v=0) = 0$

$$2 Energy: \varepsilon \stackrel{\text{def}}{=} \sum_{\alpha} y_{\alpha} \varepsilon_{\alpha} \left(\frac{z_{\alpha}}{y_{\alpha}}, \frac{1}{\rho}, \frac{\psi_{\alpha}}{y_{\alpha}} \sigma \right)$$

3 Positive Entropy Production: $D_t \sigma \geq 0$

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EQUILIBRIUM SYSTEM

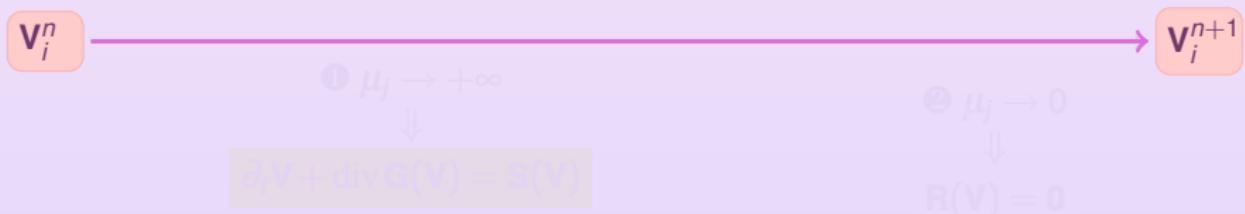
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NOTE: we can replace an EDP by an algebraic closure, for example

$$\partial_t \psi + \mathbf{u} \cdot \operatorname{grad} \psi = \frac{1}{\mu_\psi} \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \varepsilon \rightsquigarrow T_1 = T_2.$$

Numerical Scheme

$$\partial_t \mathbf{V} + \operatorname{div} \mathbf{G}(\mathbf{V}) = \mathbf{S}(\mathbf{V}) + \frac{1}{\mu} \mathbf{R}(\mathbf{V})$$



Aug. System: 5-eq. iso-T

Num. Scheme: op. splitting

$\partial_t \mathbf{V} + \operatorname{div} \mathbf{G}(\mathbf{V}) = 0$ [G. ALLAIRE and all.]

$$\mathbf{S}(\mathbf{V}) = \mathbf{S}_{\text{ad}}(\mathbf{V}) + \mathbf{S}_{\text{cond}}(\mathbf{V}) + \mathbf{S}_{\text{v}}(\mathbf{V})$$

$\partial_t \mathbf{V} = \mathbf{S}_{\text{ad}}(\mathbf{V})$ [J. U. BRACKBILL and all.]

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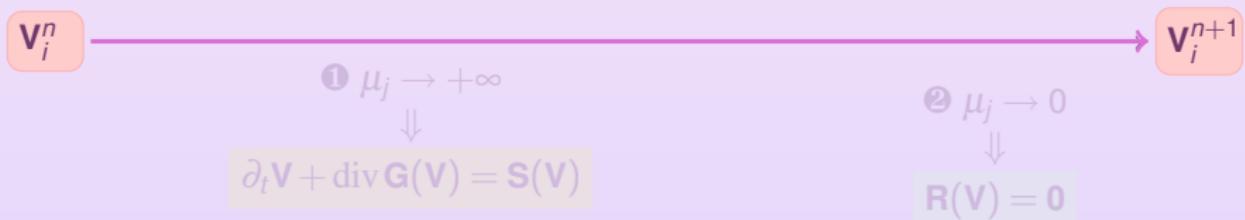
update fractions

$$(y, z, \psi)$$

solving the
Phase Change
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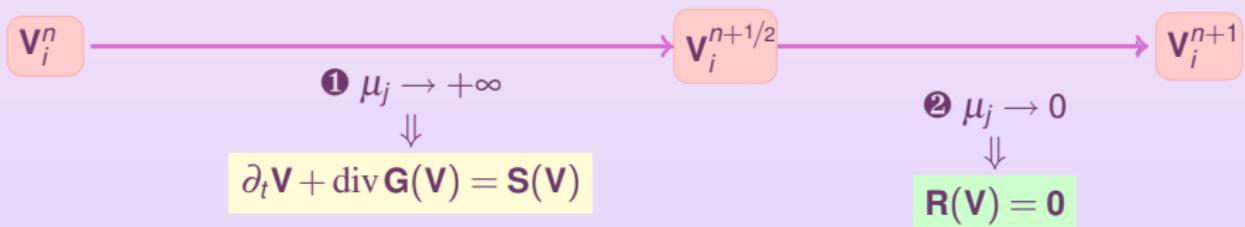
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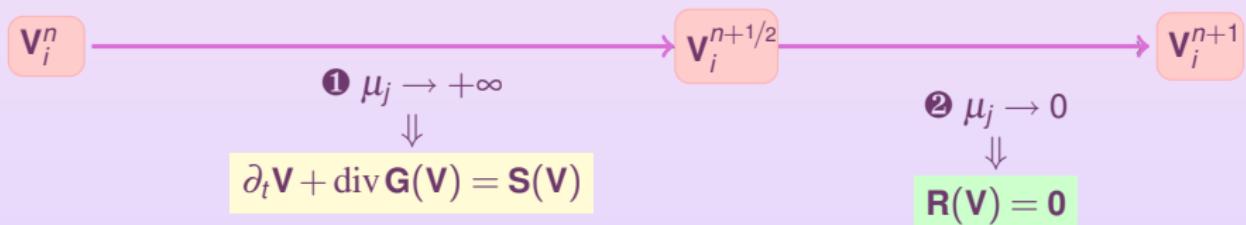
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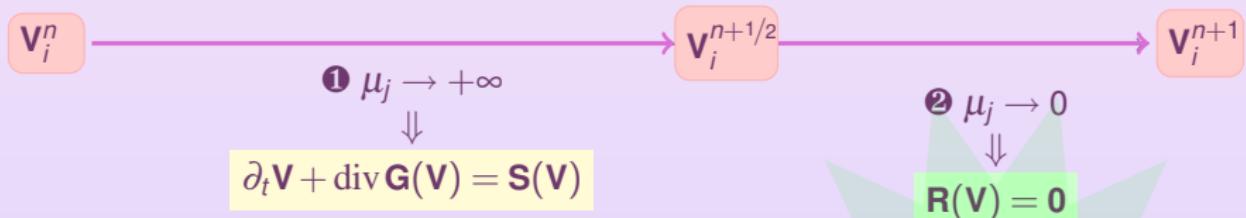
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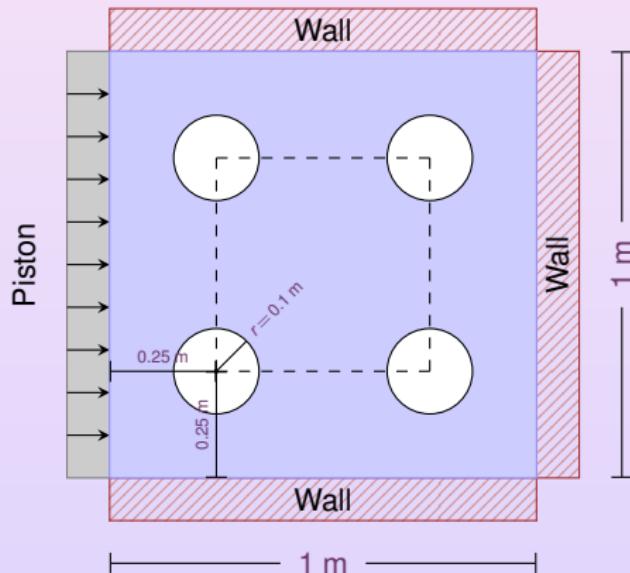
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3 Numerical Approximation

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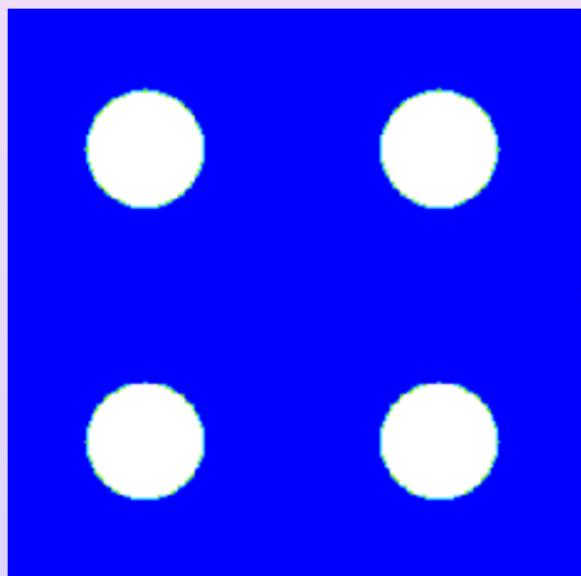
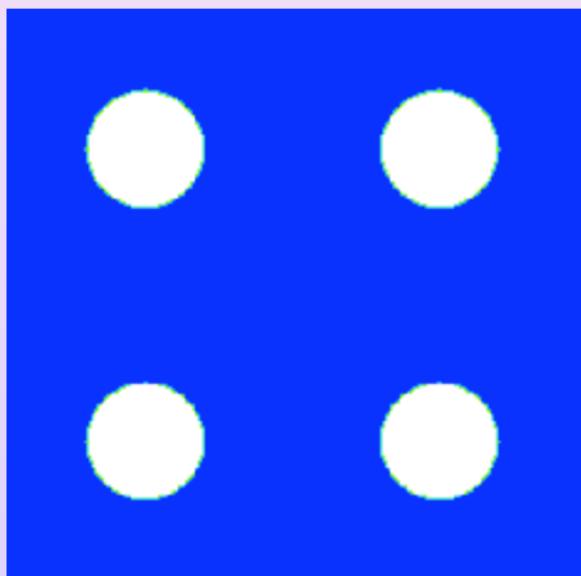
5 Conclusion

Compression of Vapor Bubbles



Compression of 4 Vapor Bubbles involving two Stiffened Gases for water and steam.
The piston moves towards right at constant speed $u_p = 30 \text{ m/s}$.

Compression of Vapor Bubbles

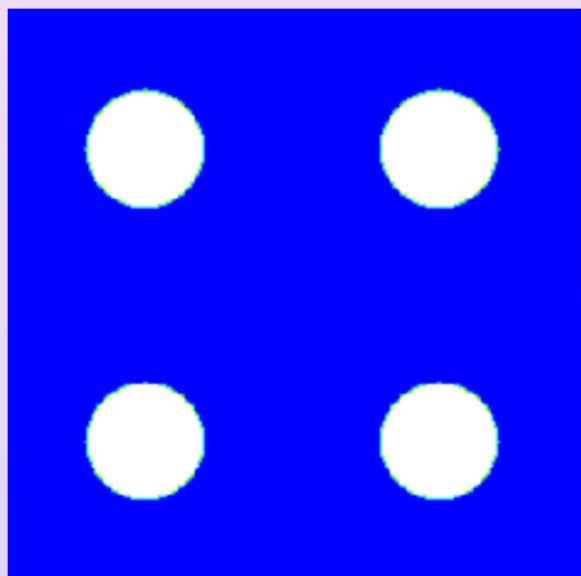
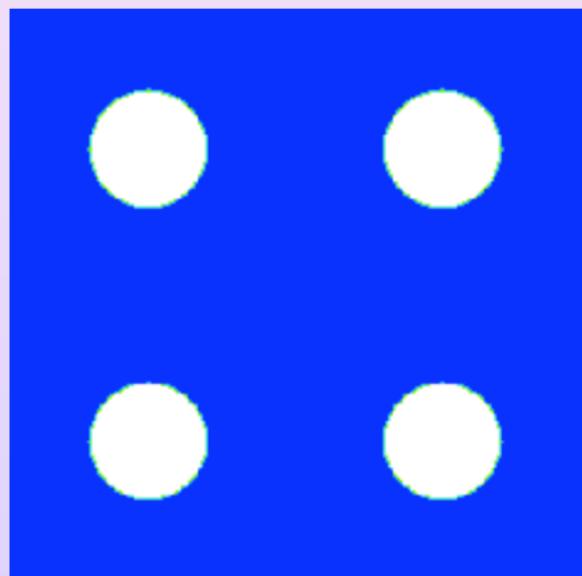
Mass Fraction y Density ρ 

◀ Geometry

▶ Play

▶ Skip

Compression of Vapor Bubbles

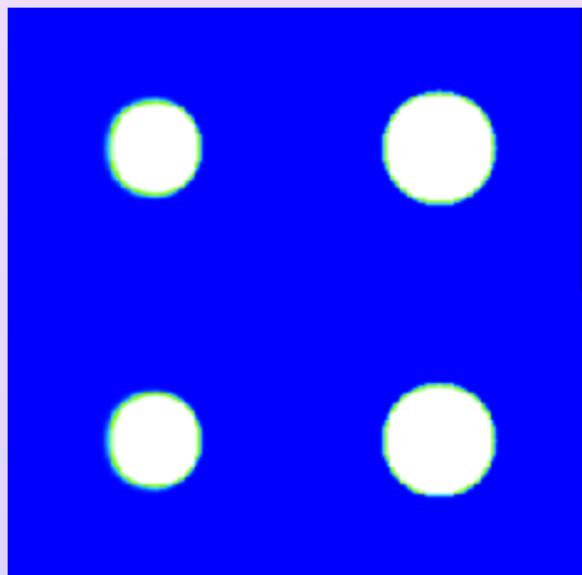
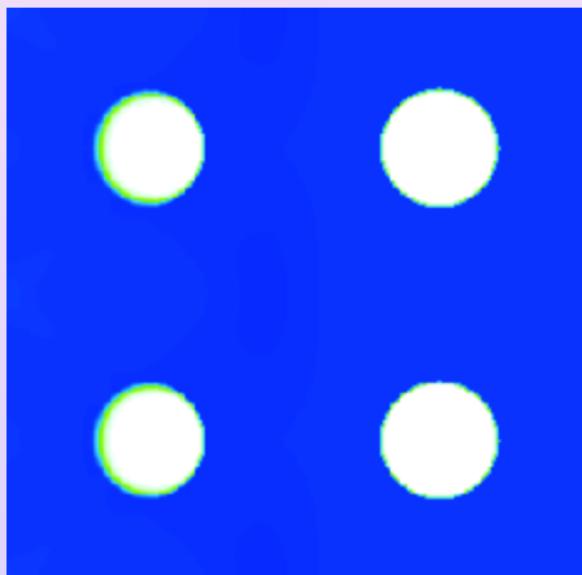
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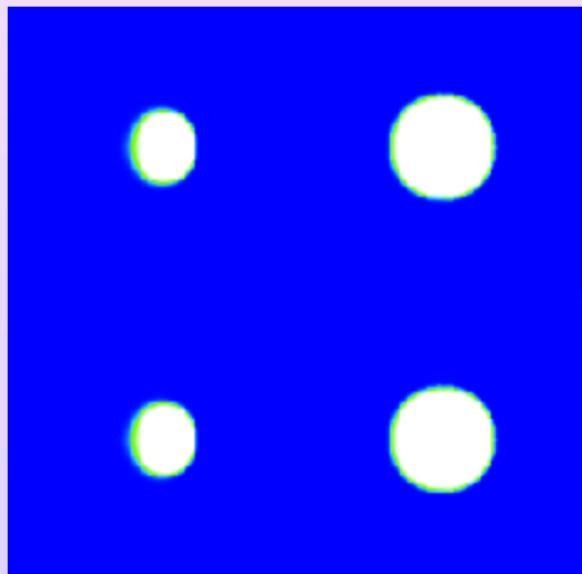
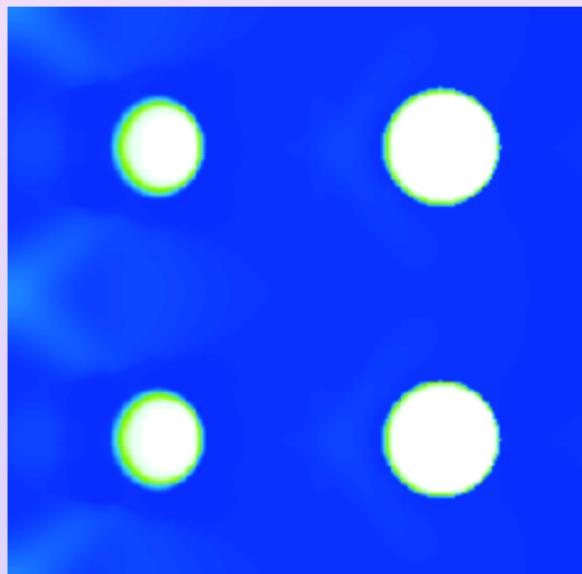
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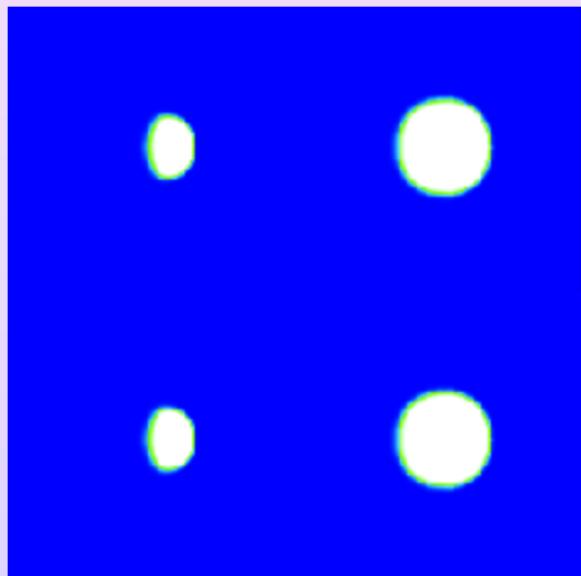
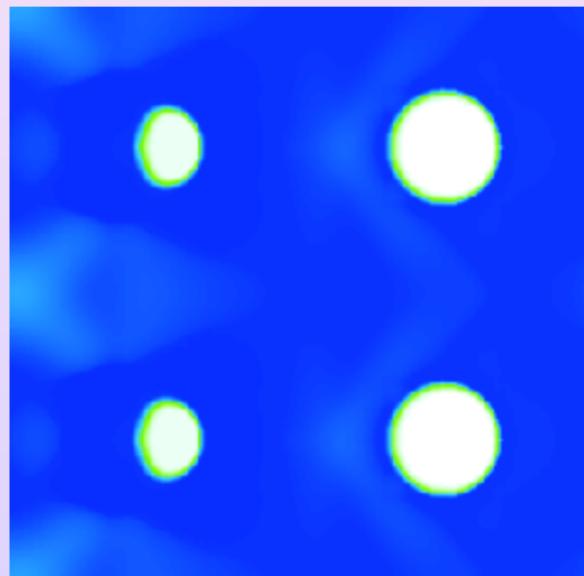
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◀ Geometry

▶ Play

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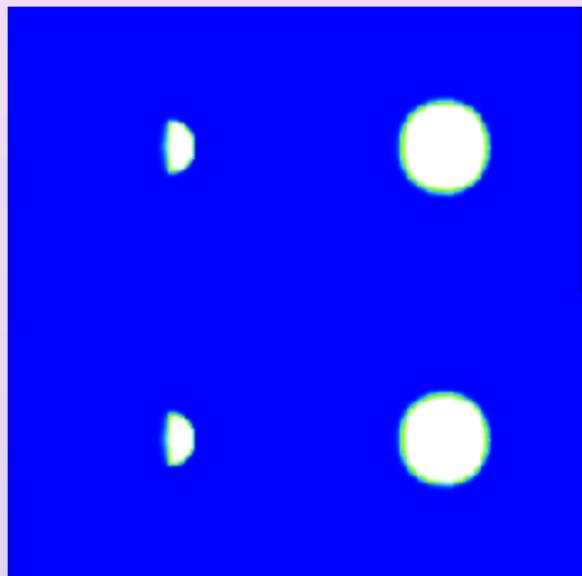
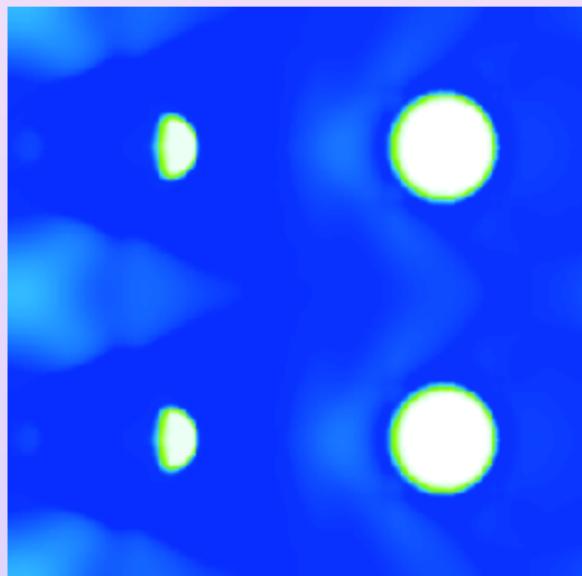
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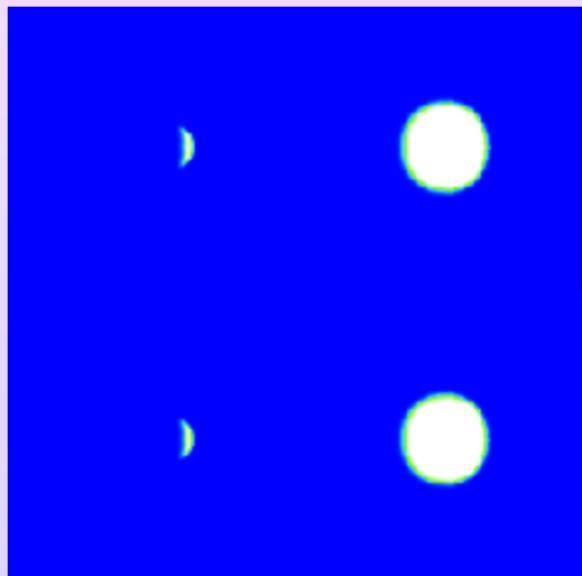
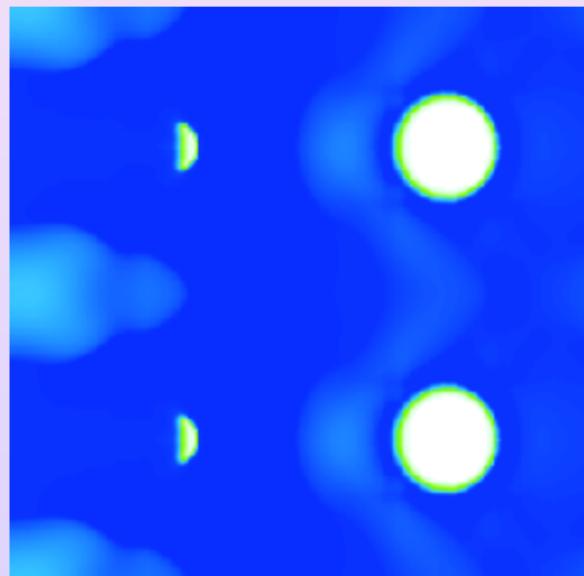
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◀ Geometry

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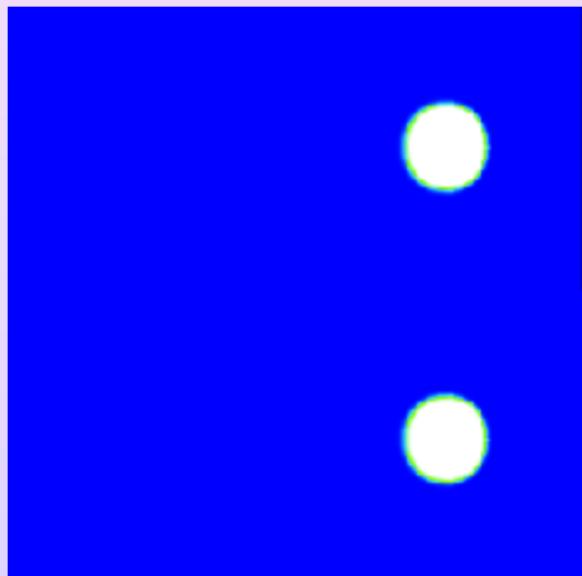
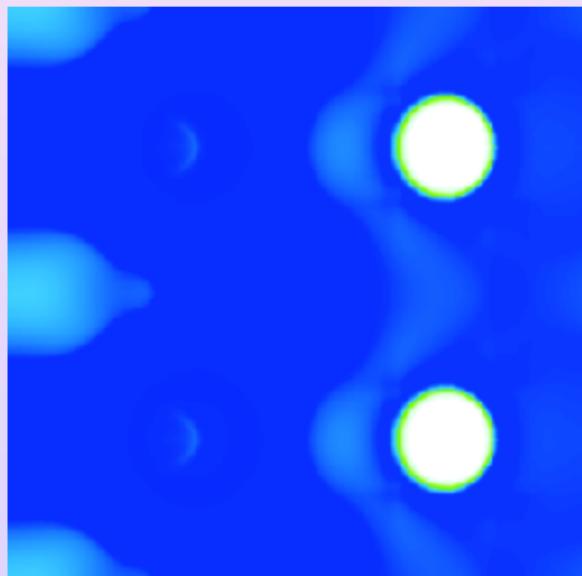
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Compression of Vapor Bubbles

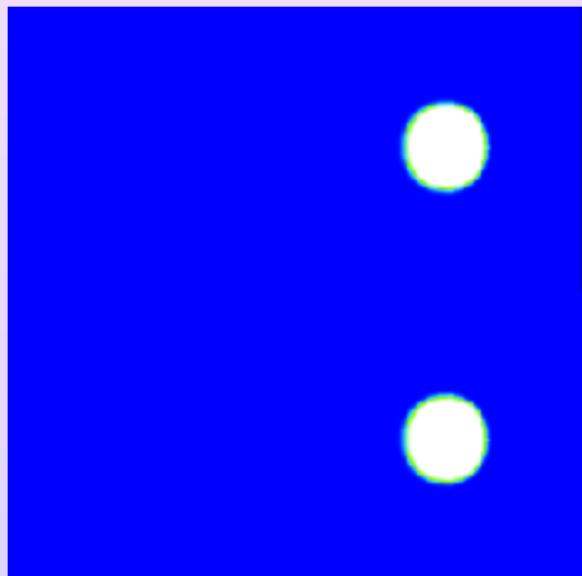
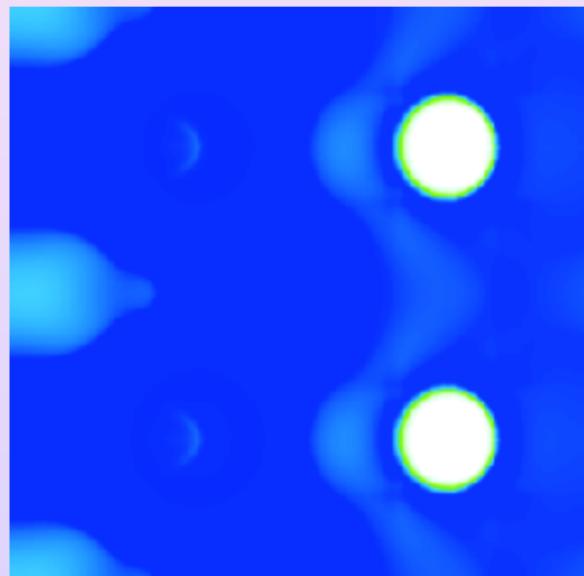
Mass Fraction y Density ρ 

◀ Geometry

▶ Play

▶ Skip

Compression of Vapor Bubbles

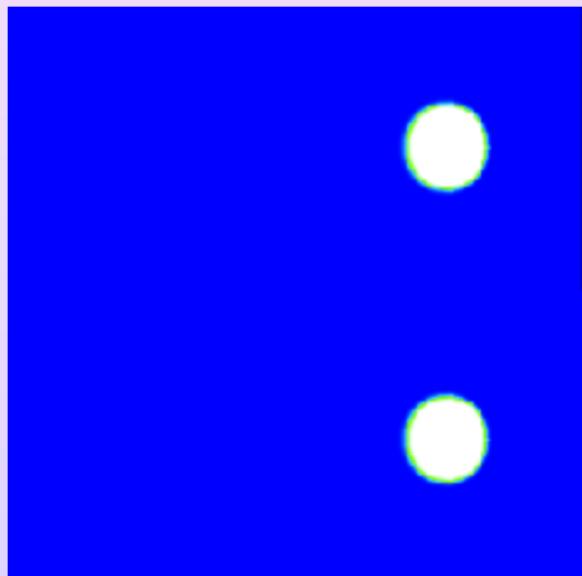
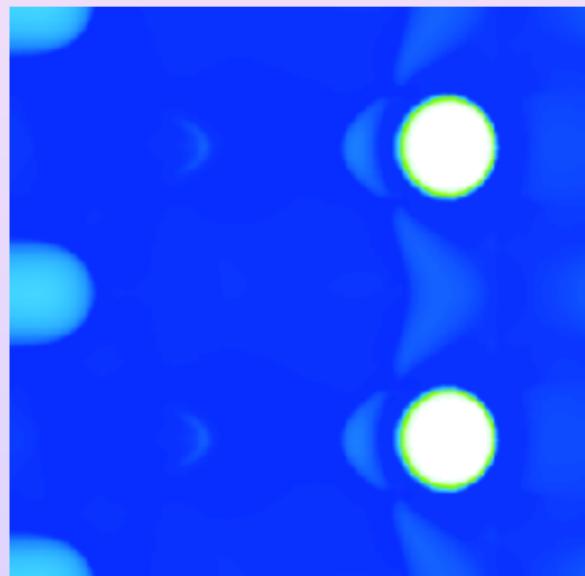
Mass Fraction y Density ρ 

◀ Geometry

▶ Play

▶ Skip

Compression of Vapor Bubbles

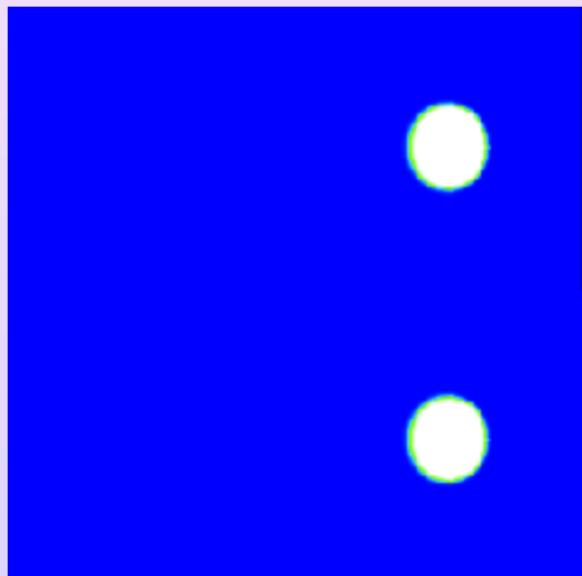
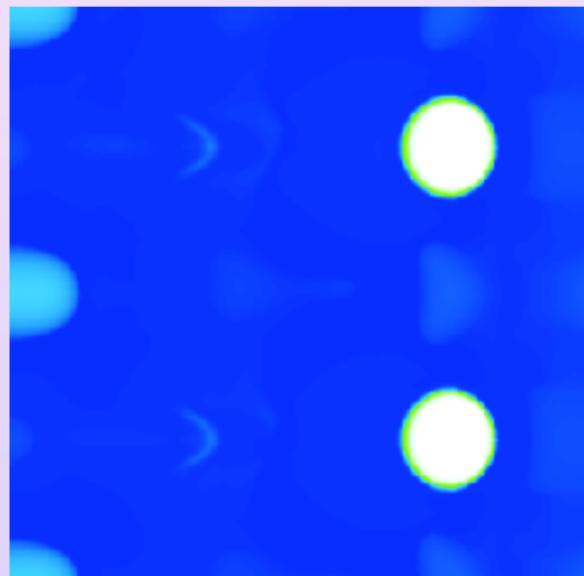
Mass Fraction y Density ρ 

◀ Geometry

▶ Play

▶ Skip

Compression of Vapor Bubbles

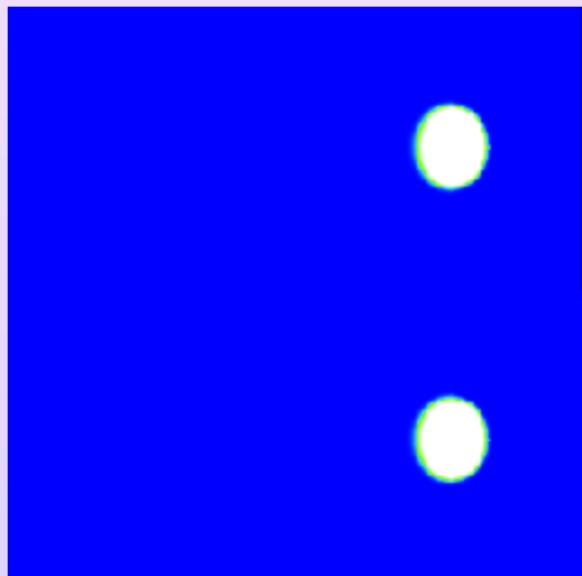
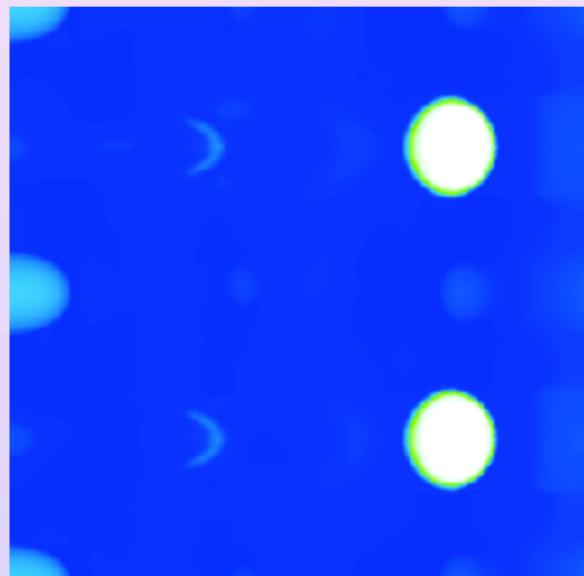
Mass Fraction y Density ρ 

◀ Geometry

▶ Play

▶ Skip

Compression of Vapor Bubbles

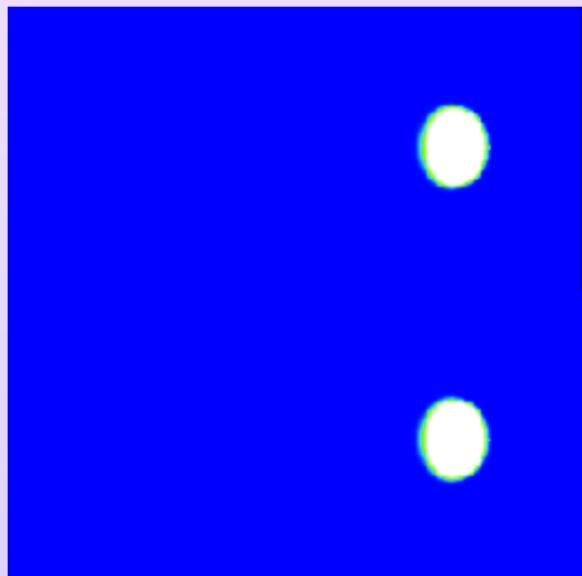
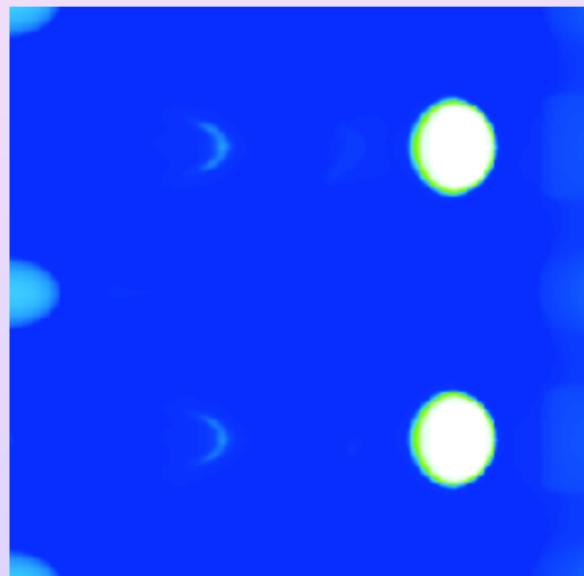
Mass Fraction y Density ρ 

◀ Geometry

▶ Play

▶ Skip

Compression of Vapor Bubbles

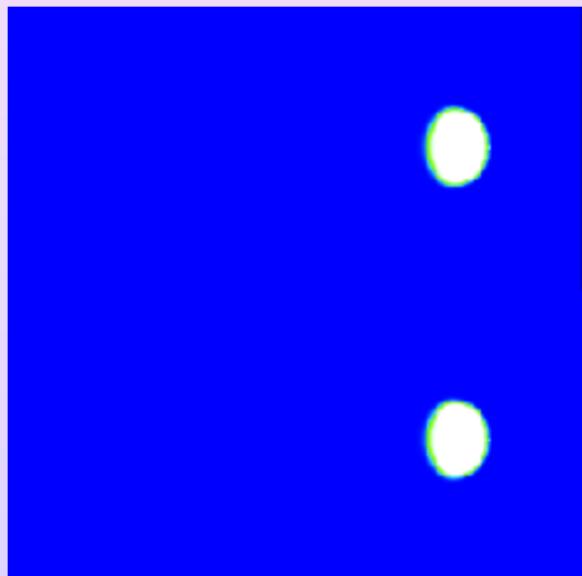
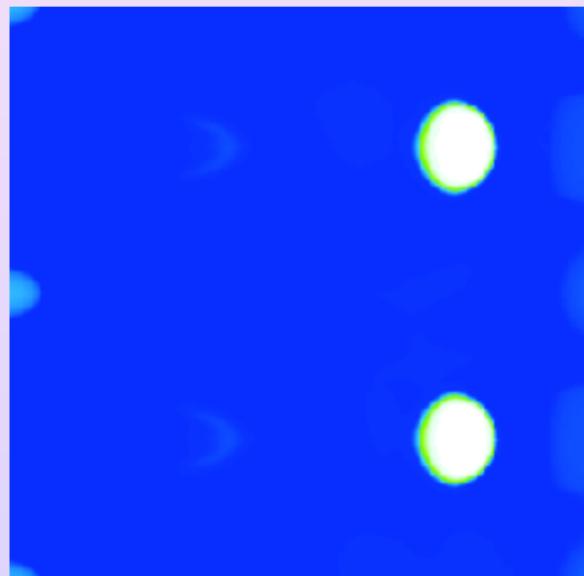
Mass Fraction y Density ρ 

◀ Geometry

▶ Play

▶ Skip

Compression of Vapor Bubbles

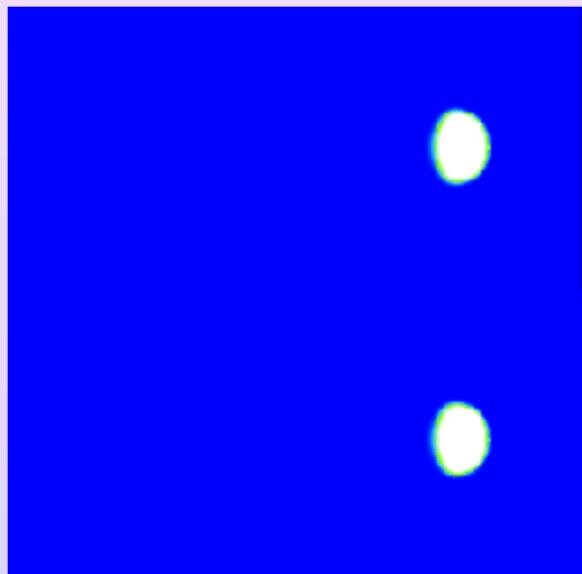
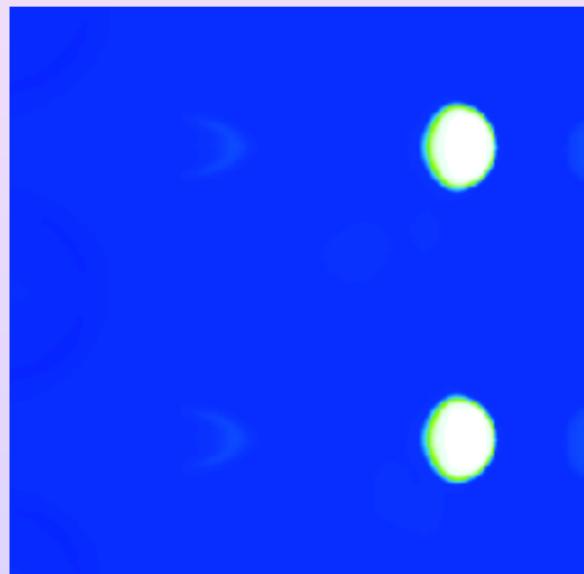
Mass Fraction y Density ρ 

◀ Geometry

▶ Play

▶ Skip

Compression of Vapor Bubbles

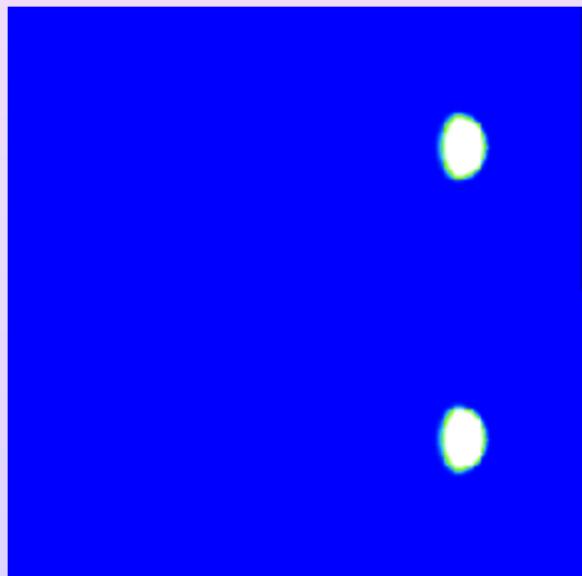
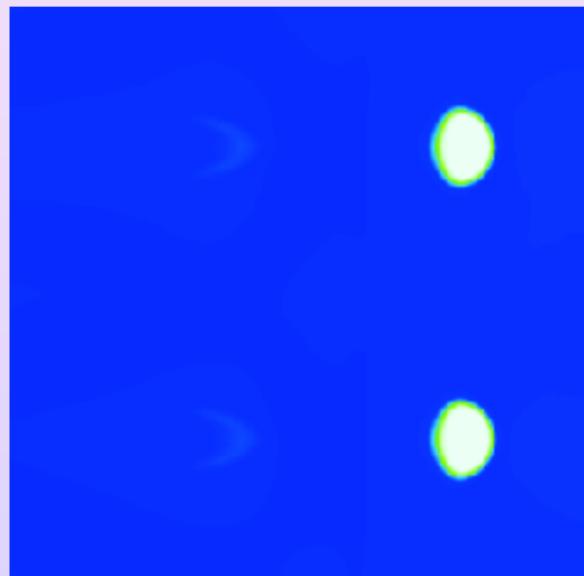
Mass Fraction y Density ρ 

◀ Geometry

▶ Play

▶ Skip

Compression of Vapor Bubbles

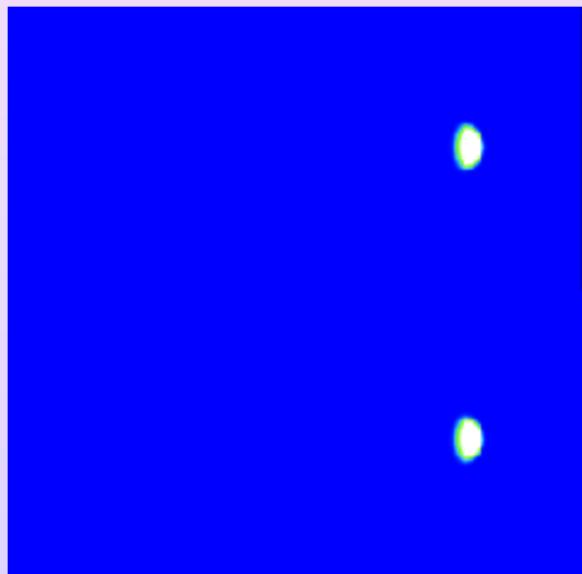
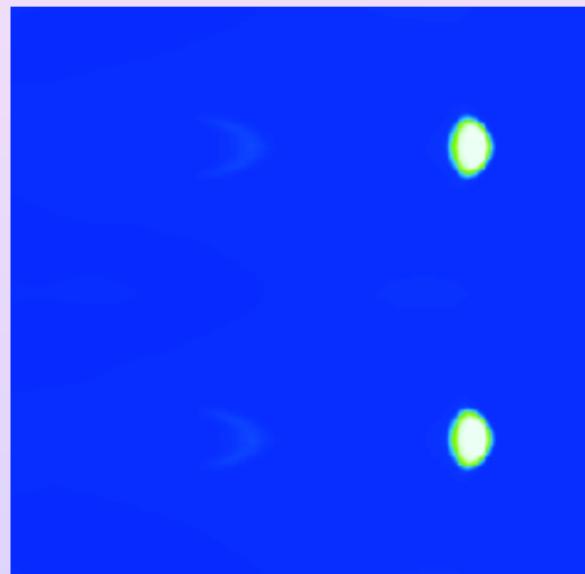
Mass Fraction y Density ρ 

◀ Geometry

▶ Play

▶ Skip

Compression of Vapor Bubbles

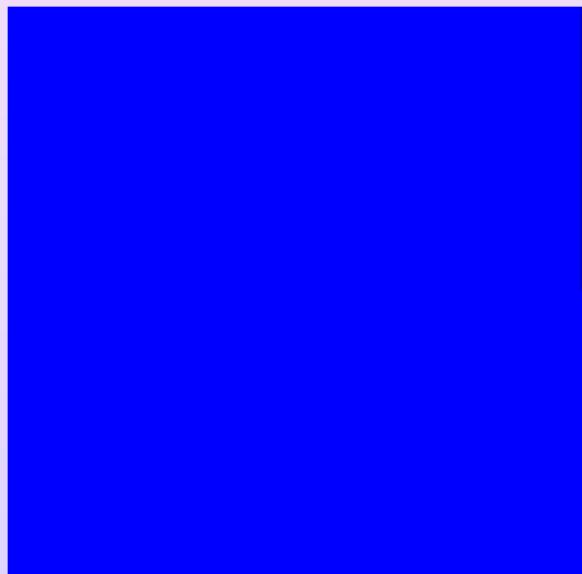
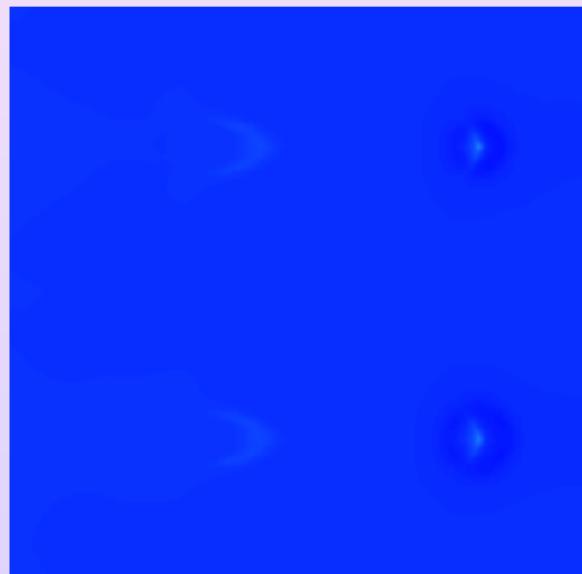
Mass Fraction y Density ρ 

◀ Geometry

▶ Play

▶ Skip

Compression of Vapor Bubbles

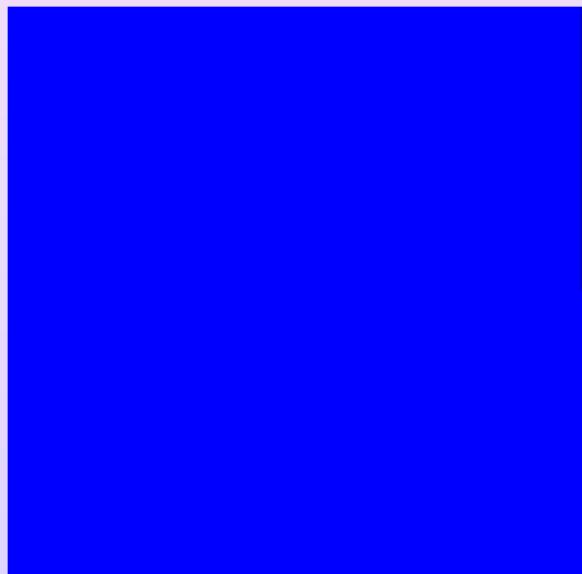
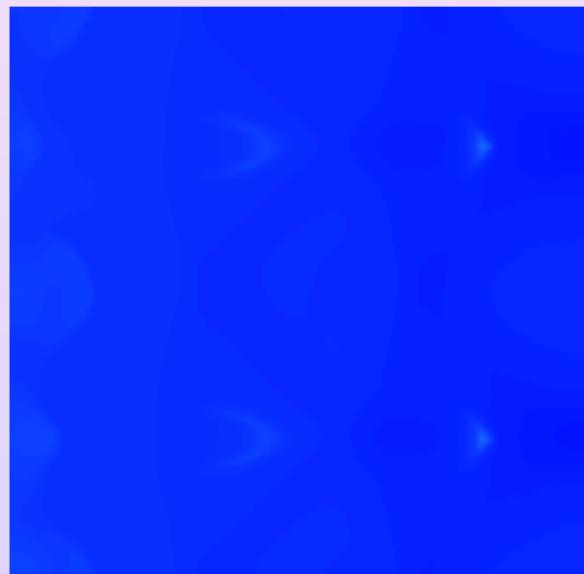
Mass Fraction y Density ρ 

◀ Geometry

▶ Play

▶ Skip

Compression of Vapor Bubbles

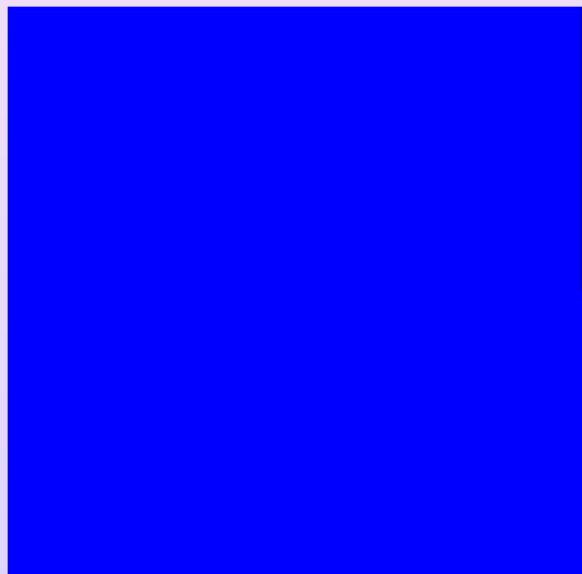
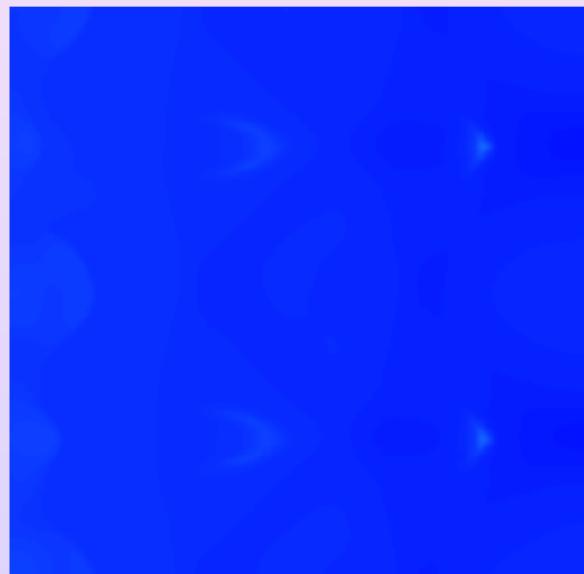
Mass Fraction y Density ρ 

◀ Geometry

▶ Play

▶ Skip

Compression of Vapor Bubbles

Mass Fraction y Density ρ 

◀ Geometry

▶ Play

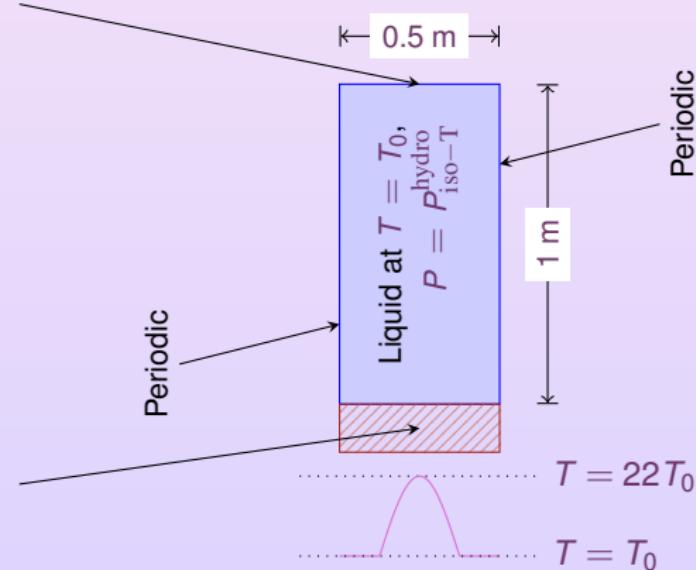
▶ Skip

Nucleating Bubble

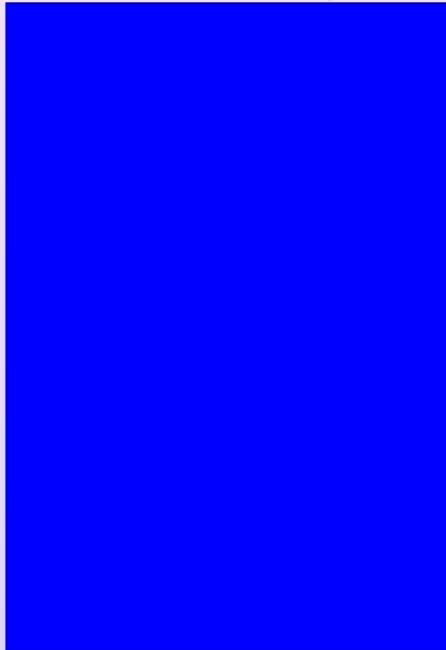
Pressure and
temperature
imposed

$$P = P^{\text{ref}} > P^{\text{sat}}(T_0), \\ T = T_0$$

Wall,
temperature imposed



Nucleating Bubble

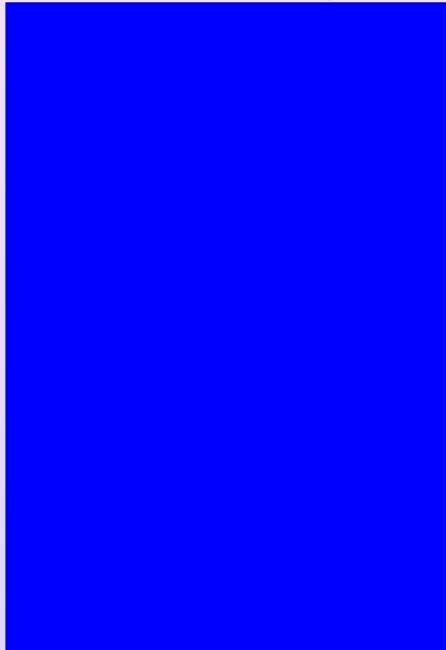
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

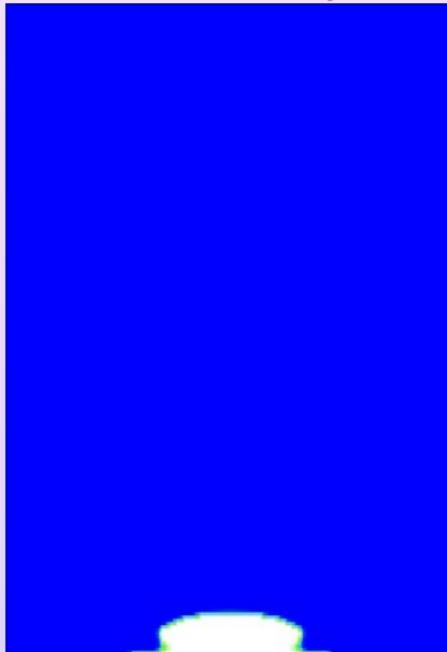
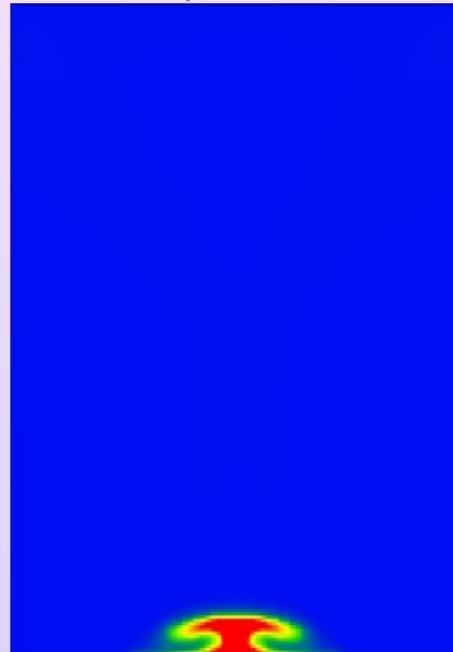
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

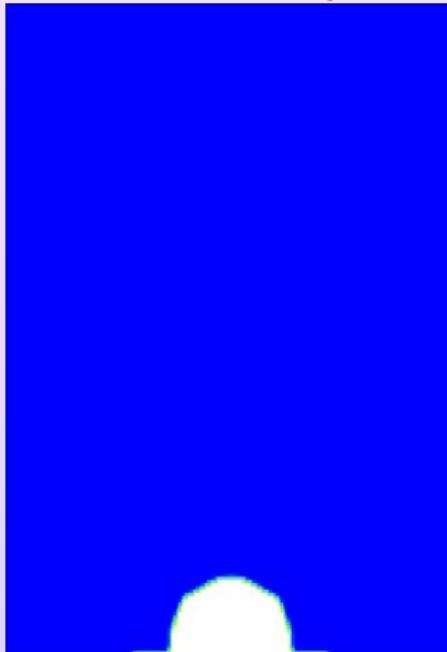
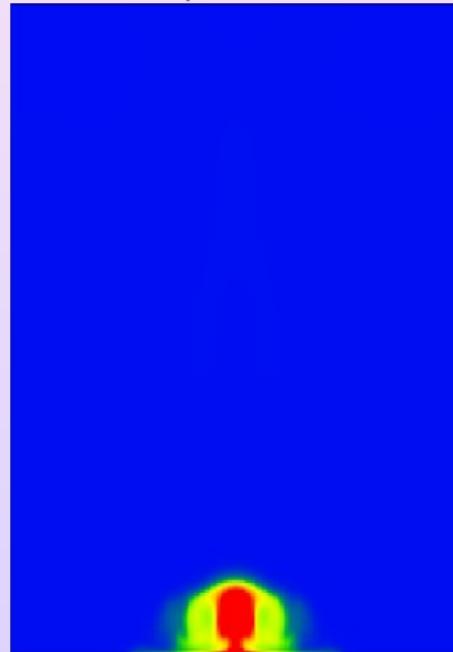
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

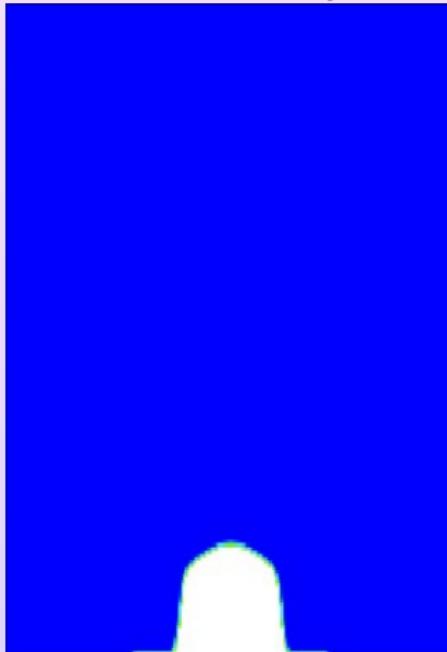
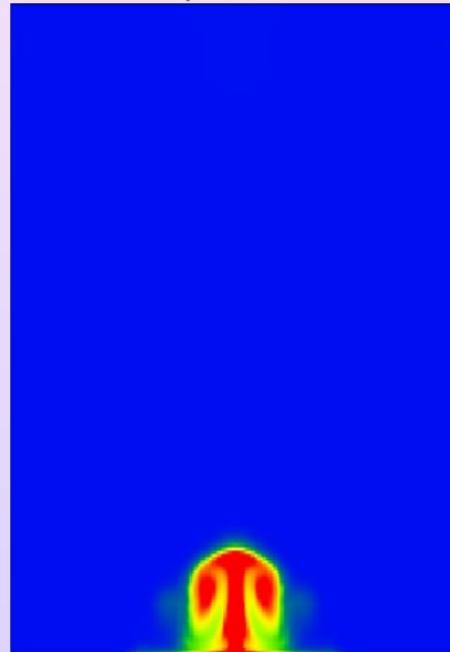
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

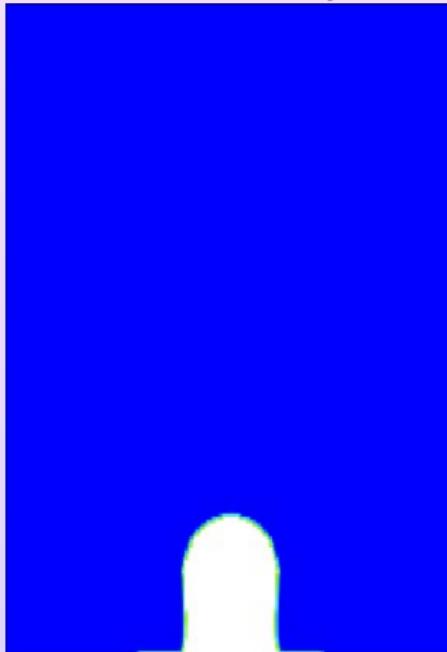
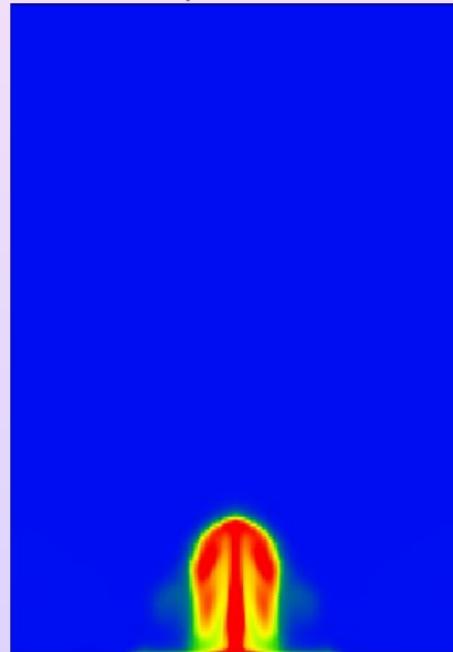
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

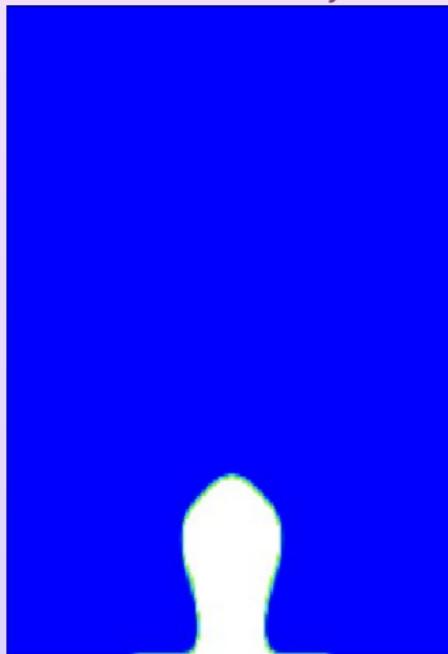
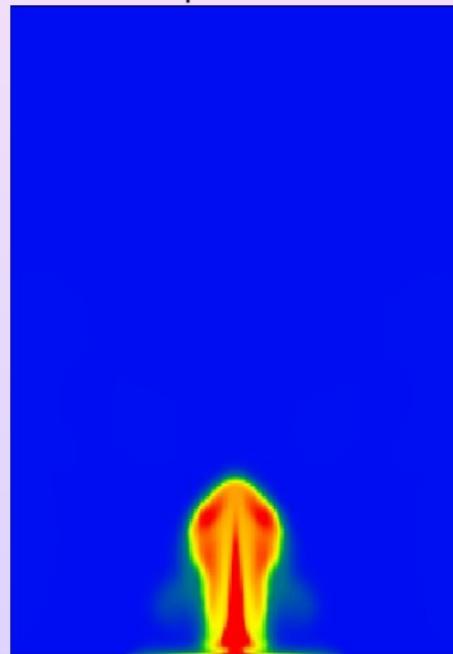
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

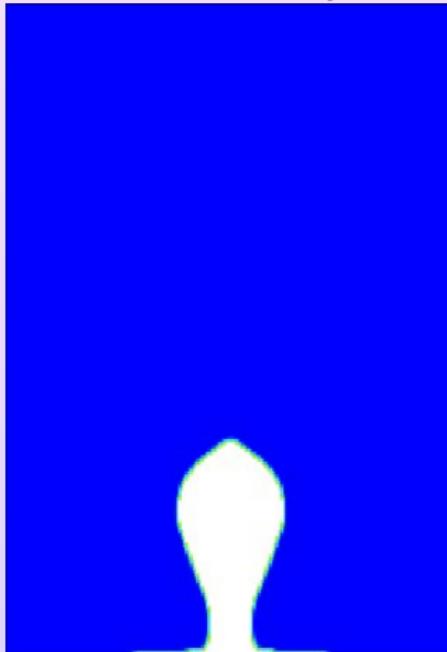
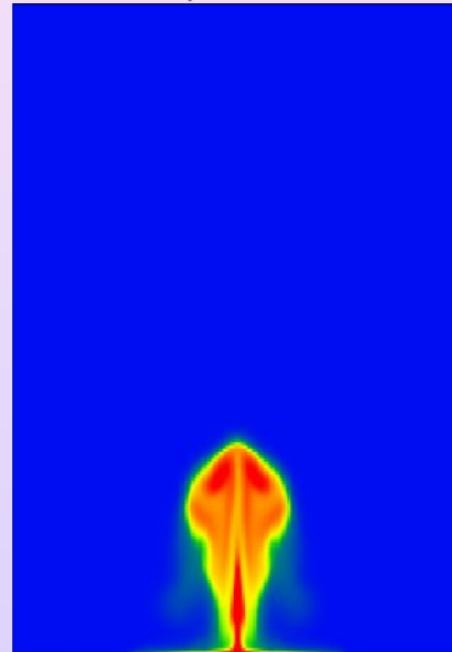
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

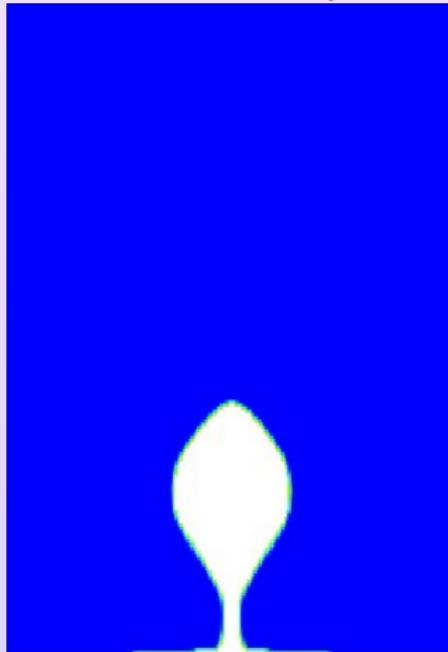
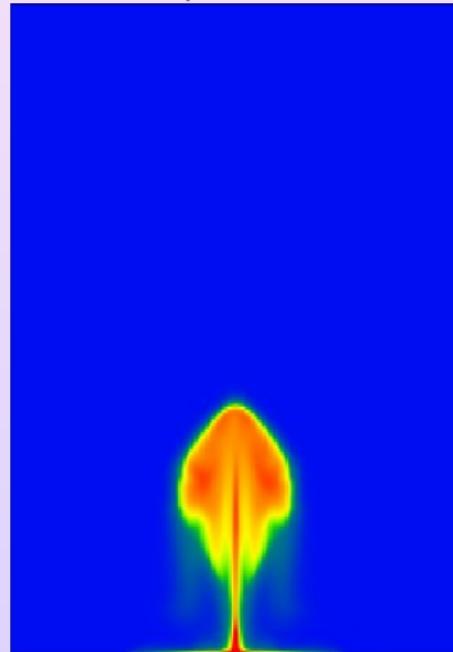
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

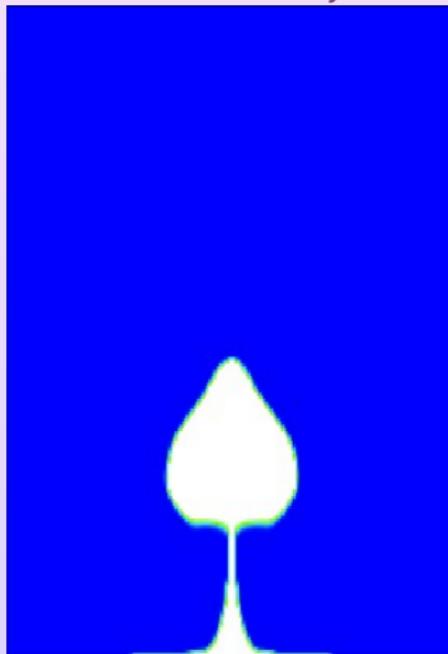
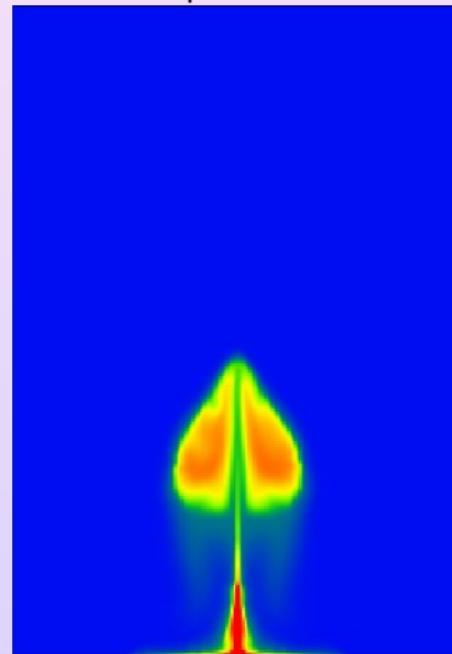
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

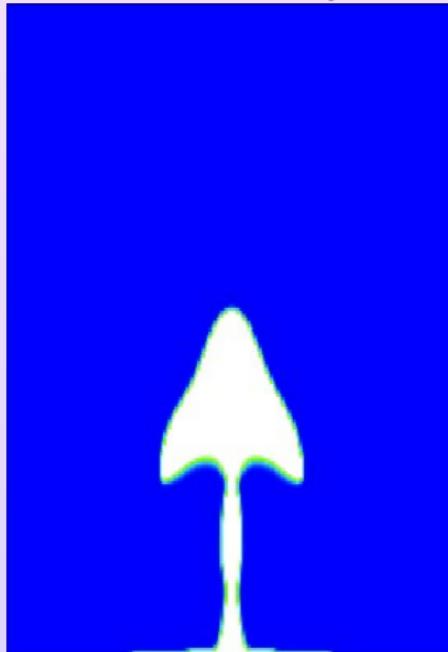
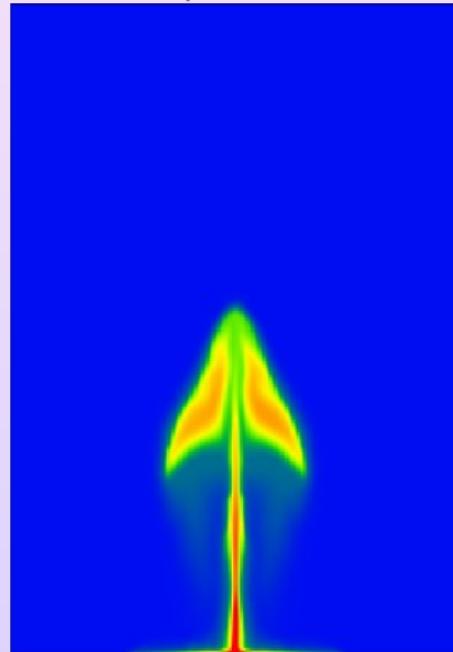
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

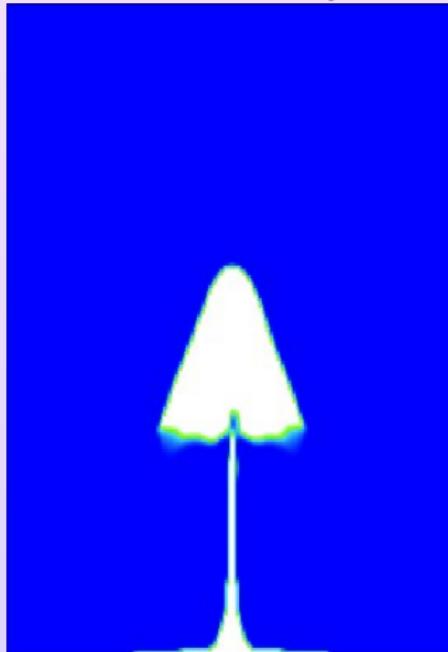
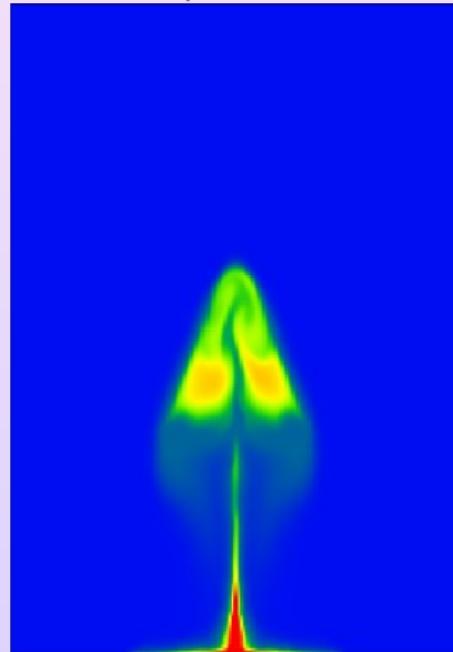
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

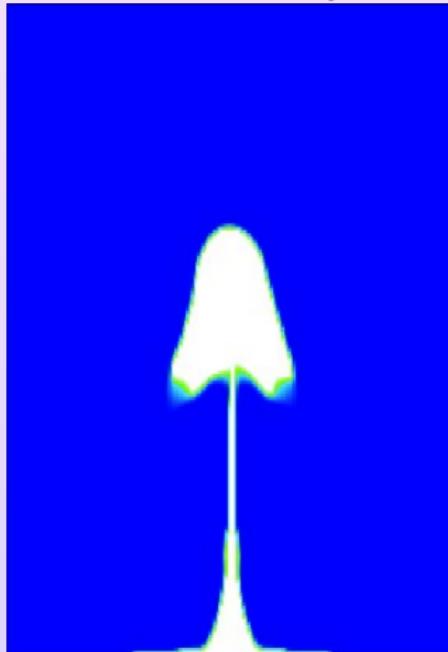
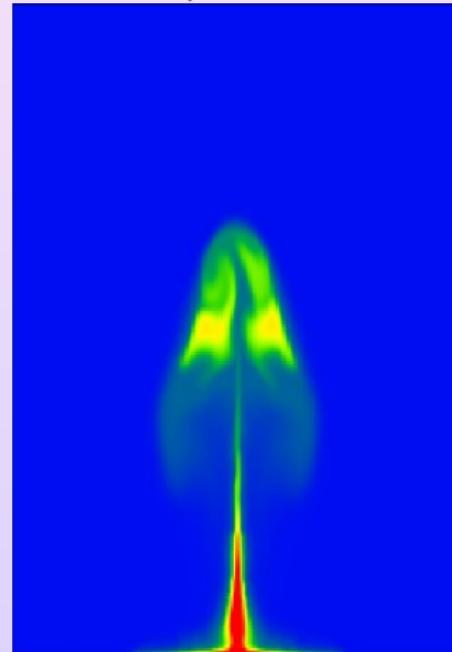
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

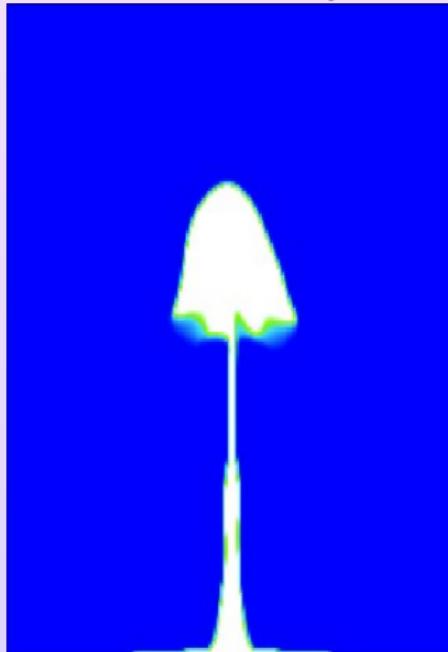
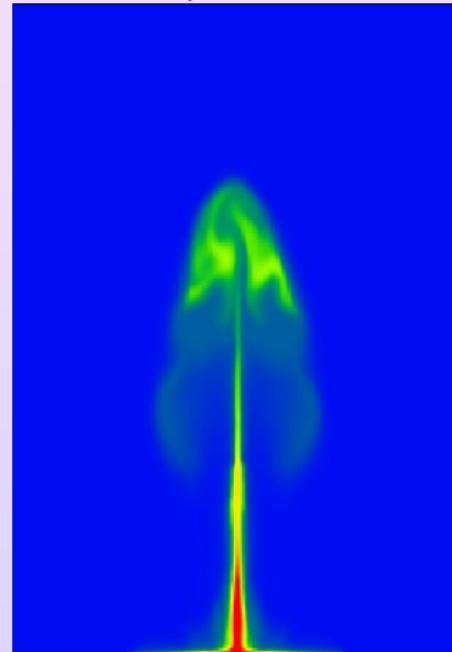
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

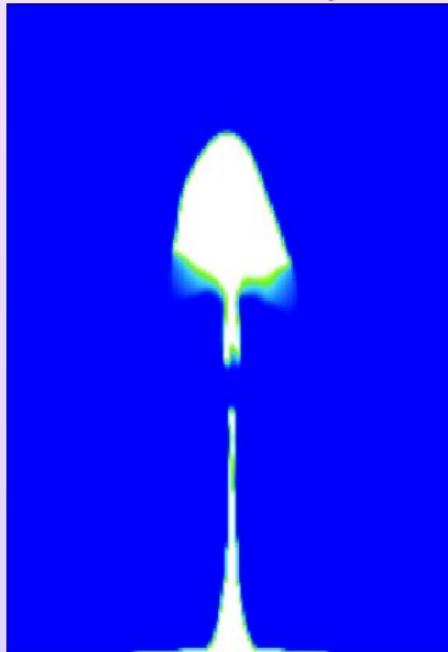
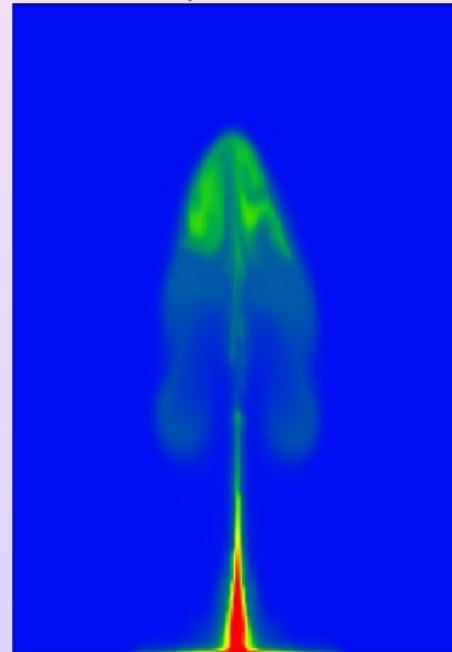
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

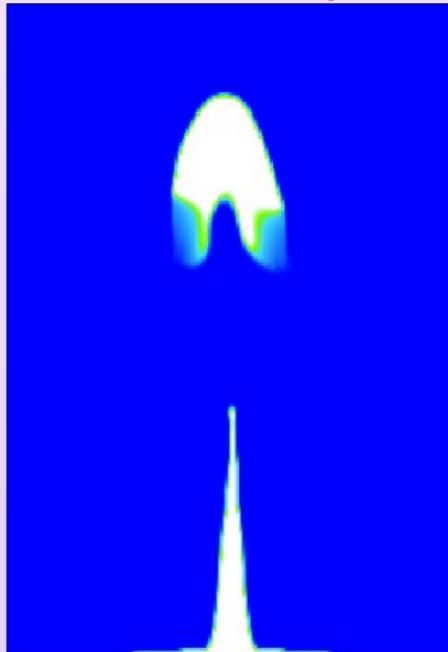
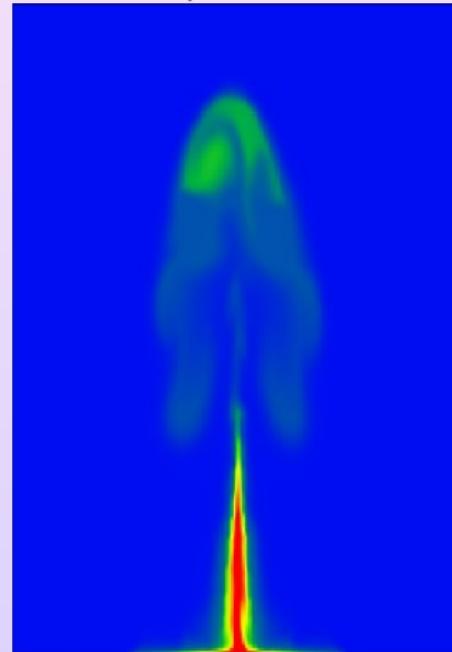
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

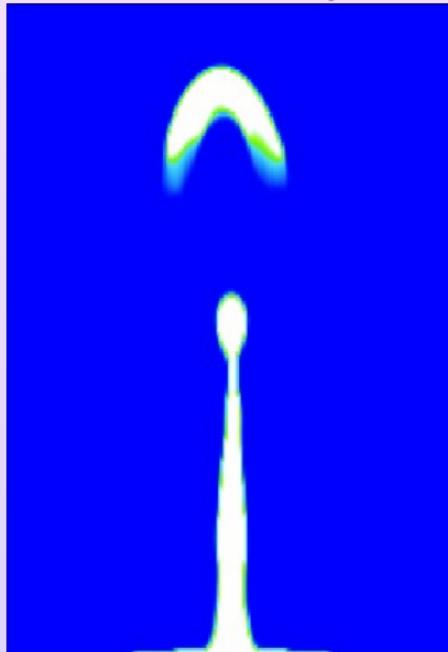
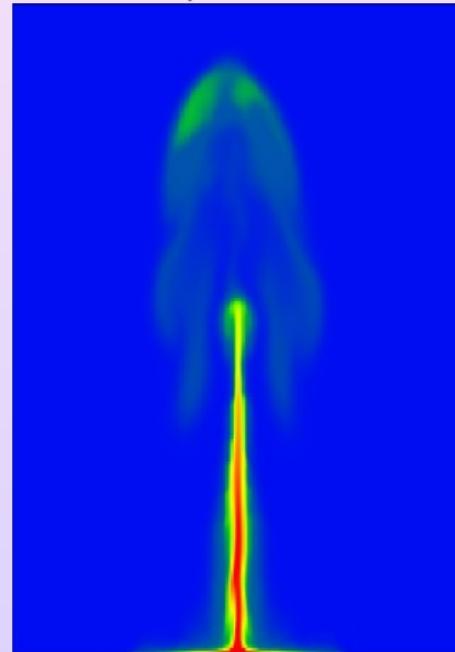
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

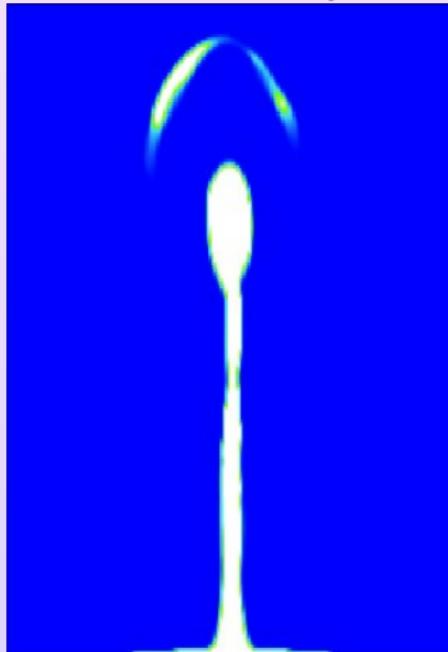
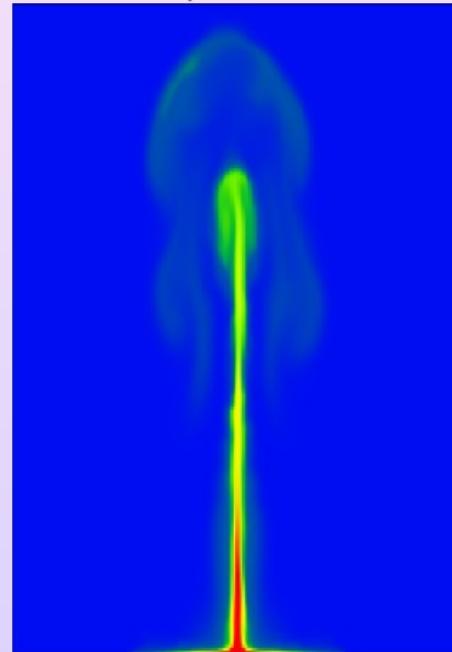
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

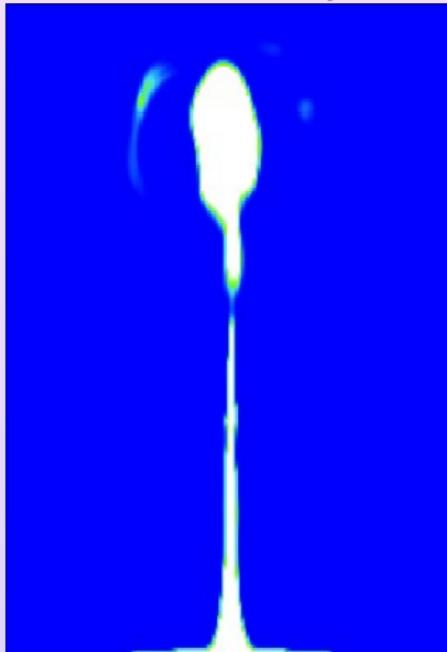
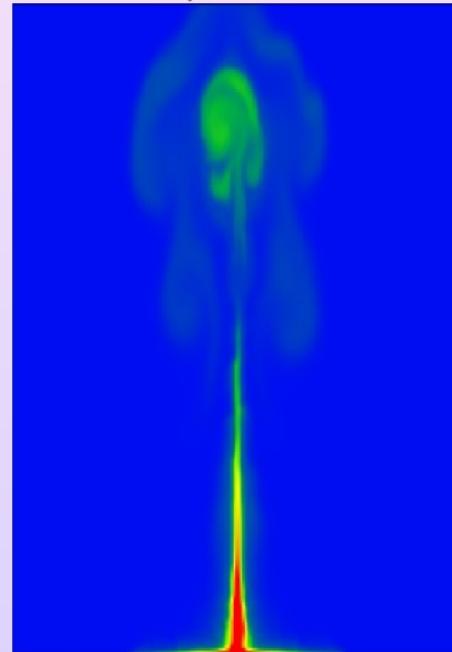
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

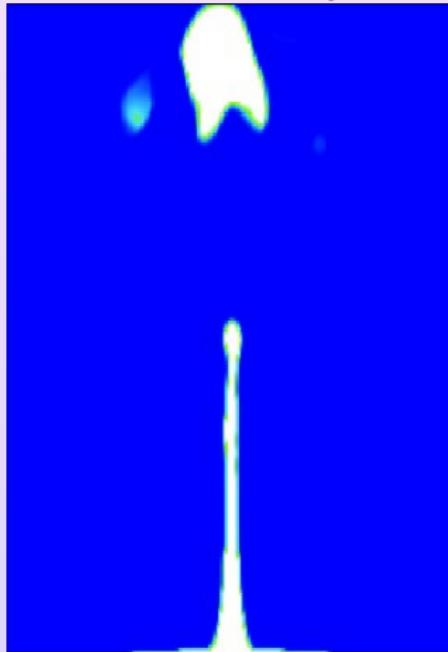
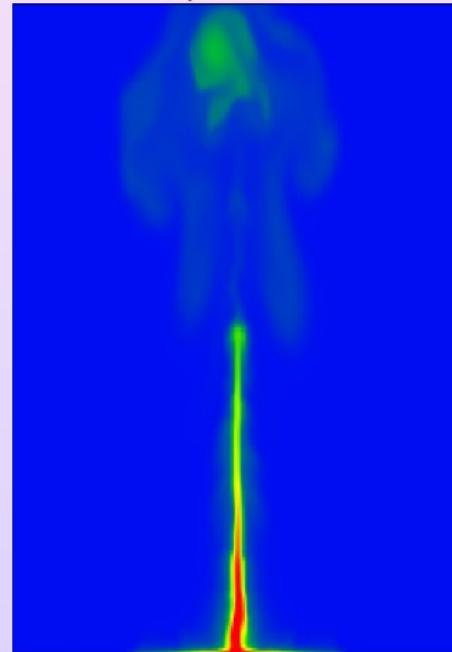
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

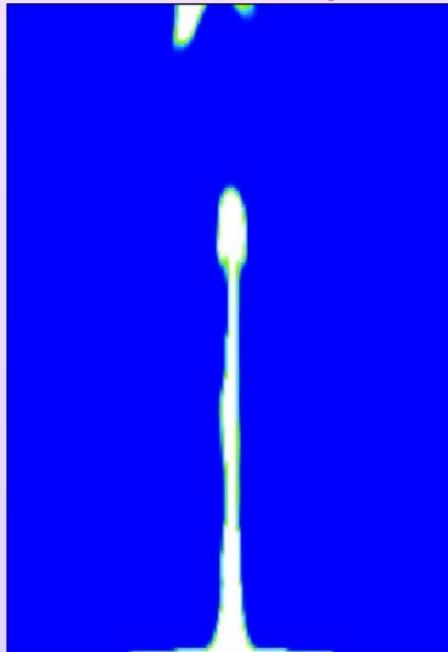
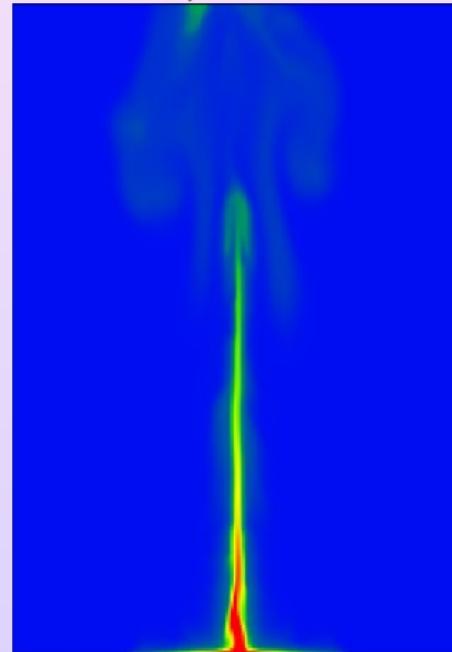
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

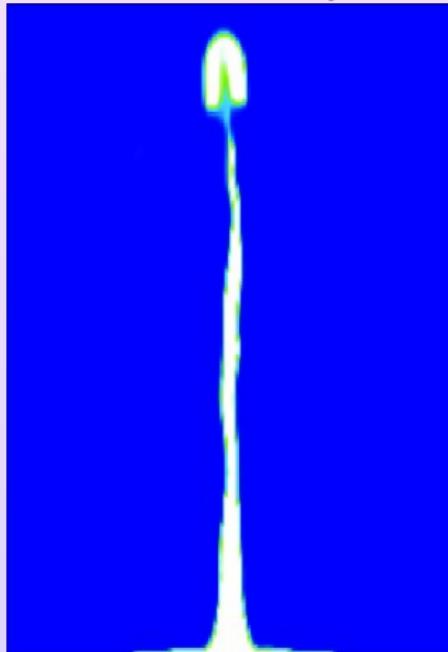
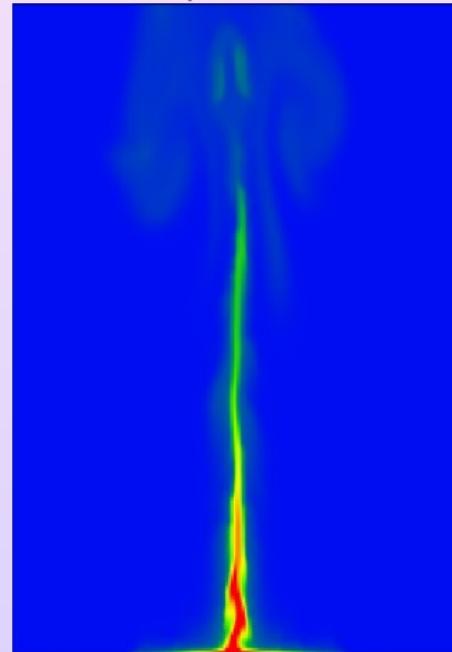
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

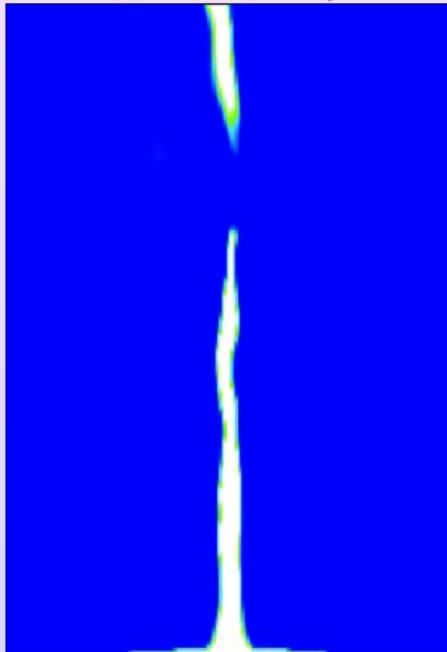
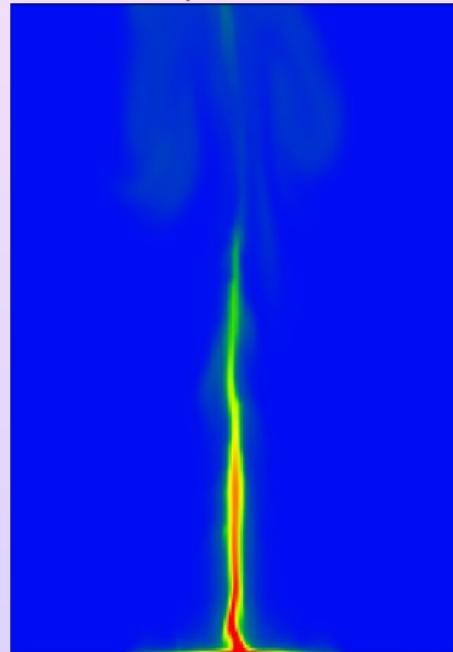
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

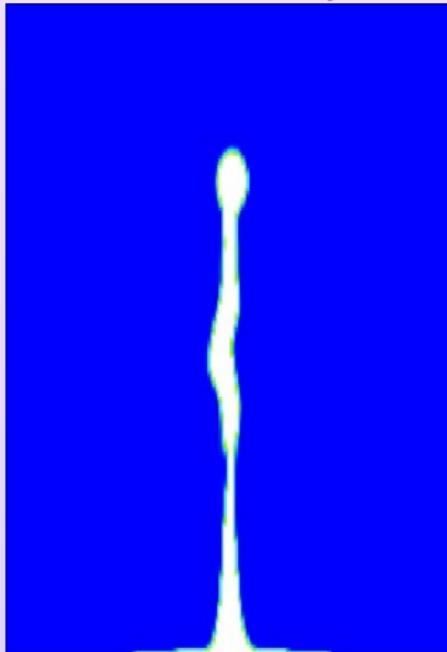
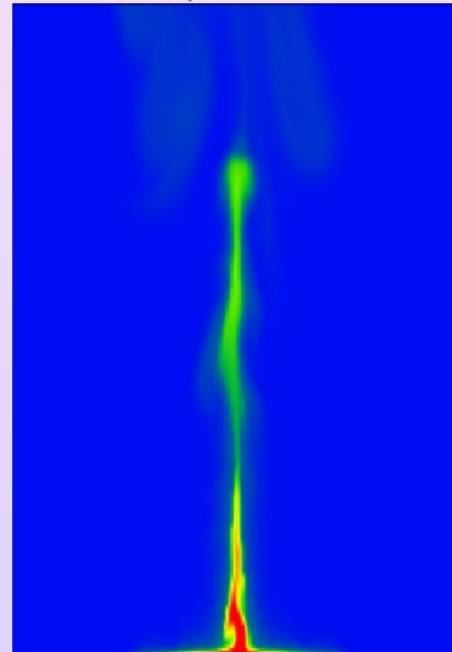
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

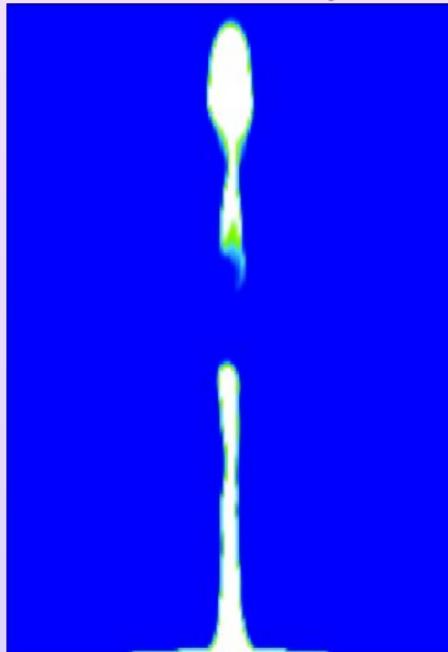
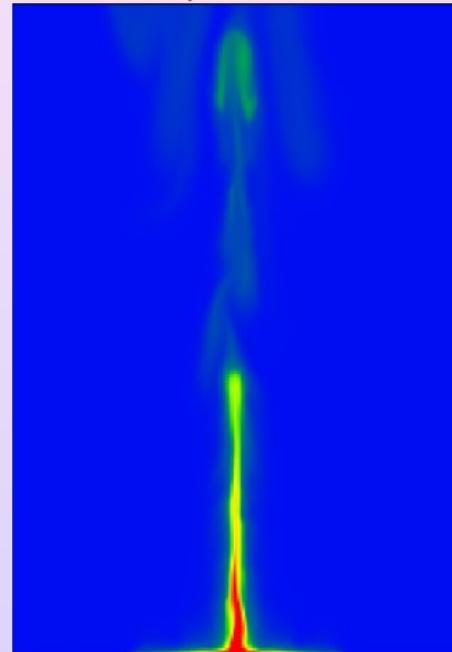
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

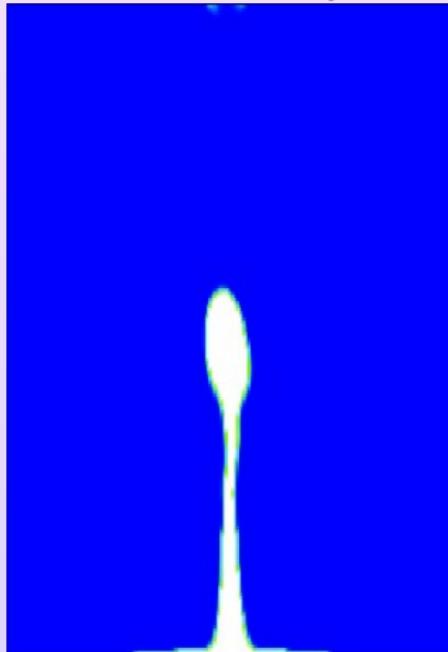
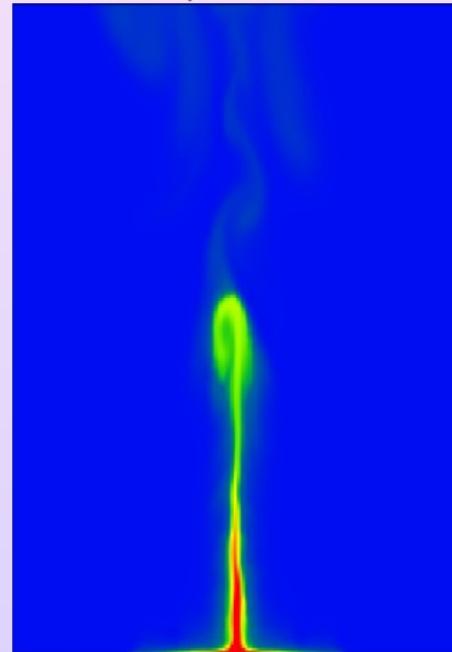
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

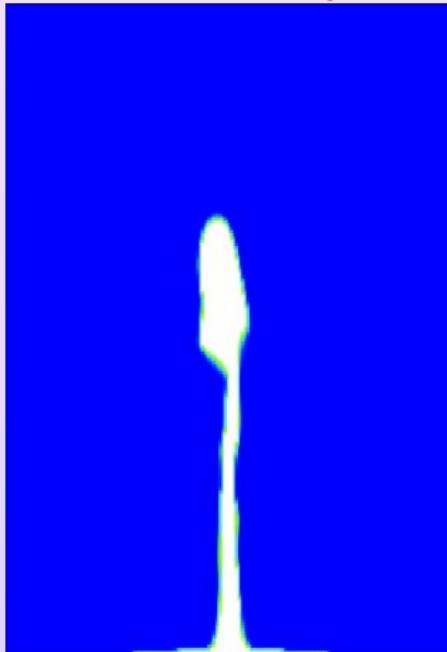
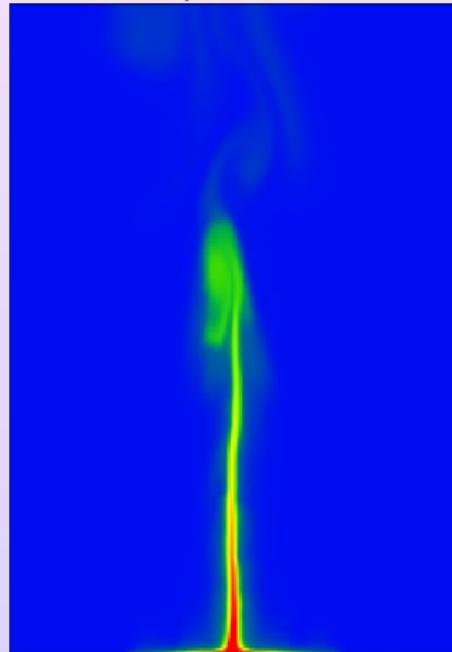
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

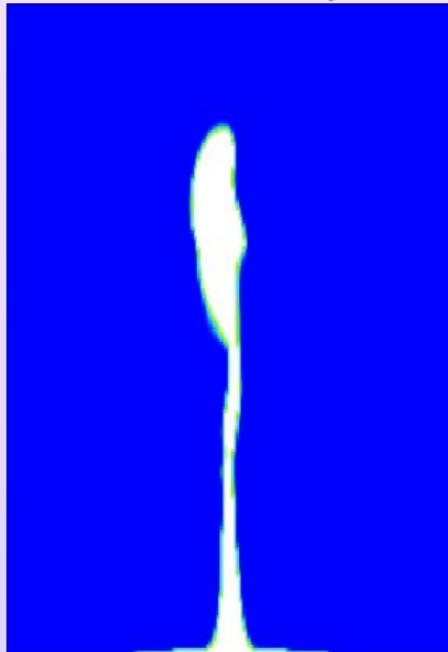
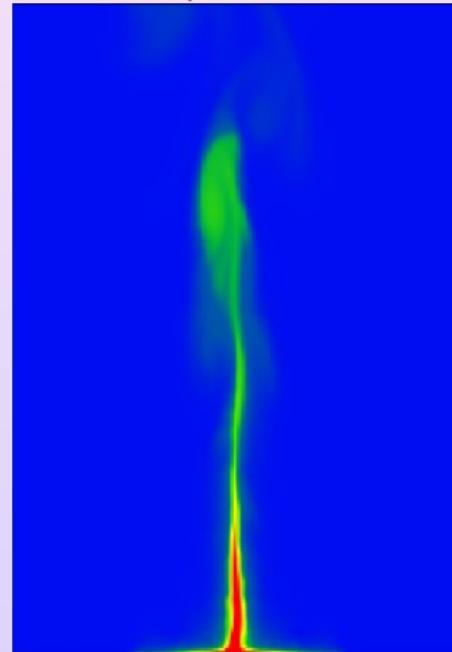
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

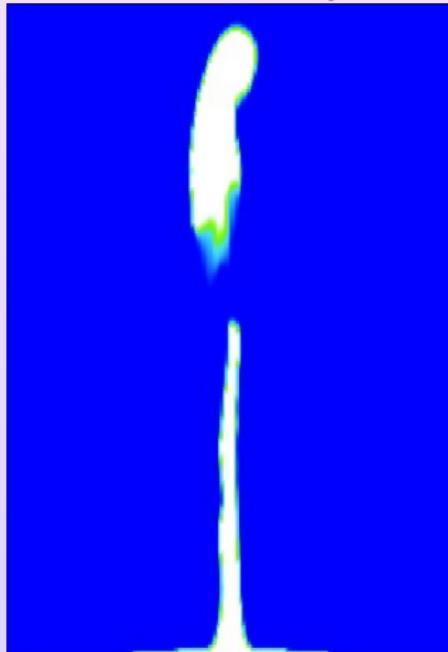
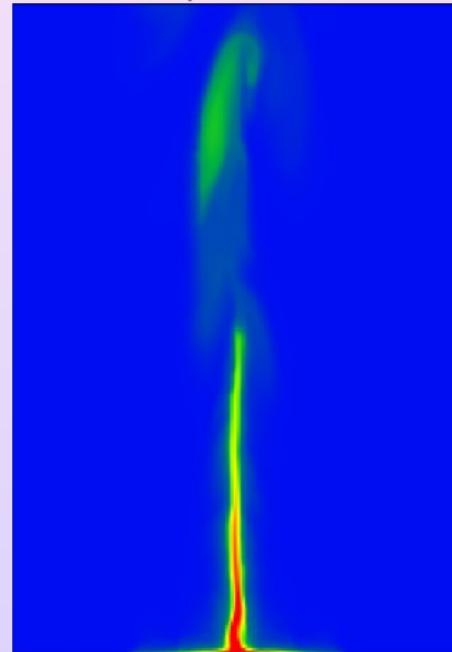
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

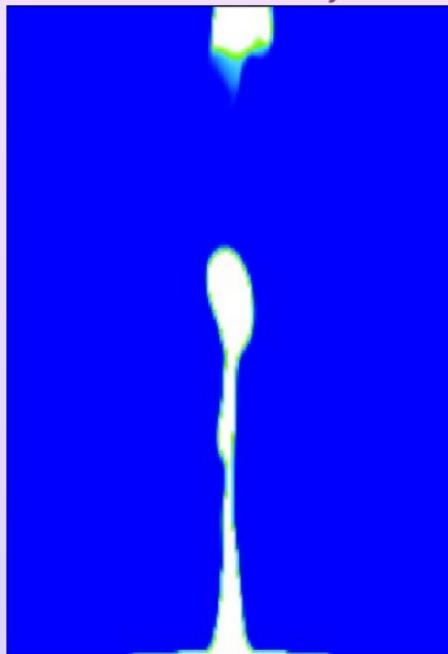
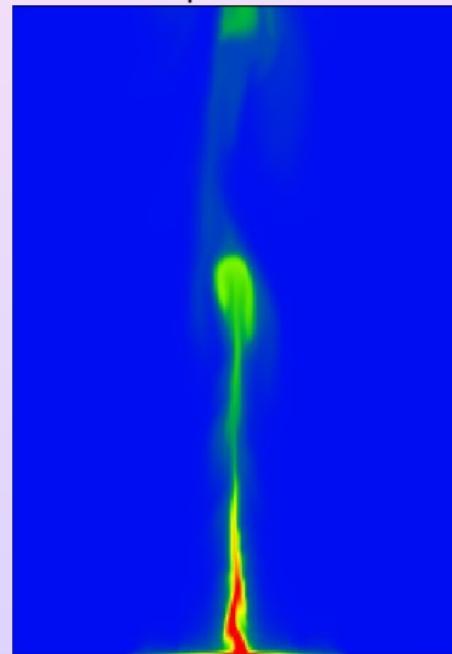
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

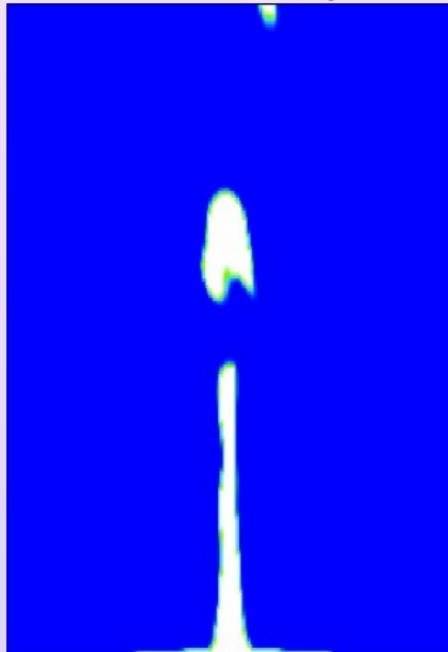
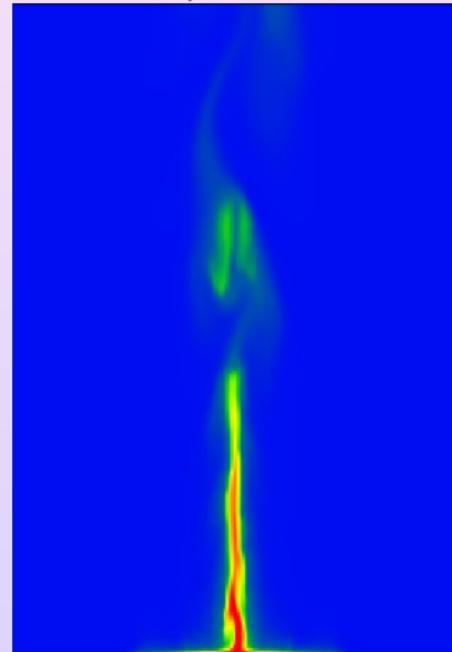
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

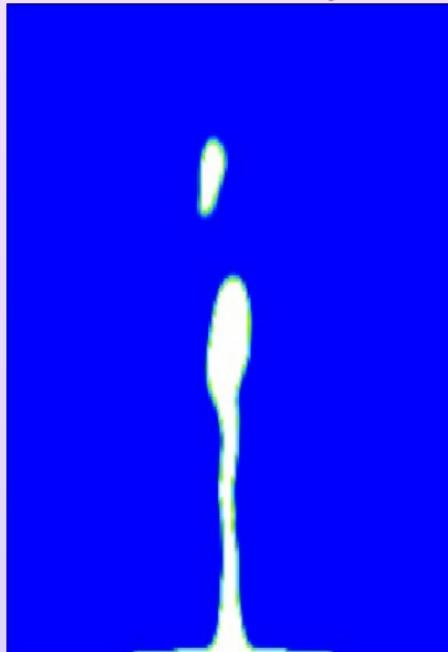
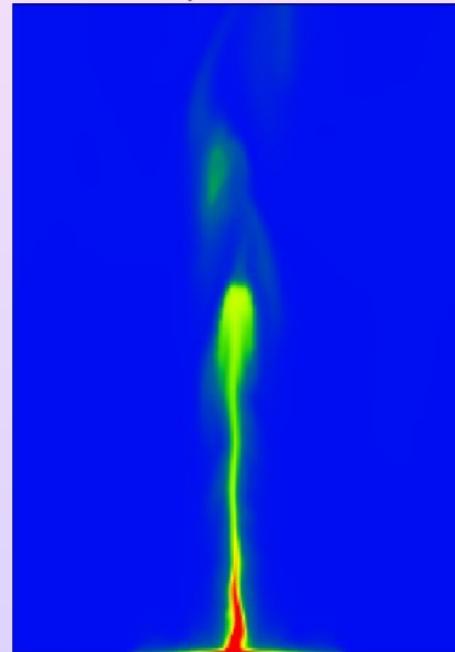
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

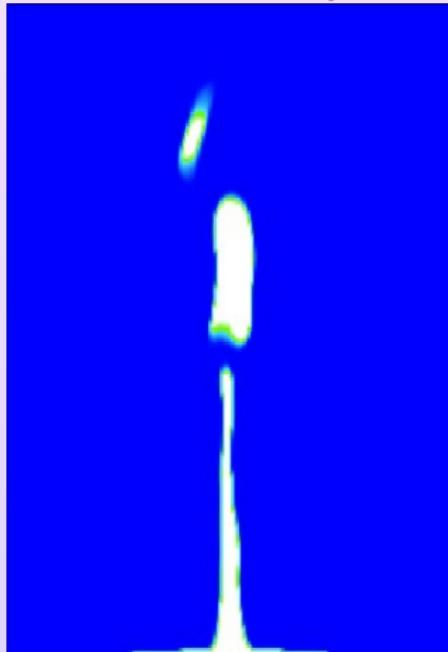
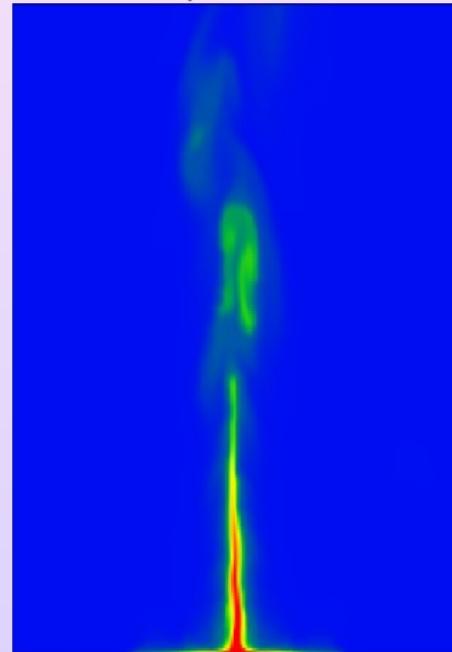
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

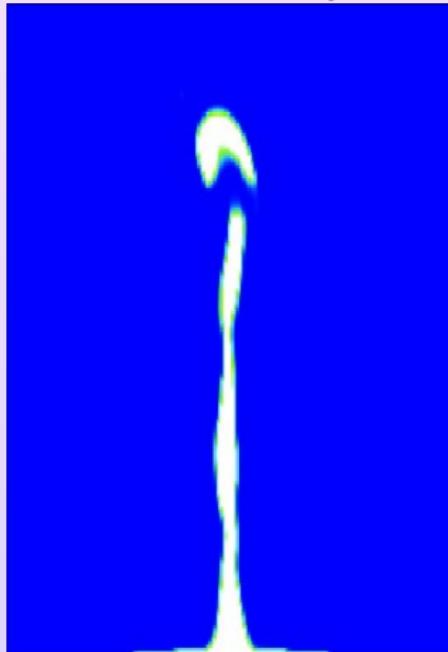
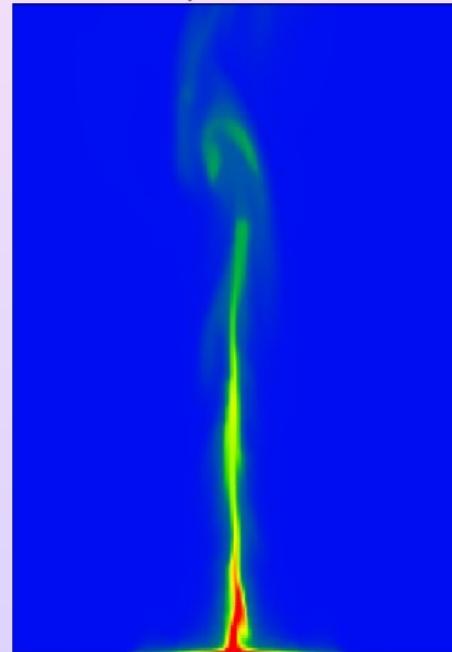
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

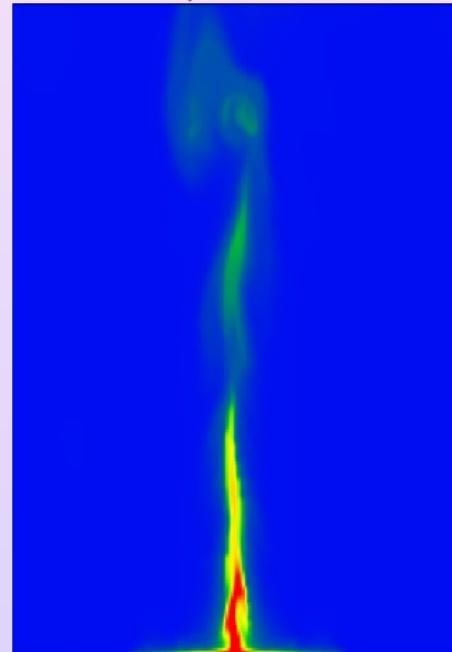
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

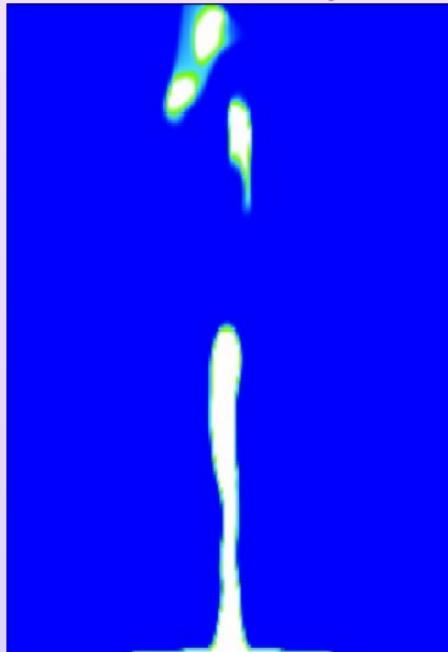
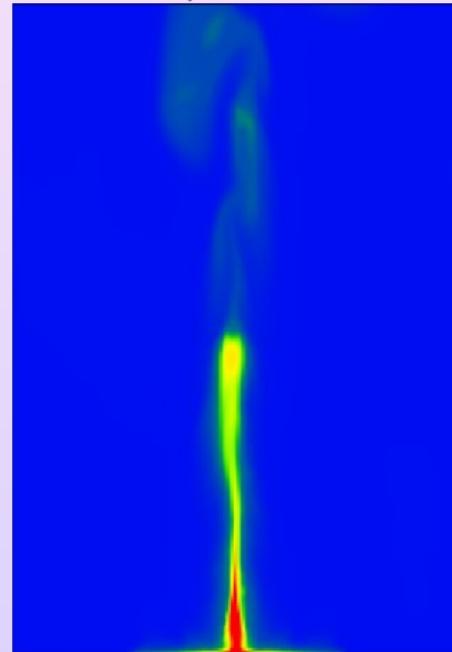
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

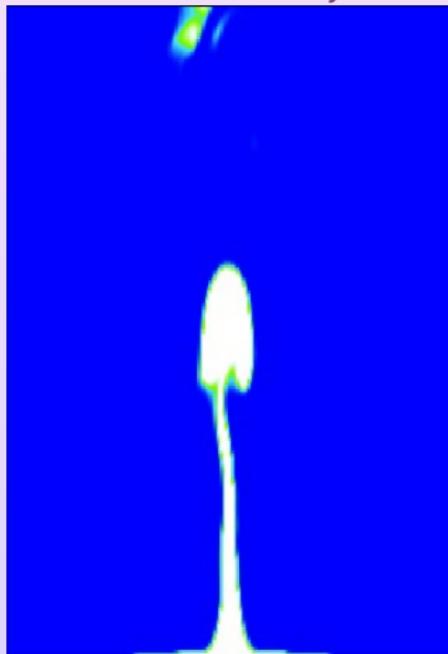
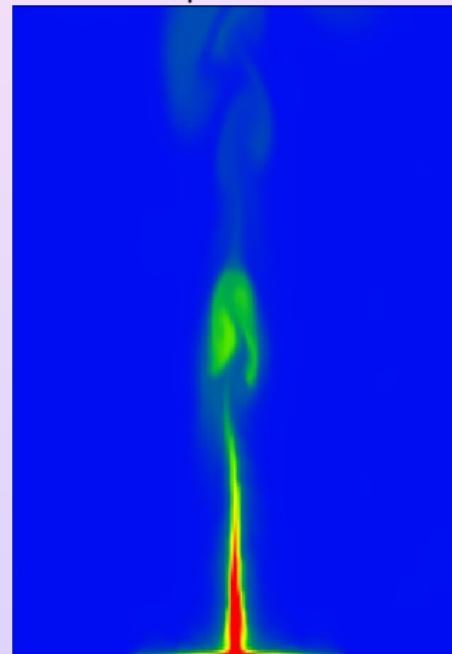
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

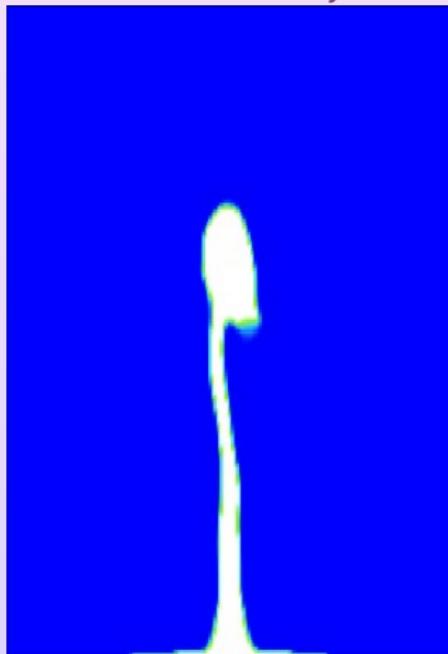
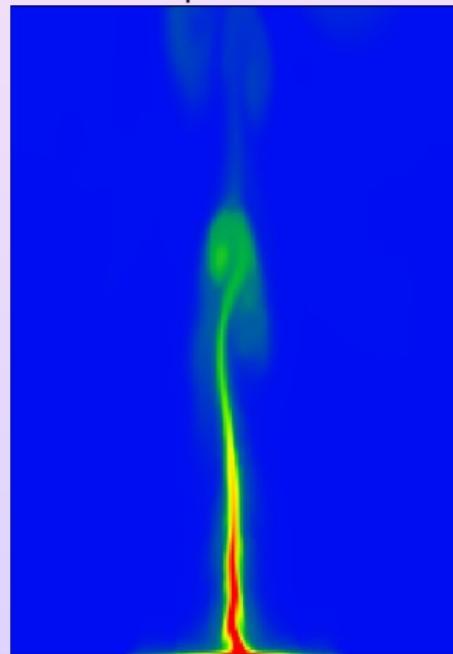
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

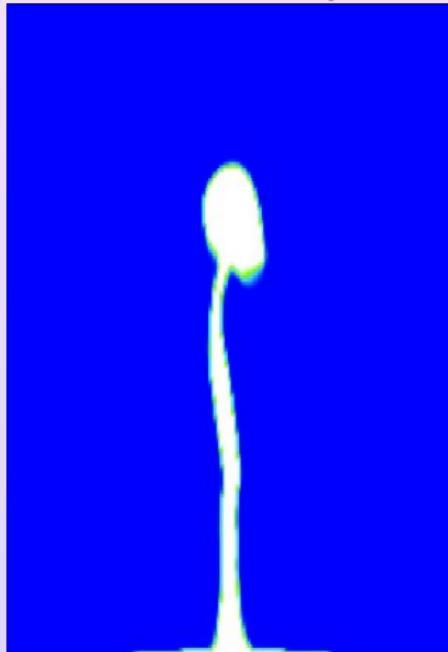
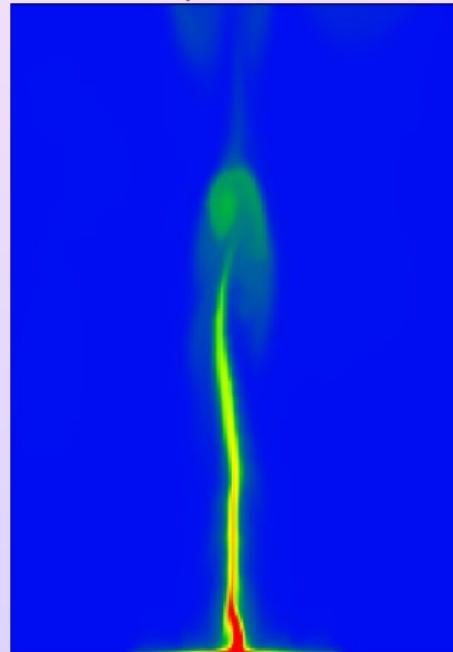
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

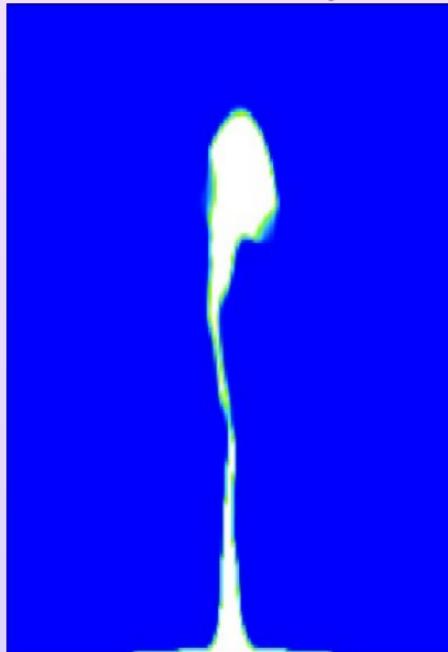
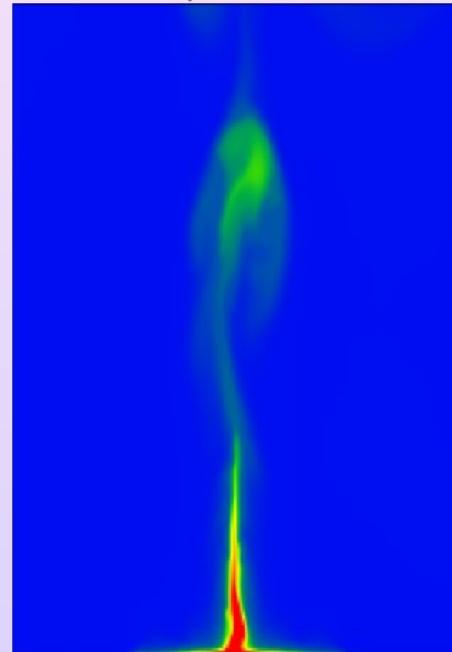
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

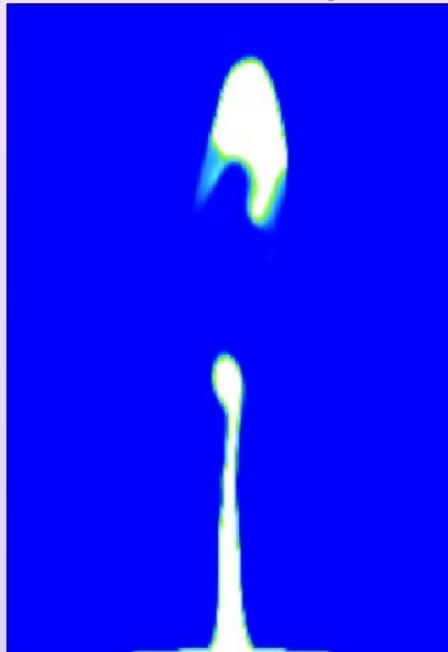
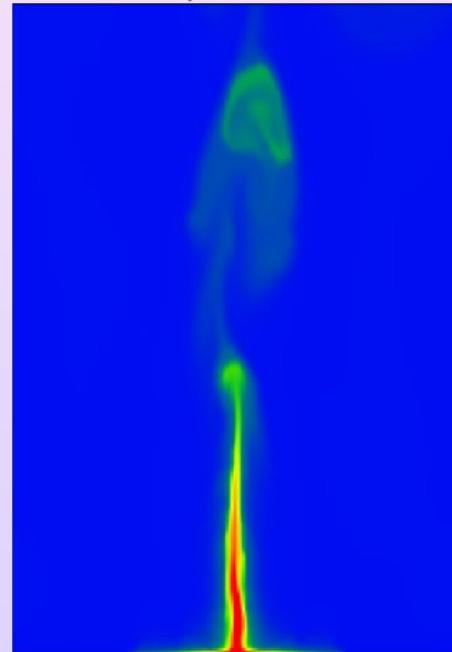
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

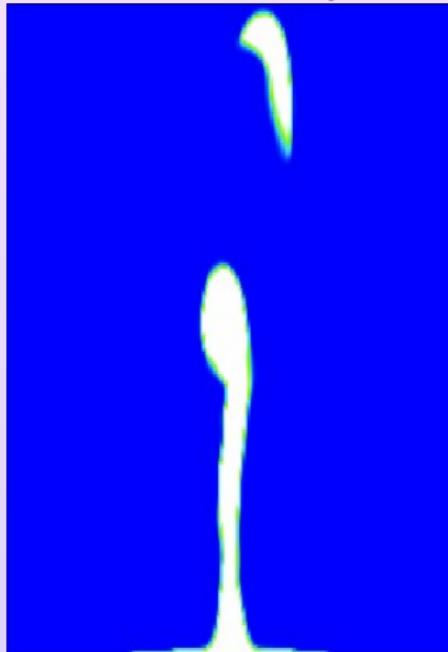
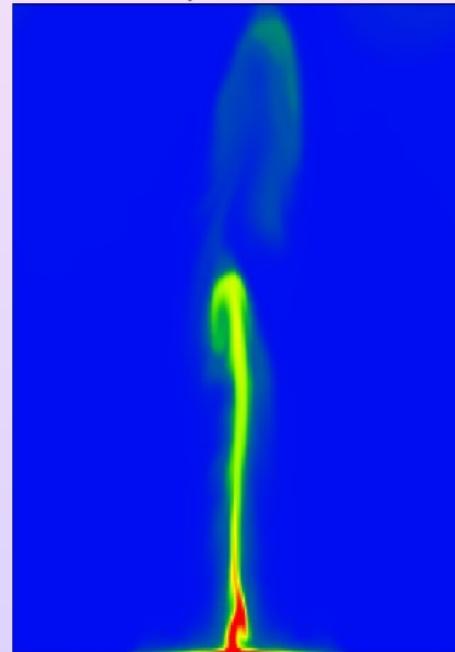
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

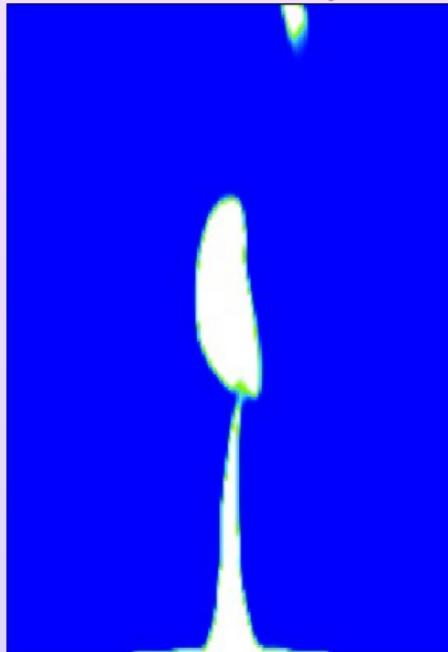
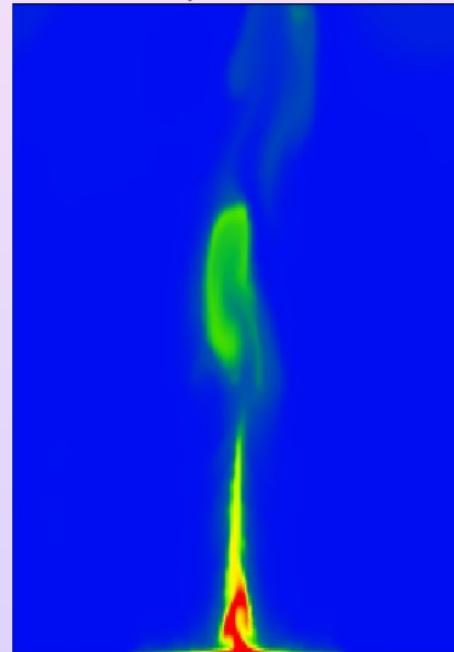
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

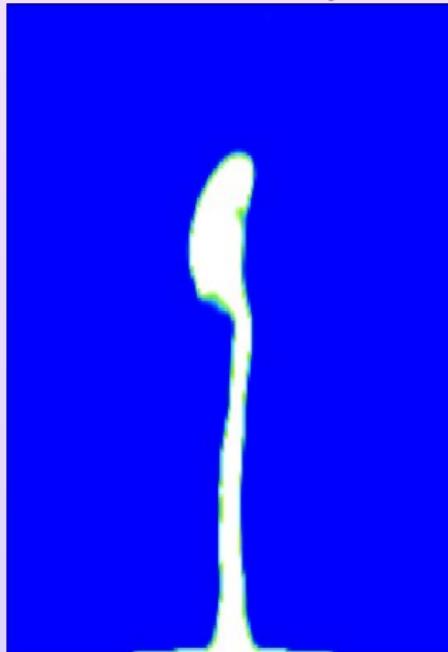
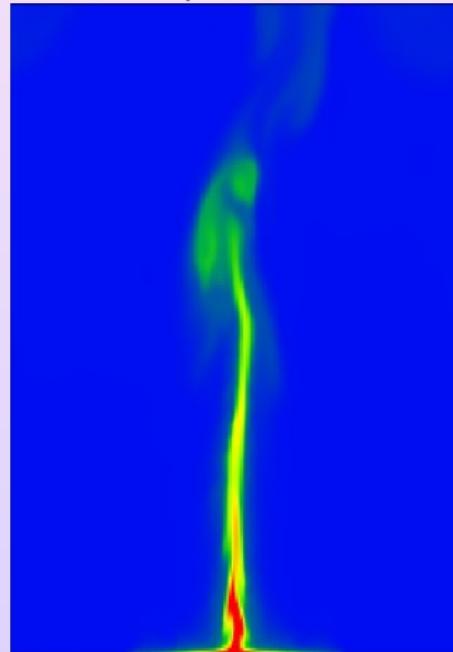
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

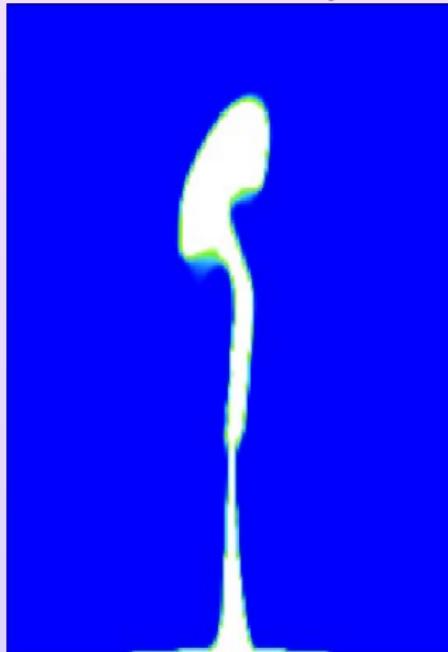
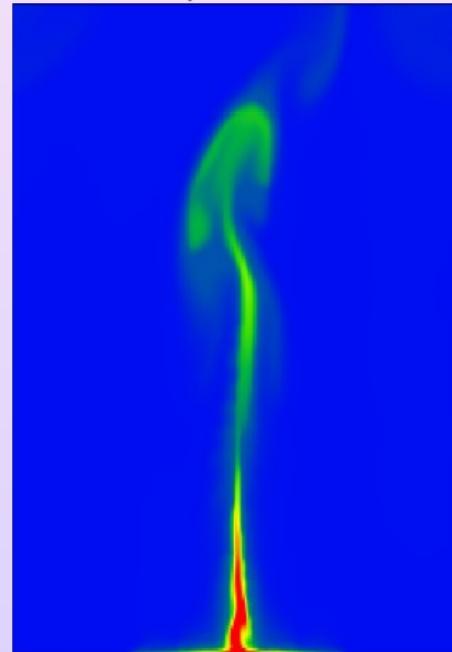
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

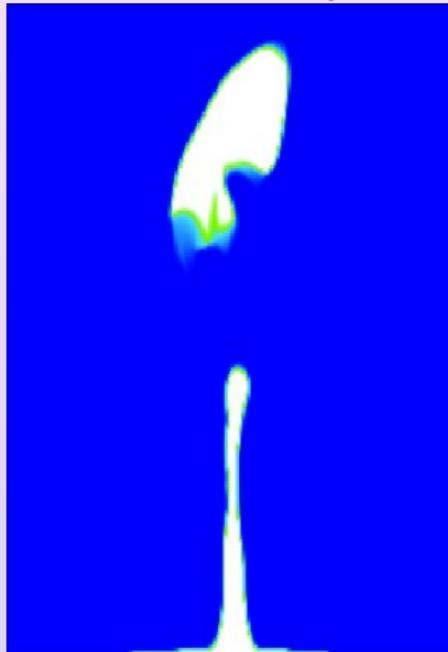
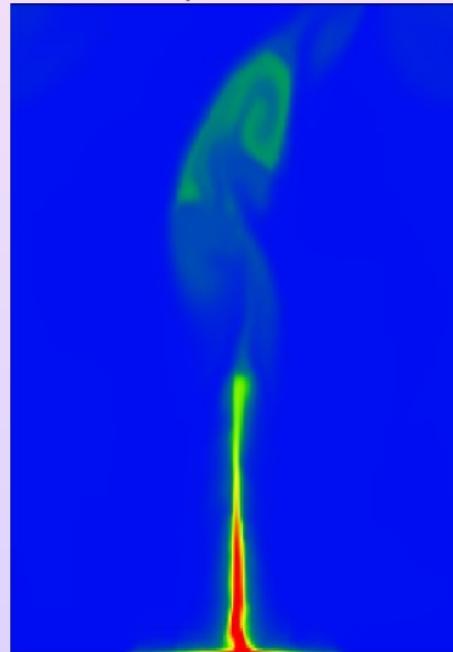
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

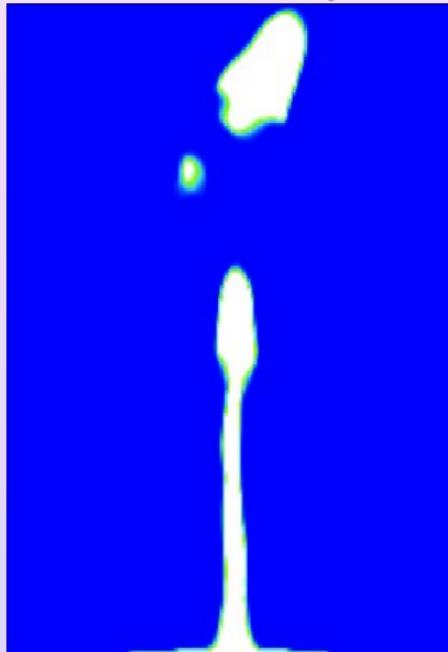
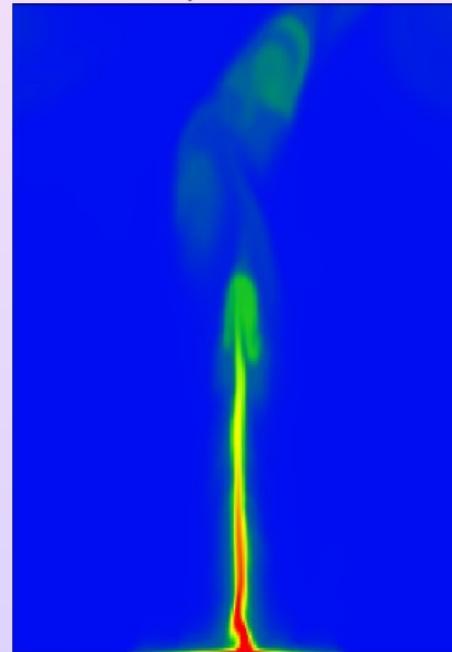
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

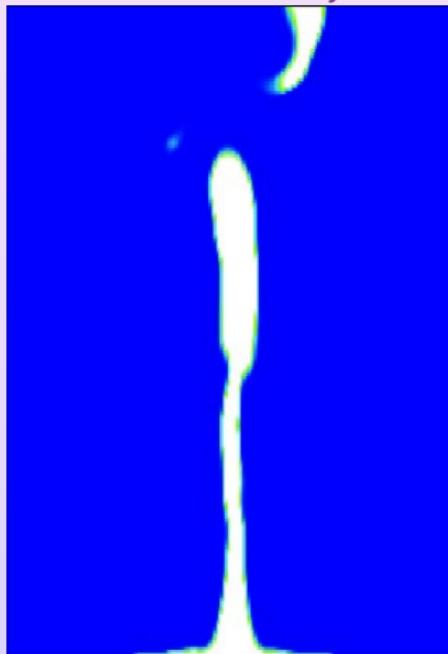
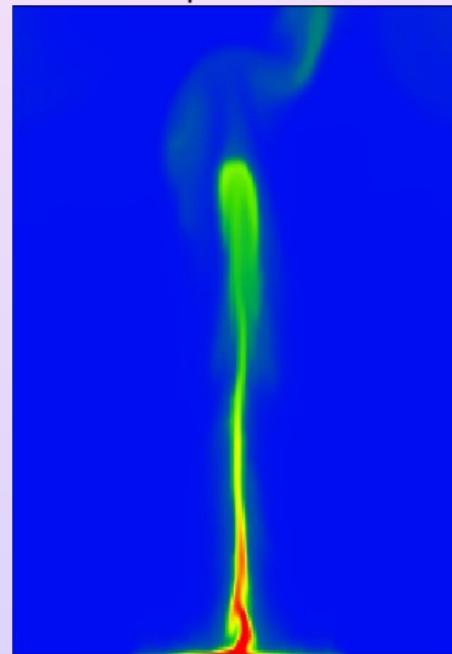
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

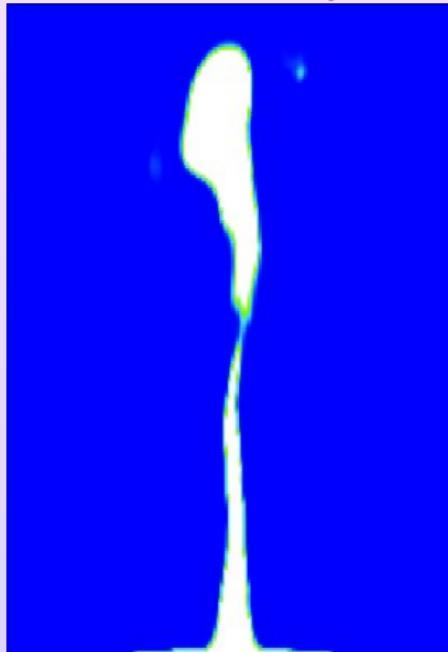
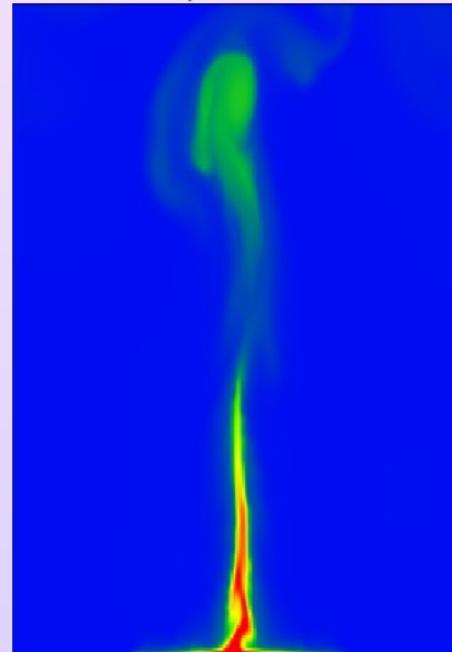
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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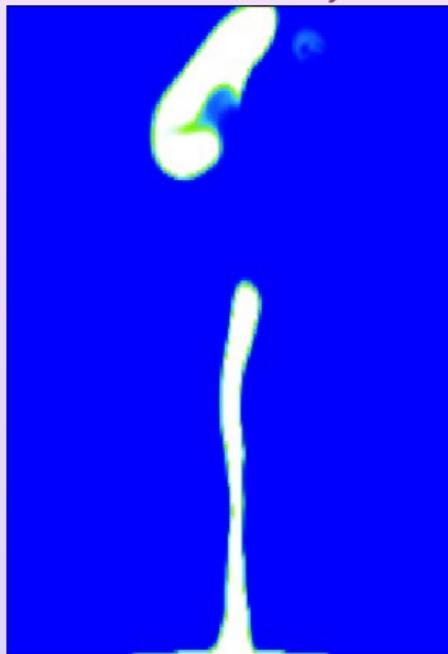
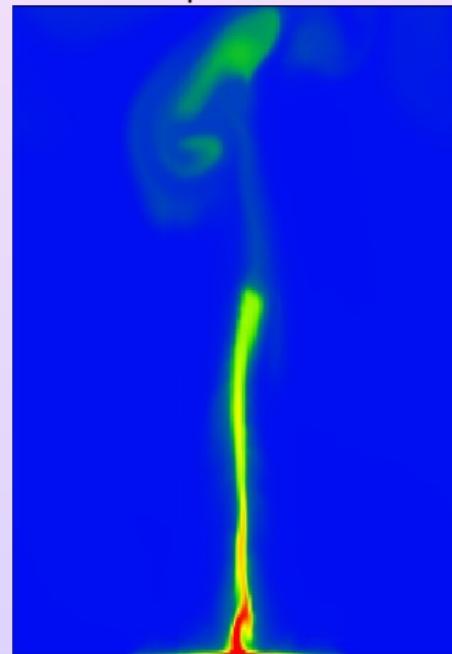
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

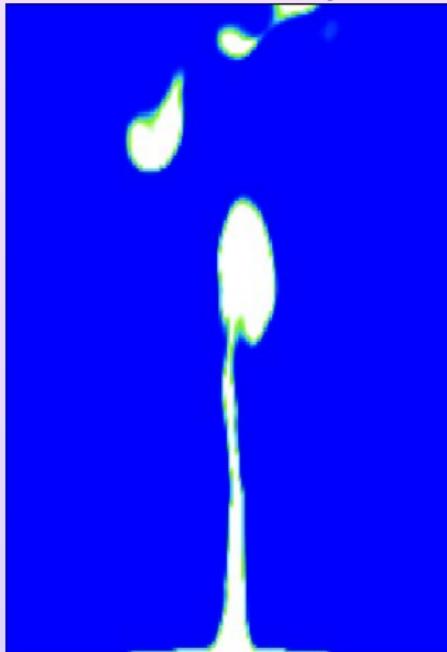
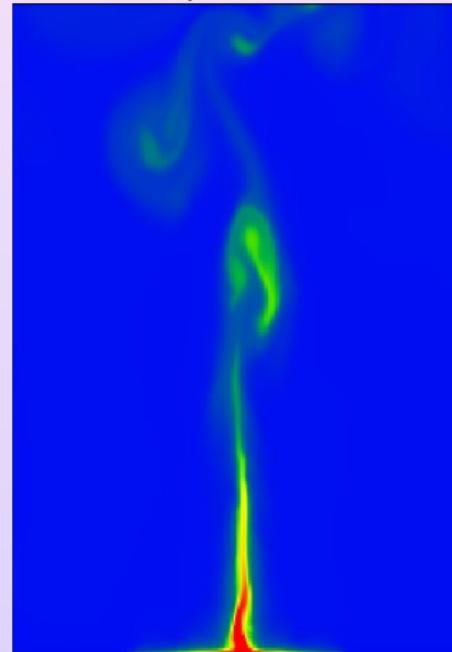
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◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

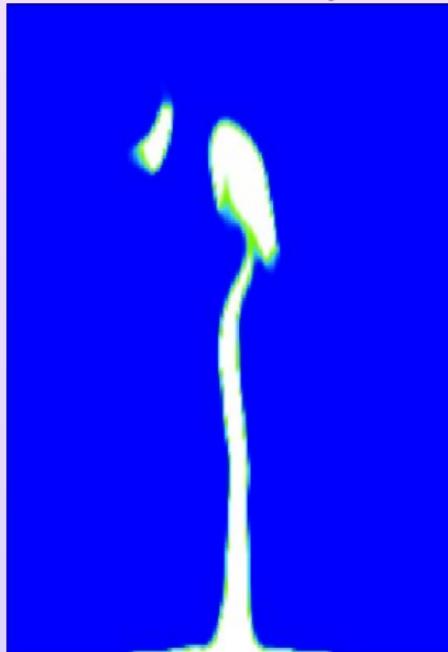
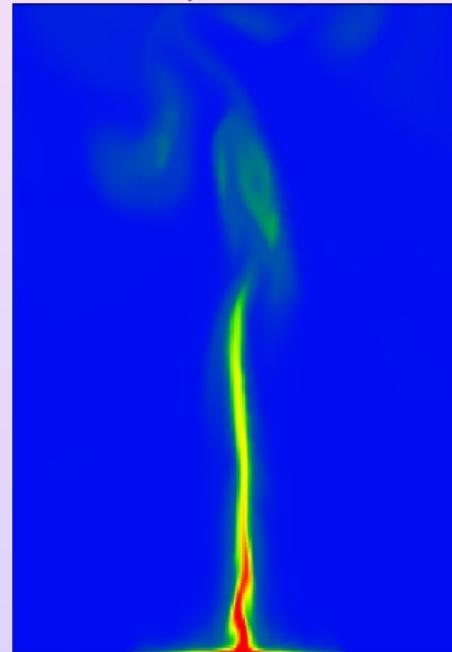
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

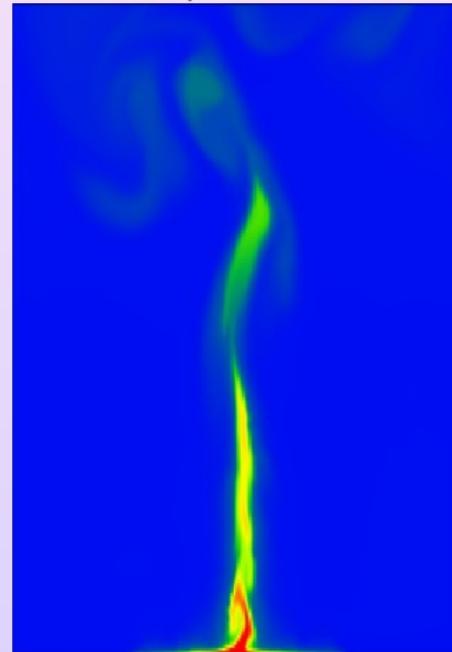
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

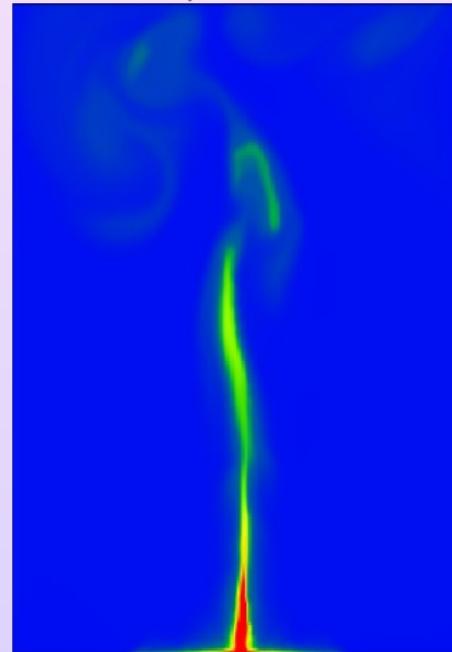
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

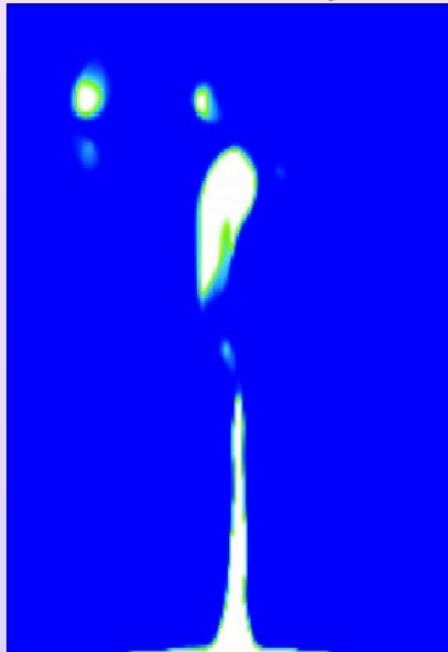
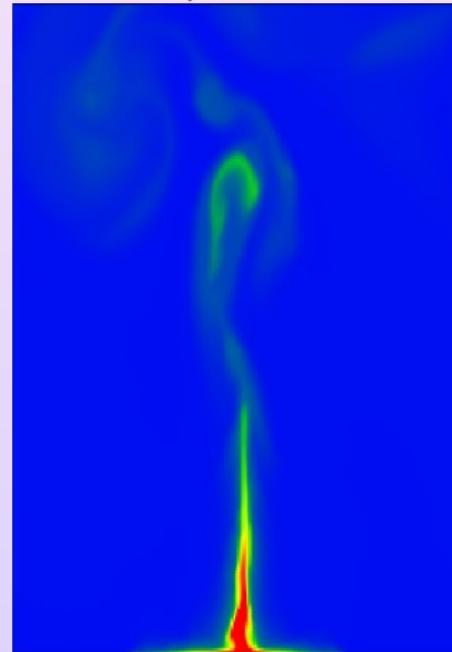
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

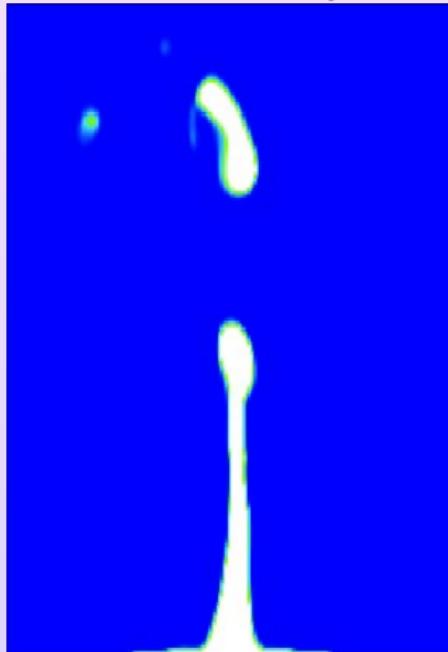
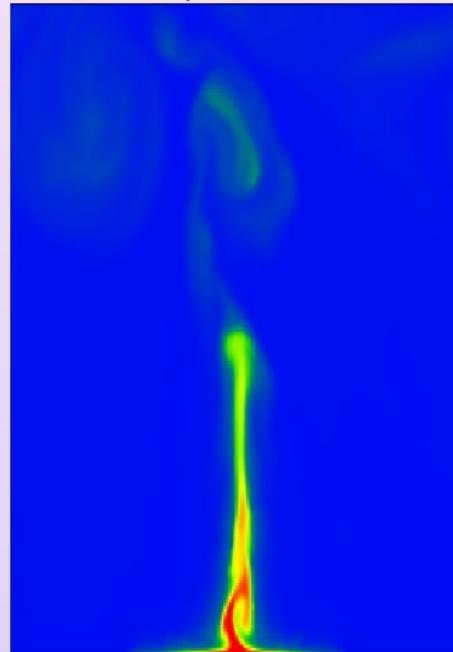
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

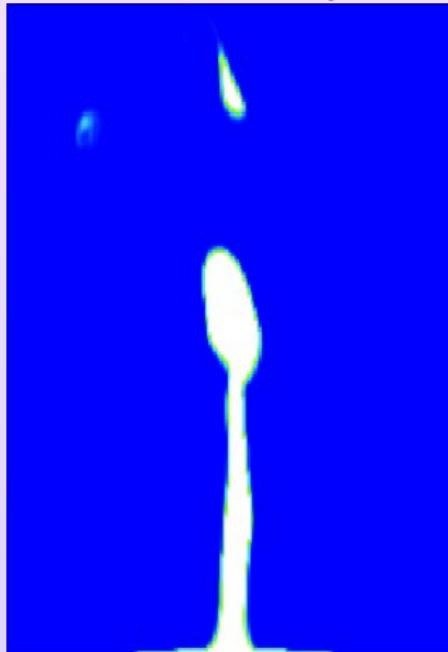
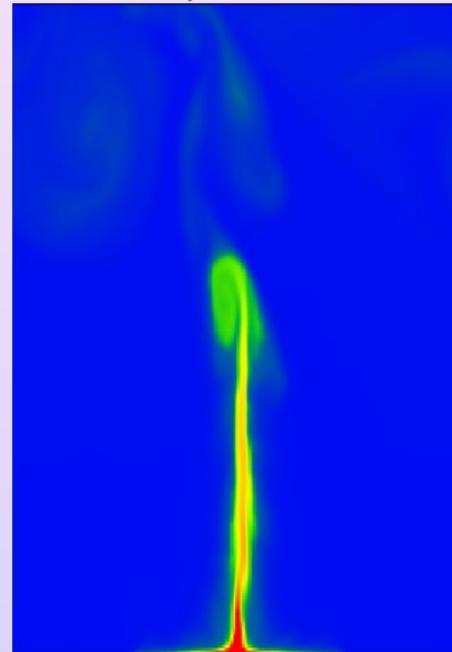
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

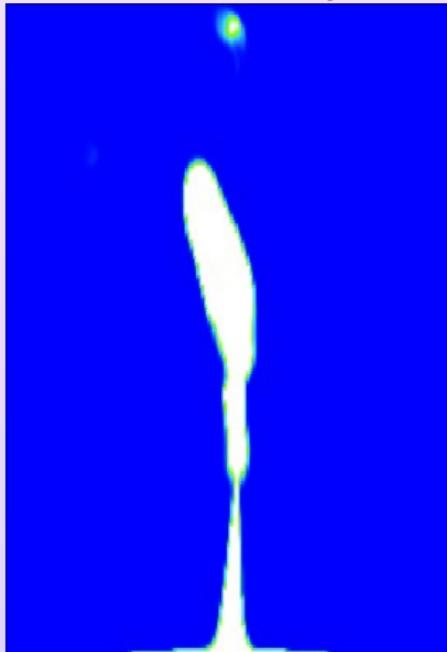
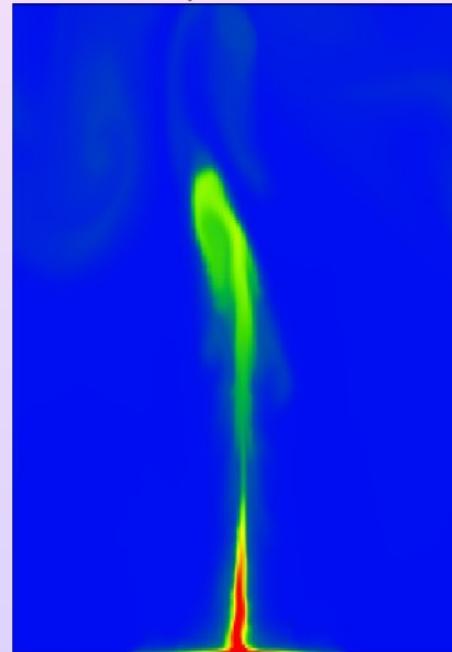
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

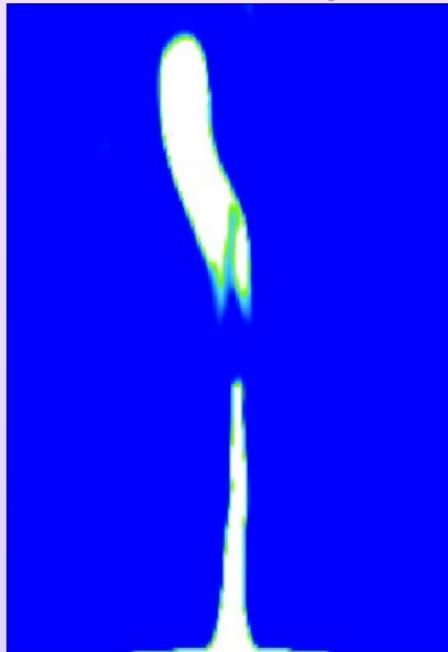
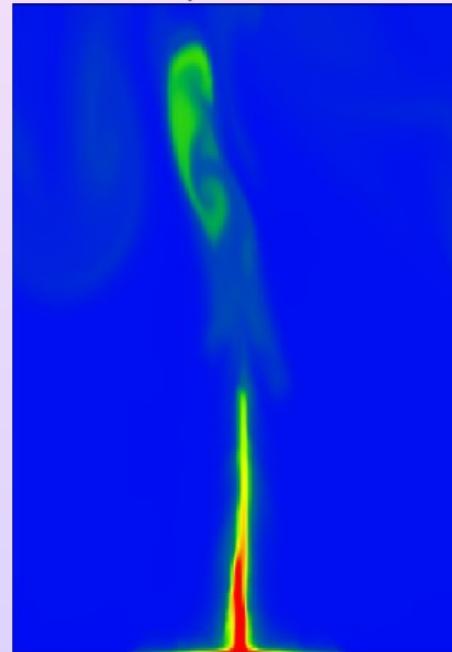
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

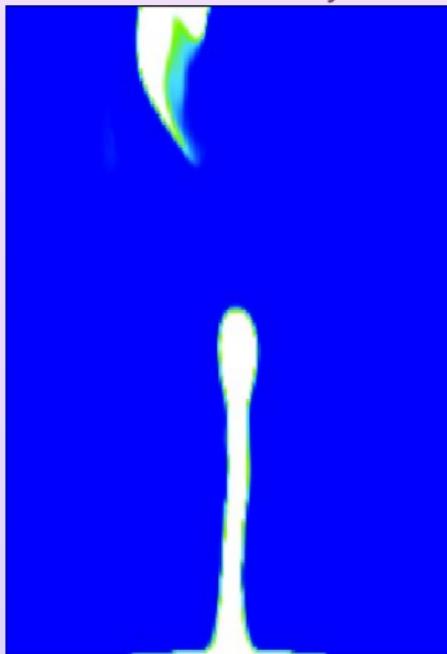
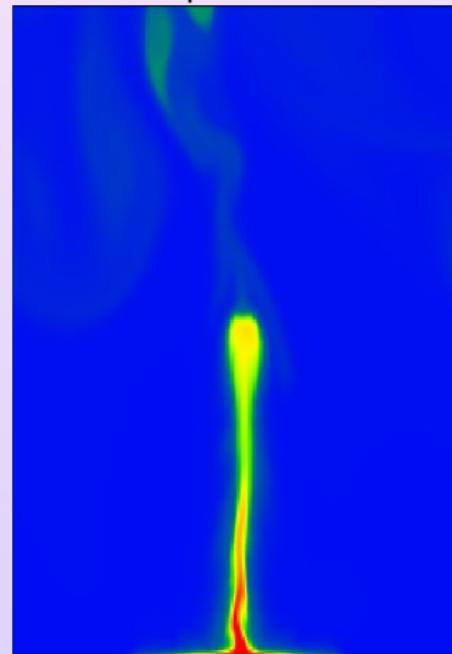
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

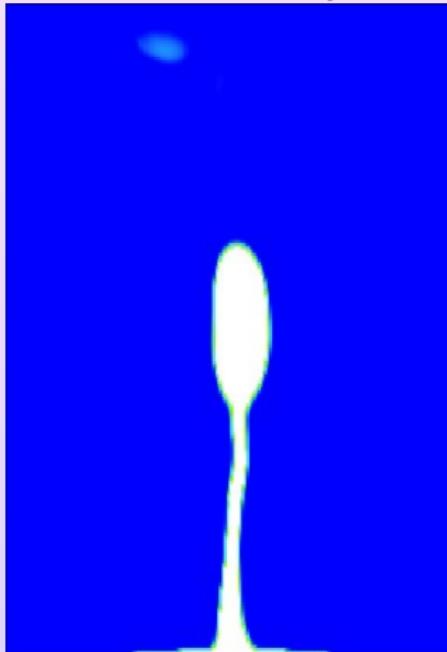
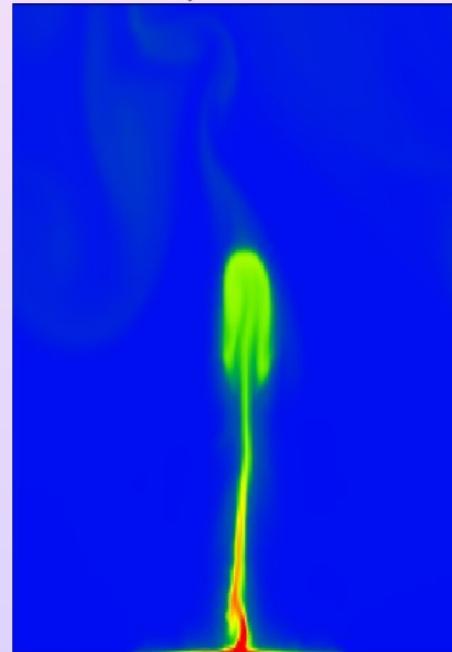
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

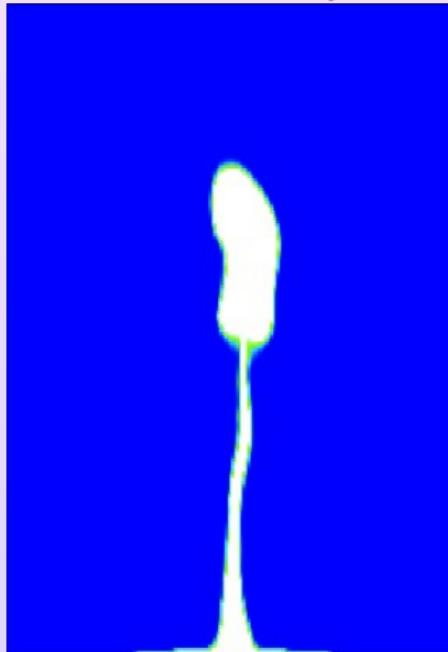
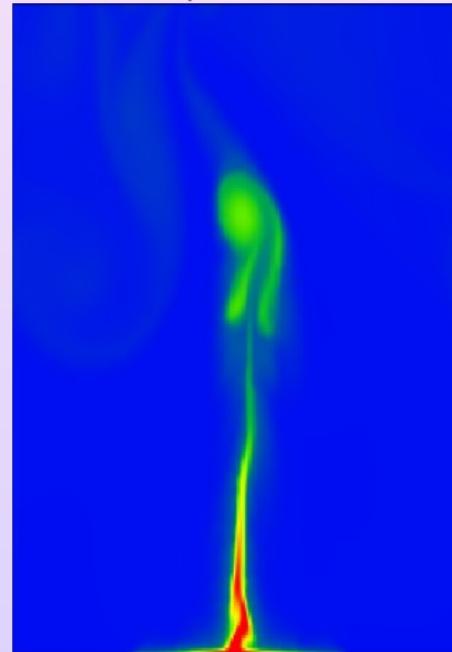
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

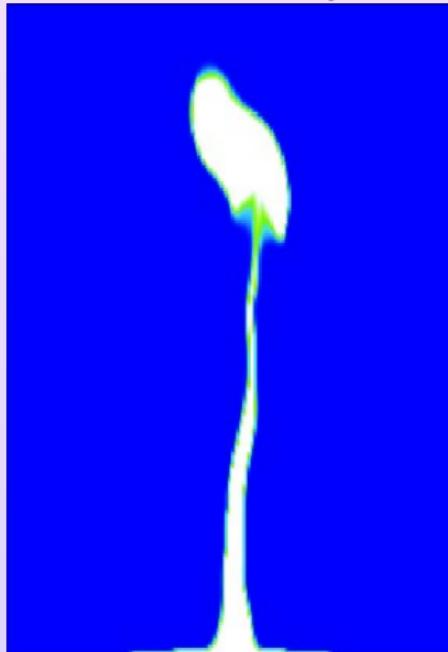
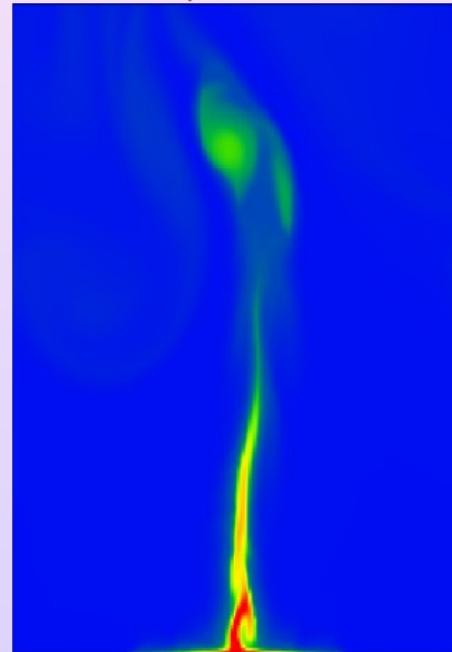
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

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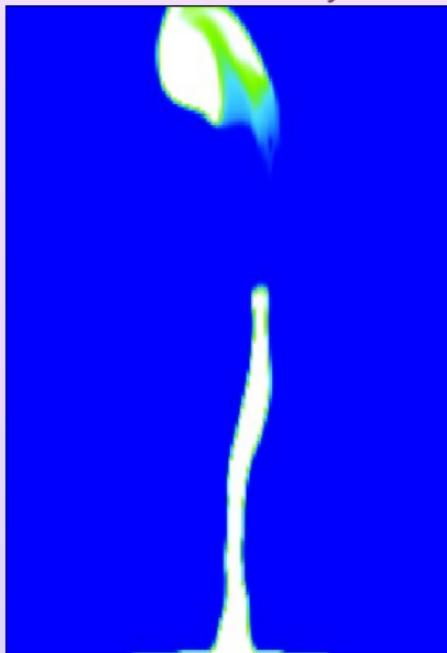
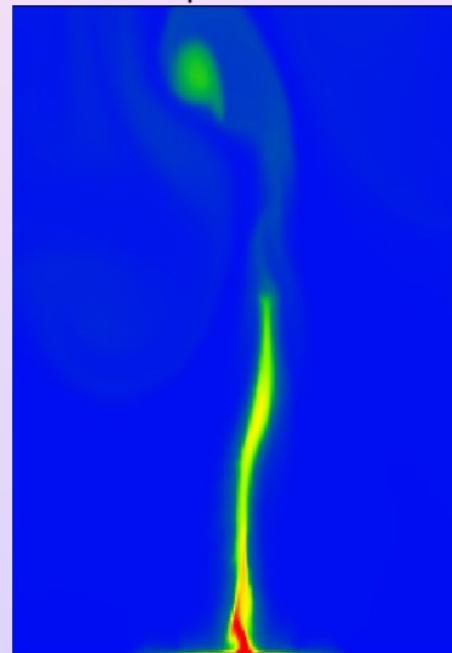
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

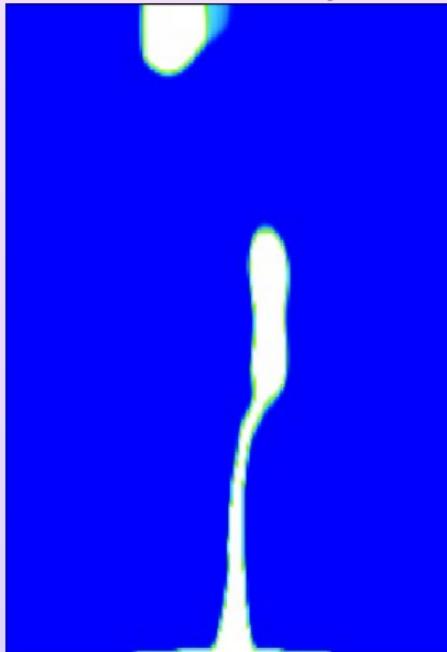
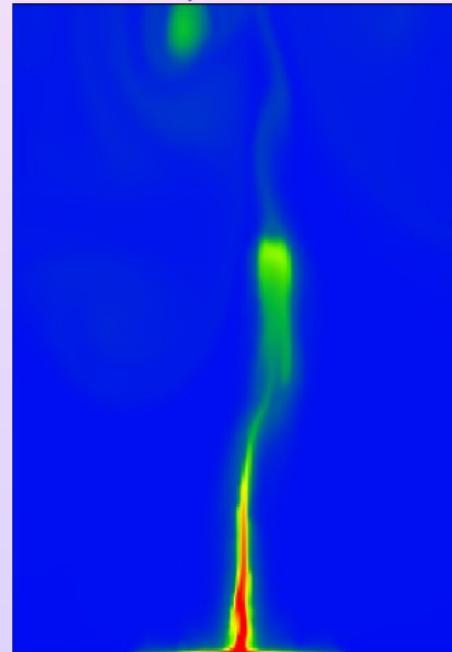
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

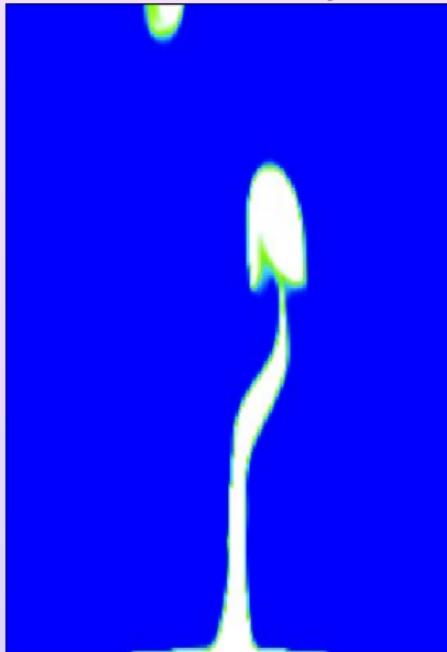
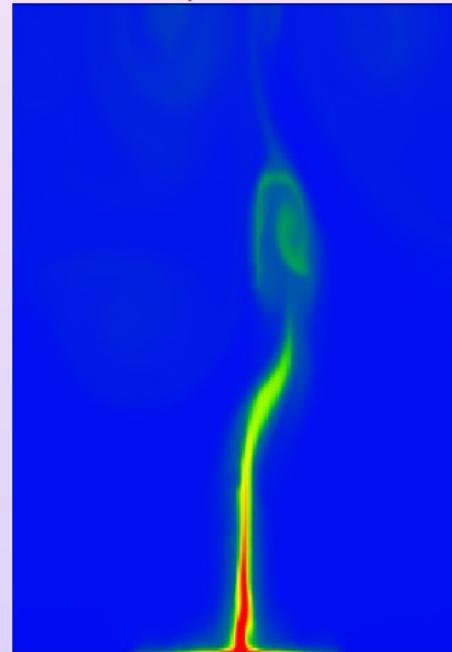
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Nucleating Bubble

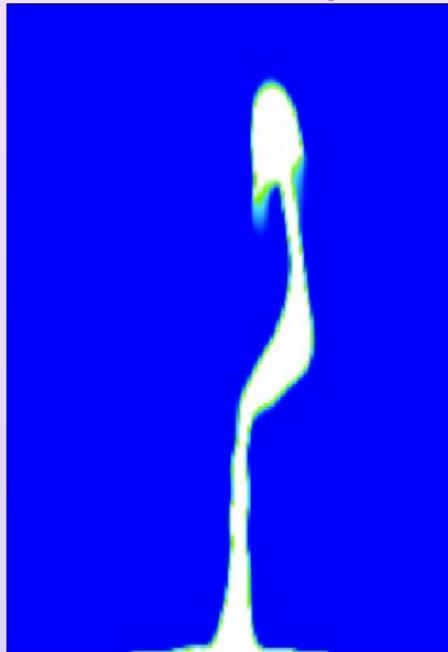
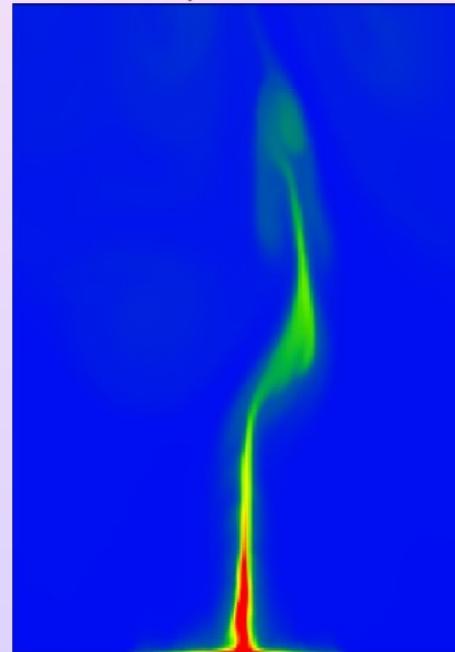
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Nucleating Bubble

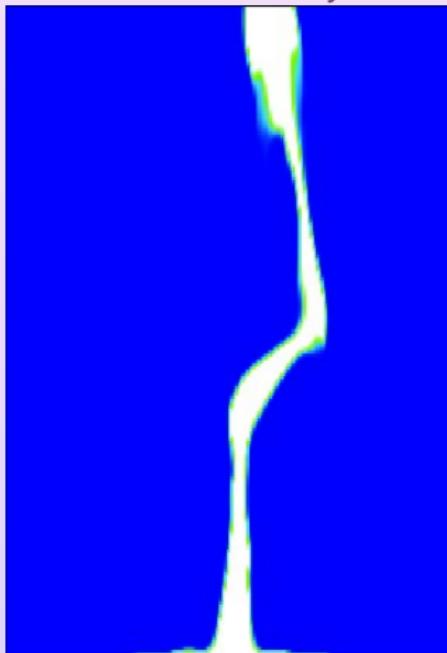
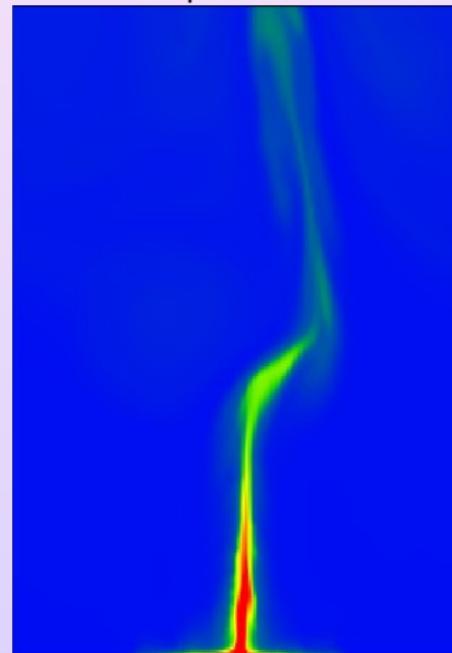
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

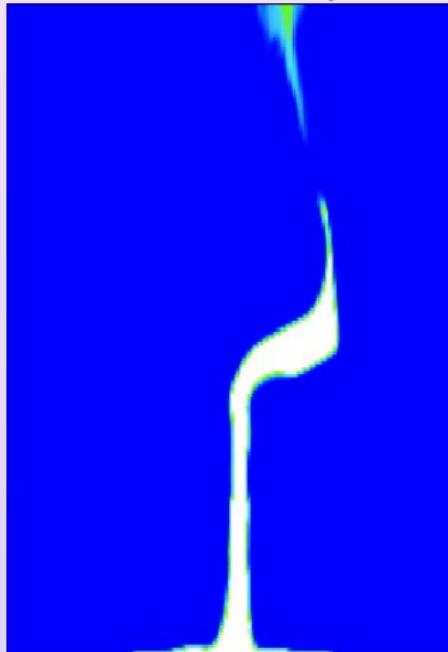
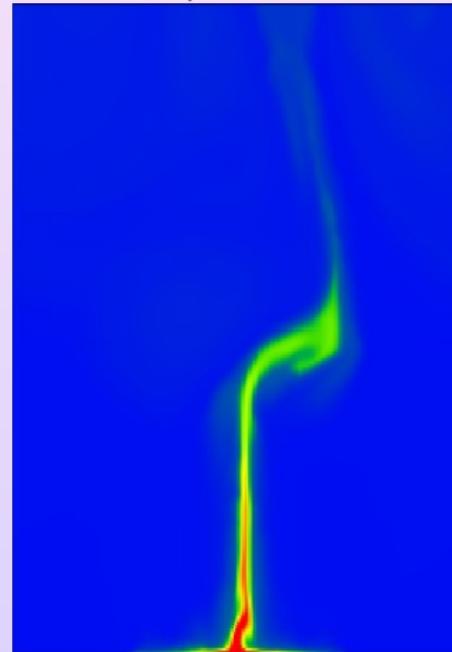
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

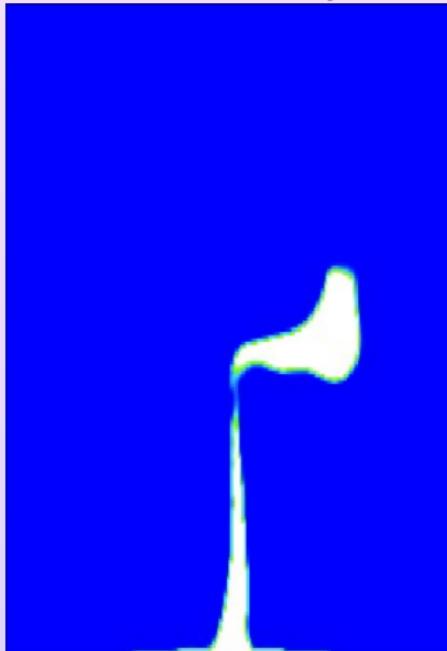
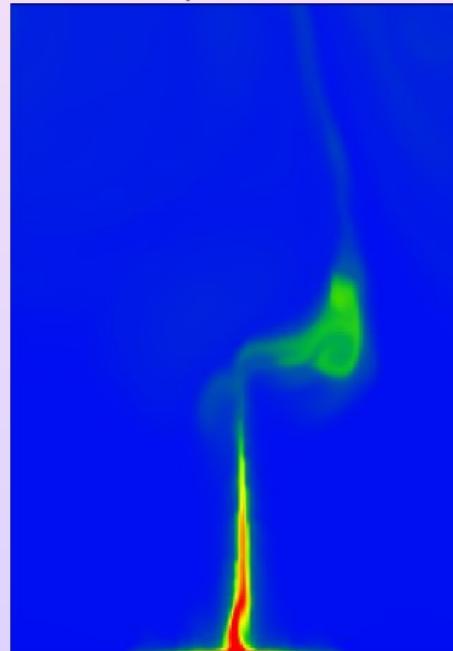
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

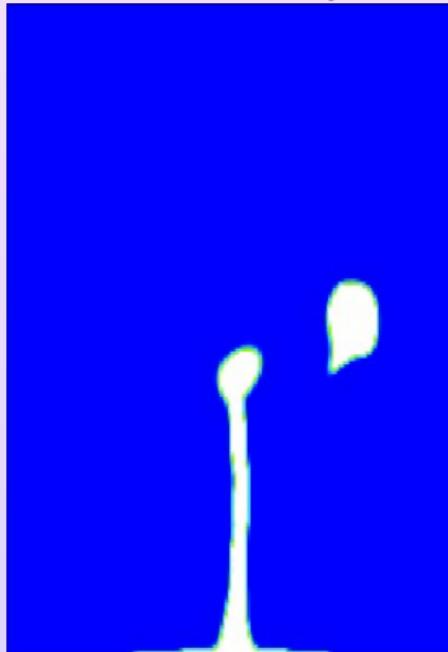
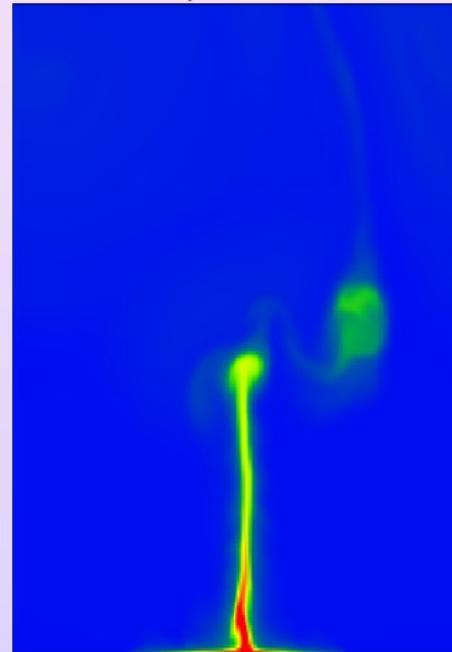
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◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

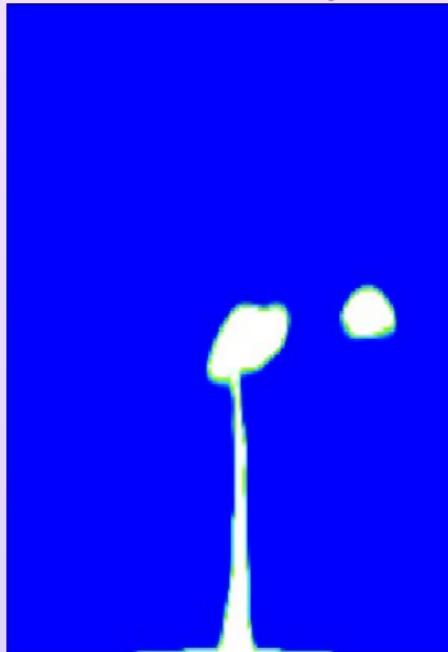
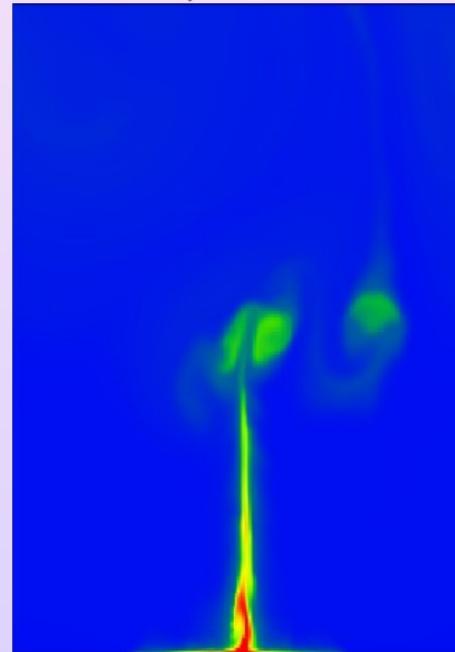
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◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

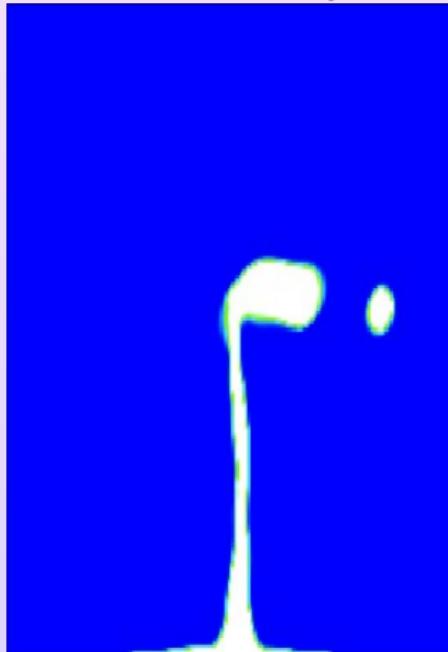
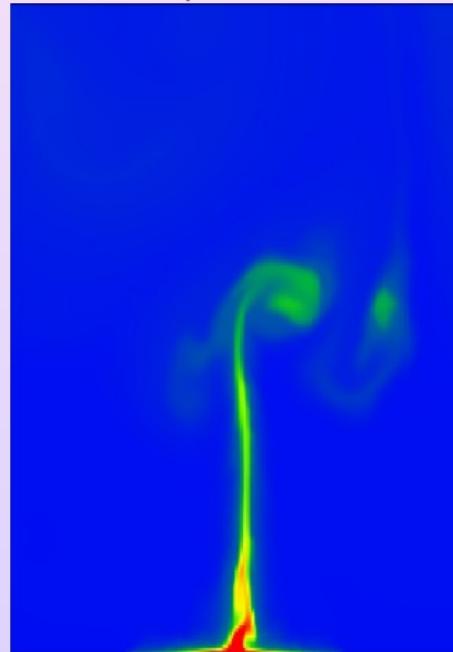
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

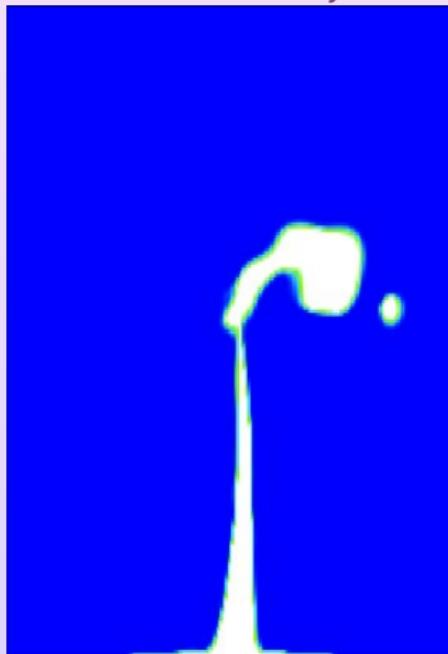
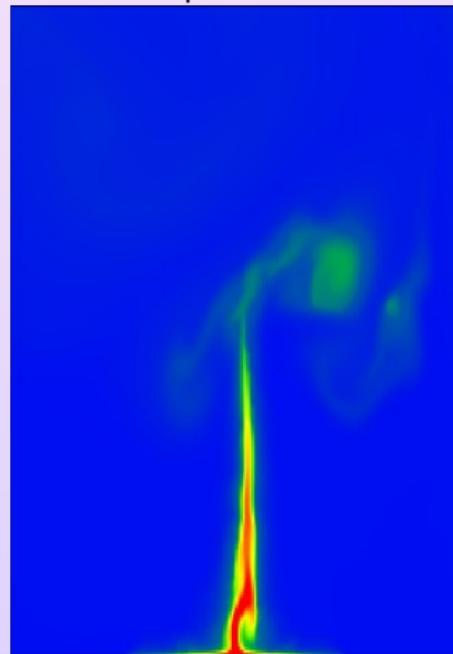
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

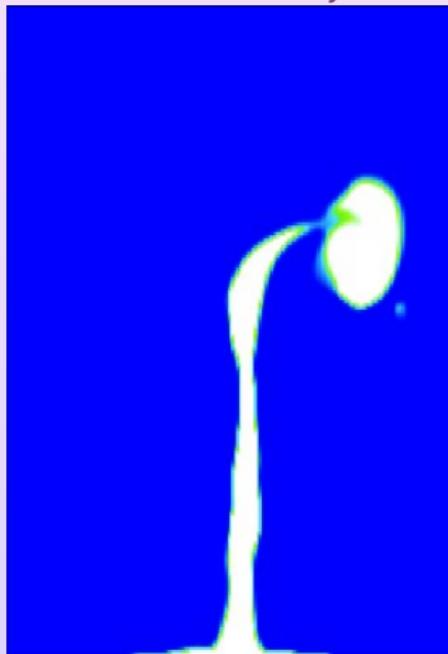
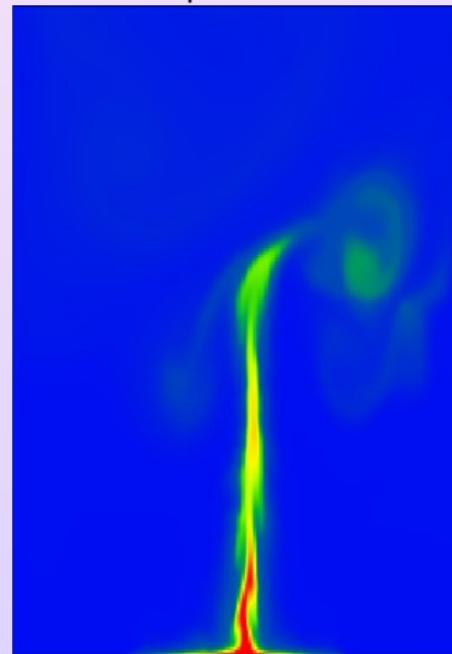
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

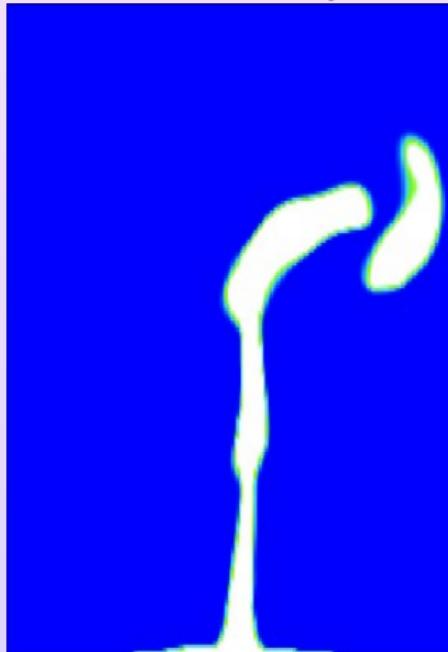
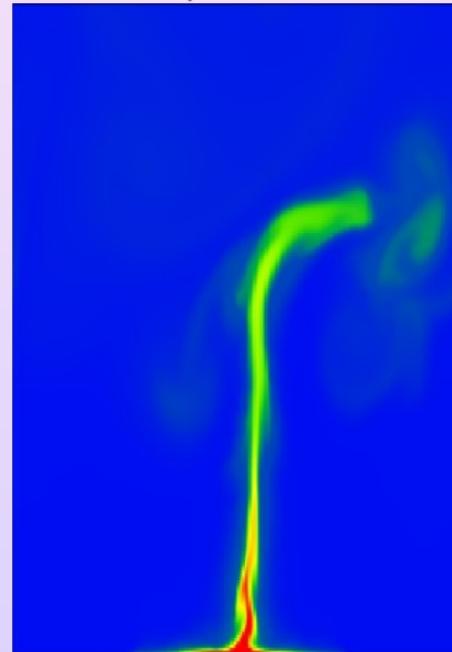
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

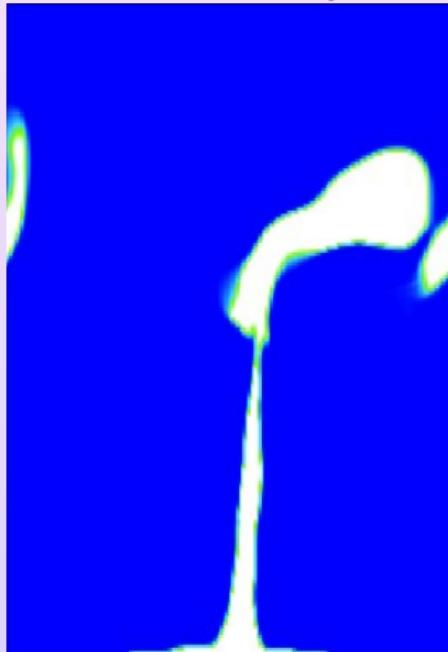
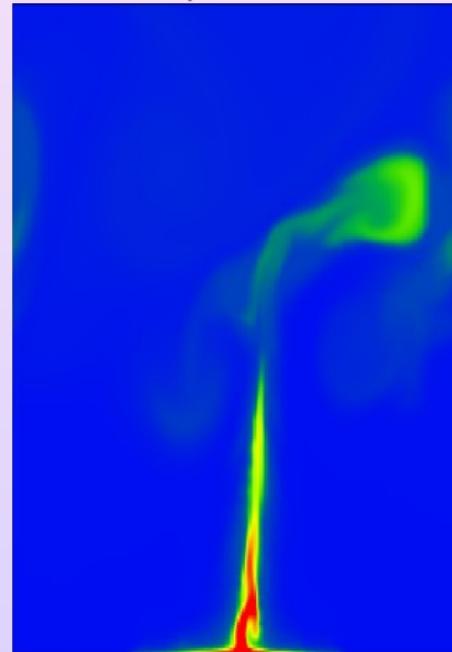
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

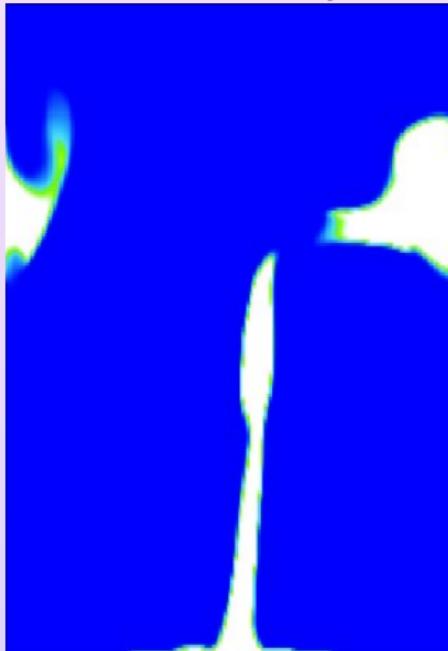
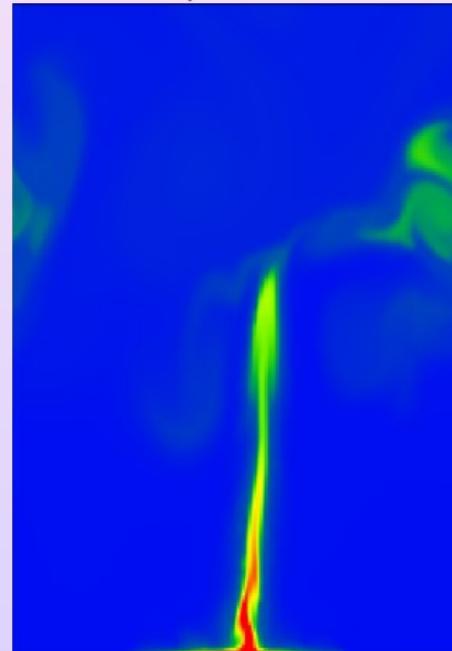
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

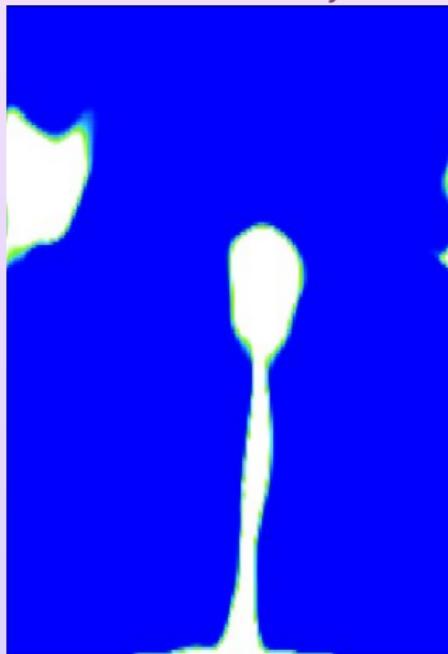
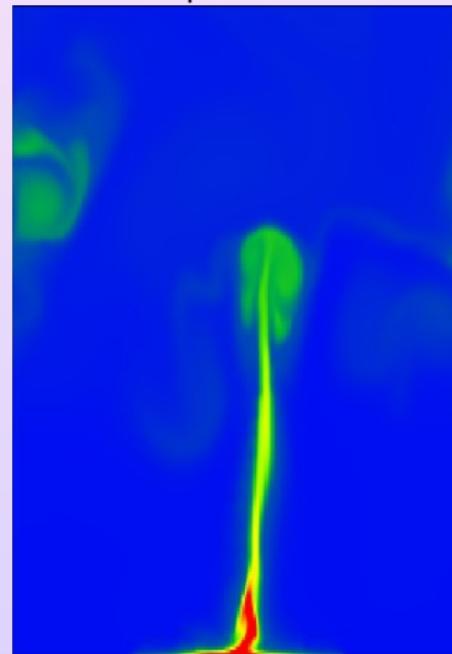
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

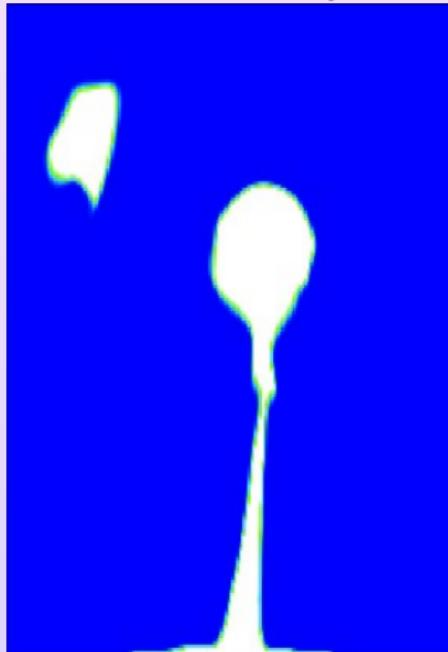
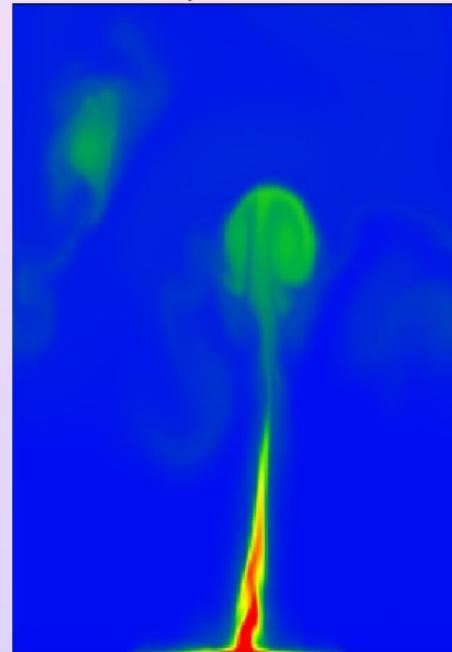
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

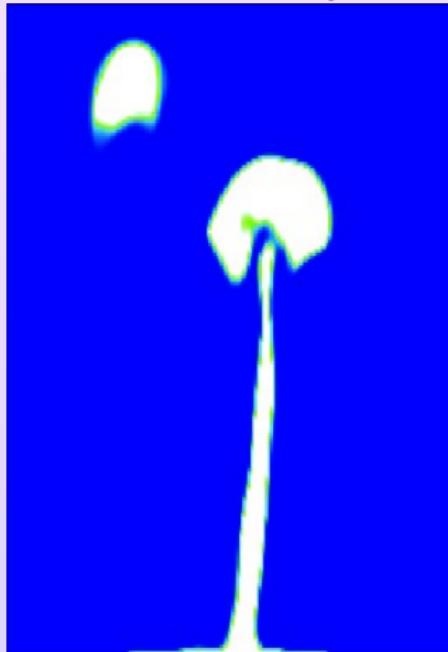
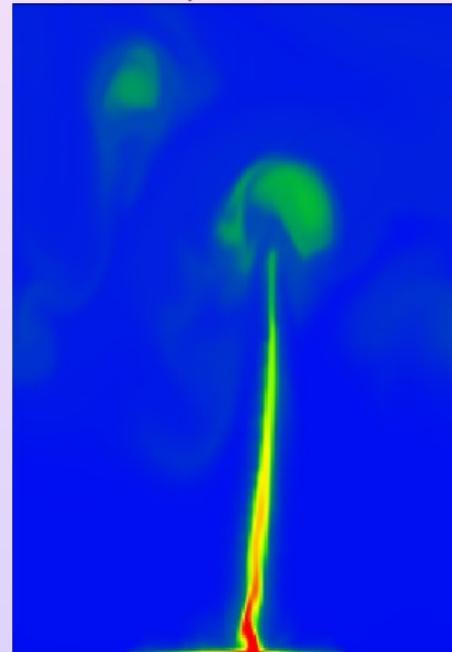
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

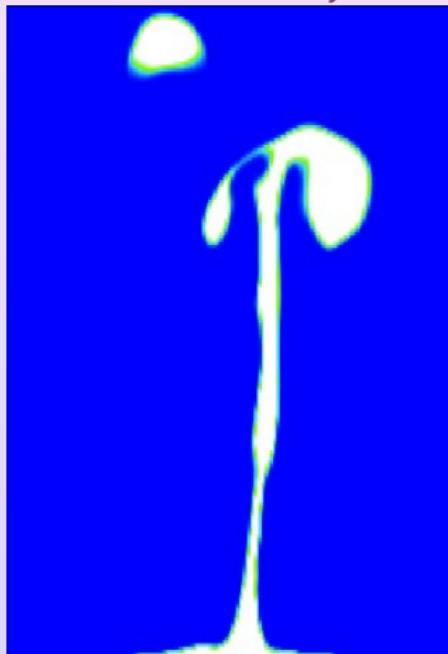
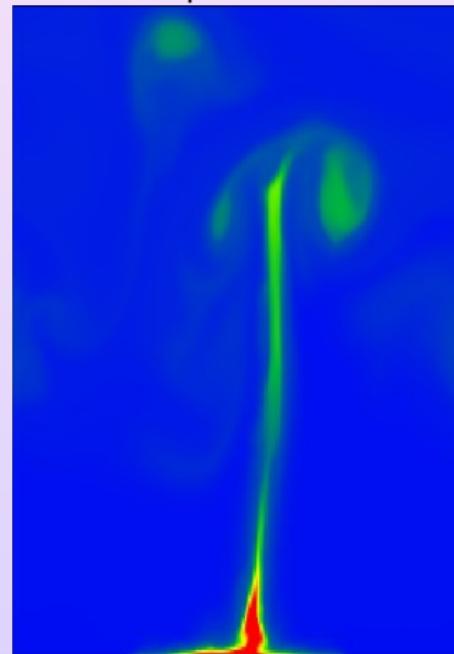
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

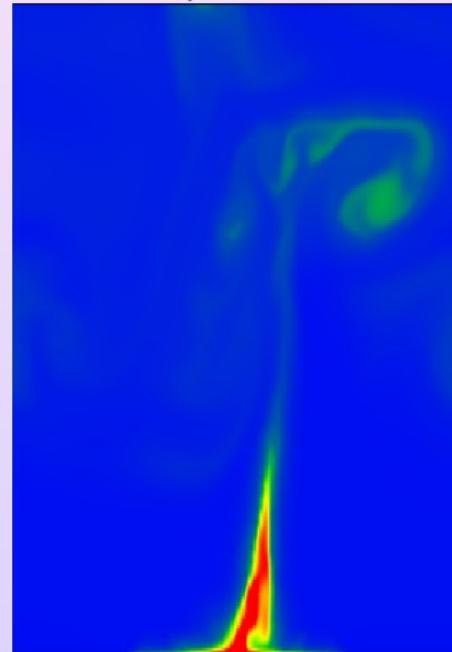
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Nucleating Bubble

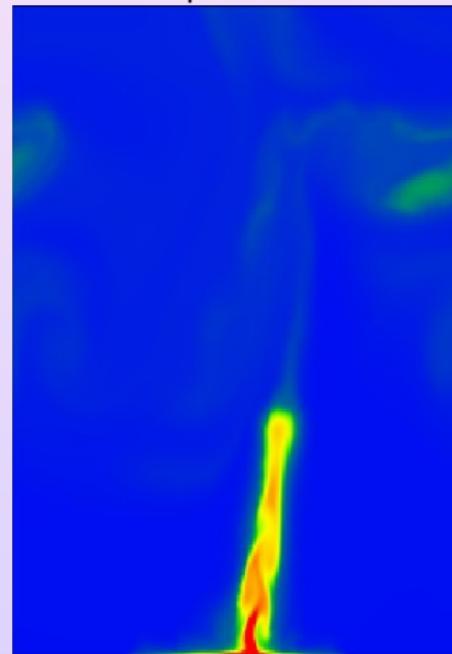
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

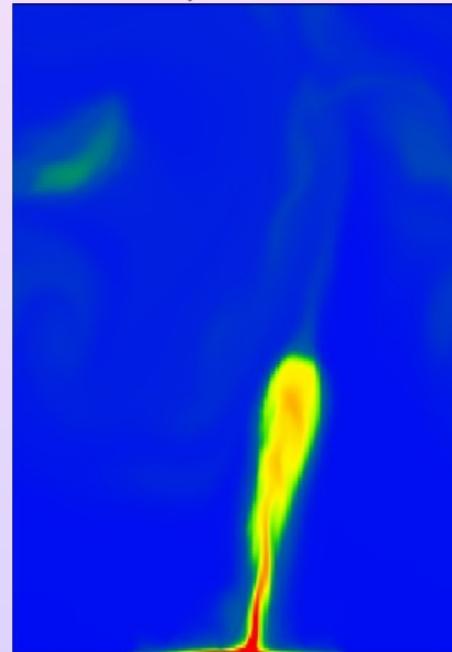
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Nucleating Bubble

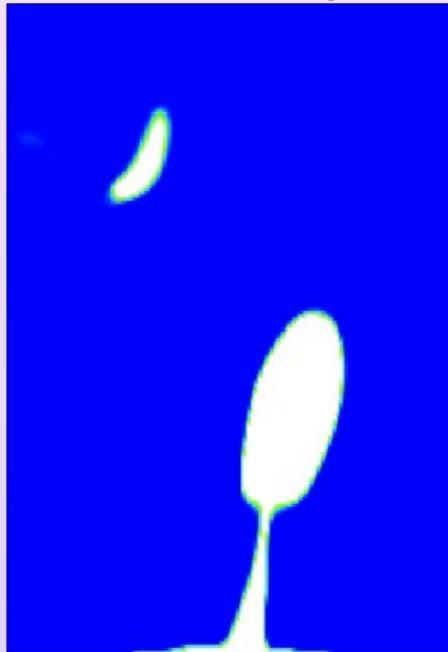
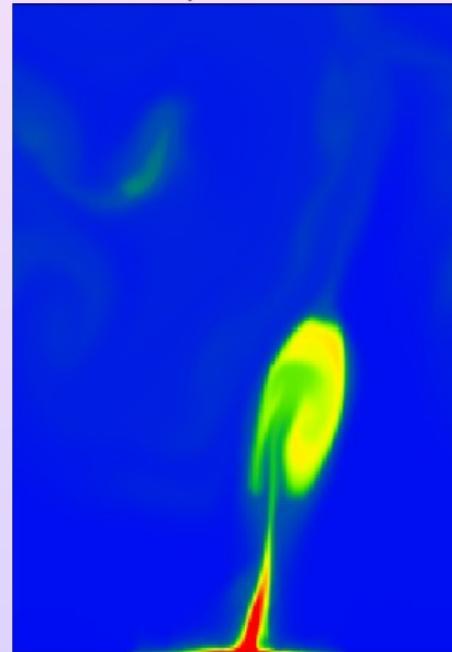
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

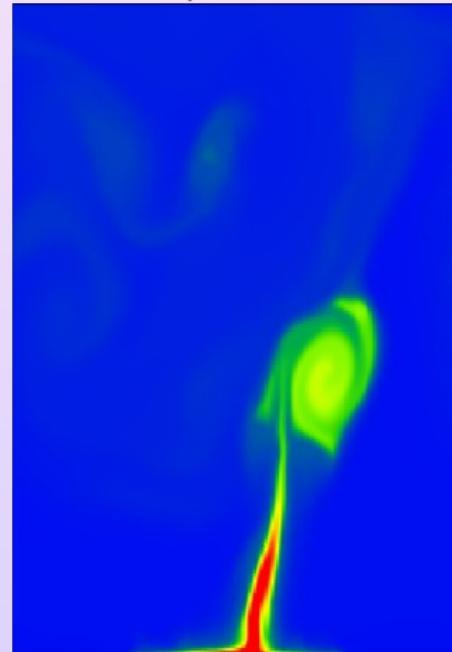
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

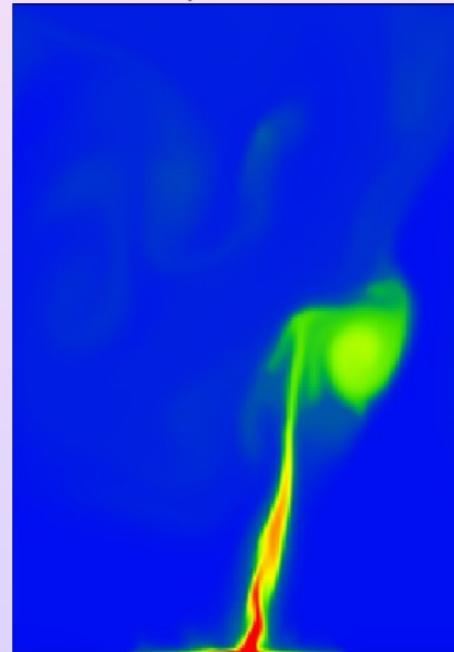
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

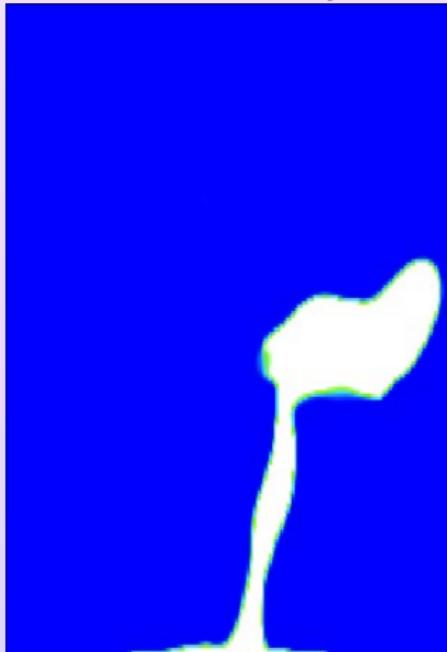
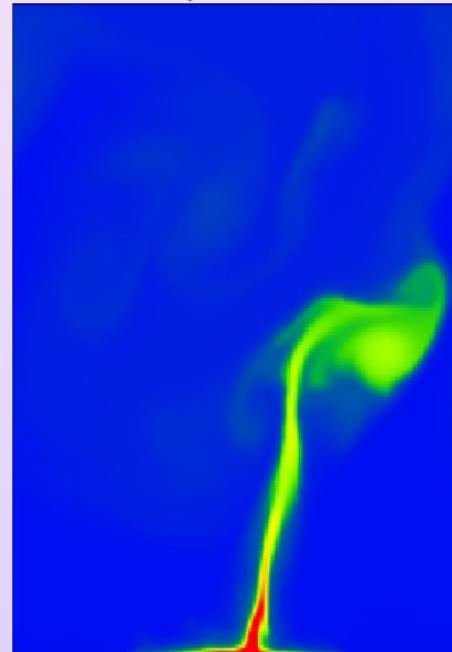
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◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

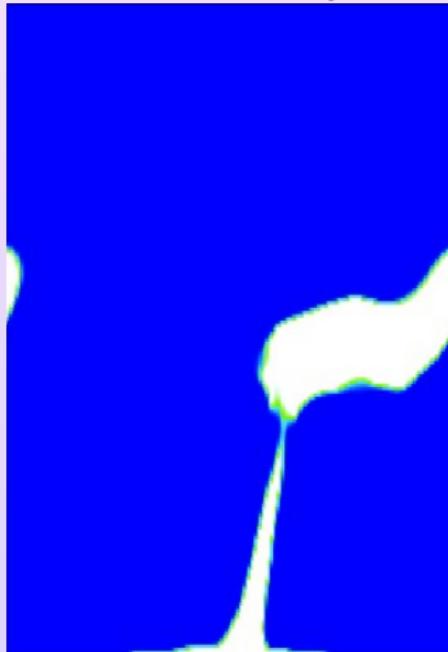
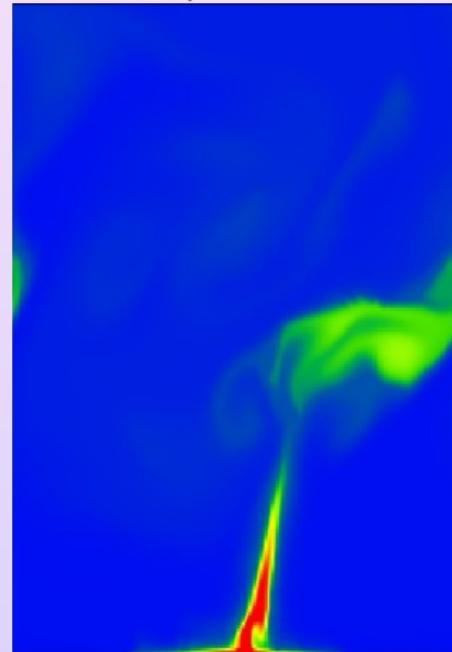
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Nucleating Bubble

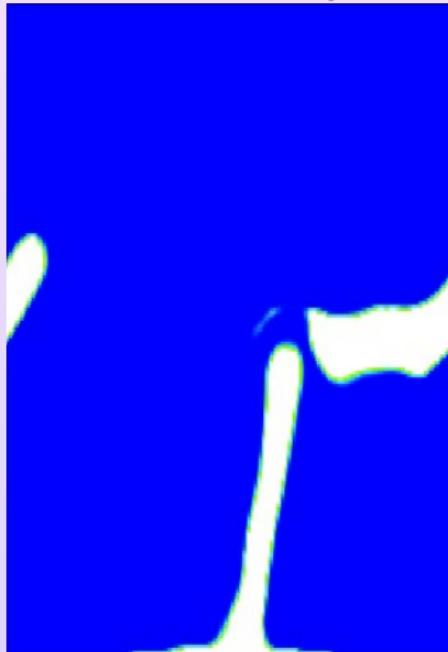
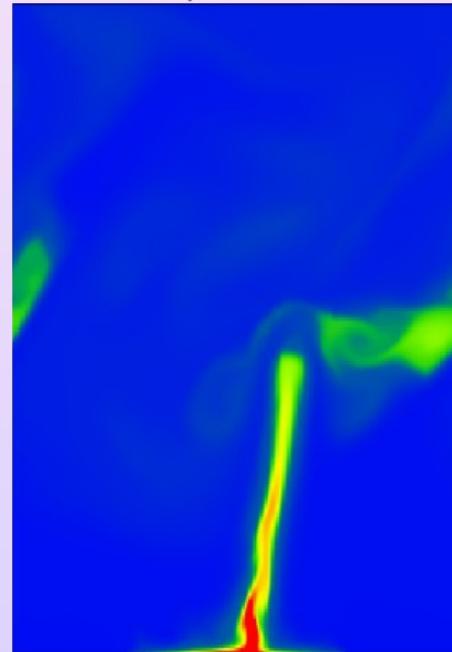
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Nucleating Bubble

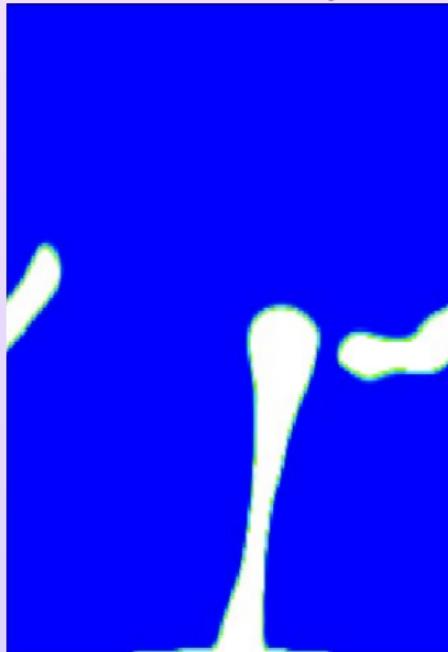
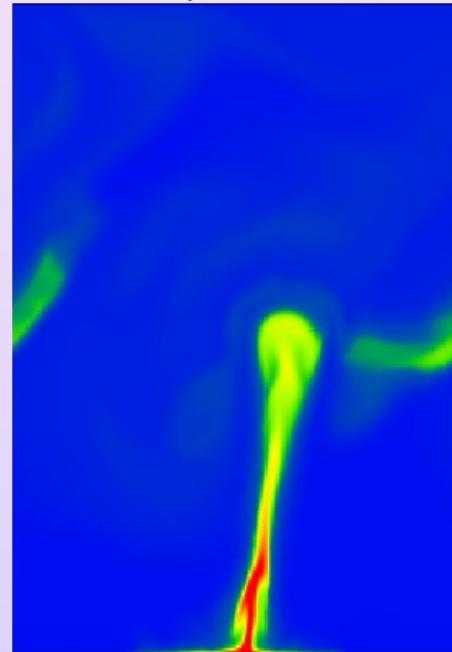
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

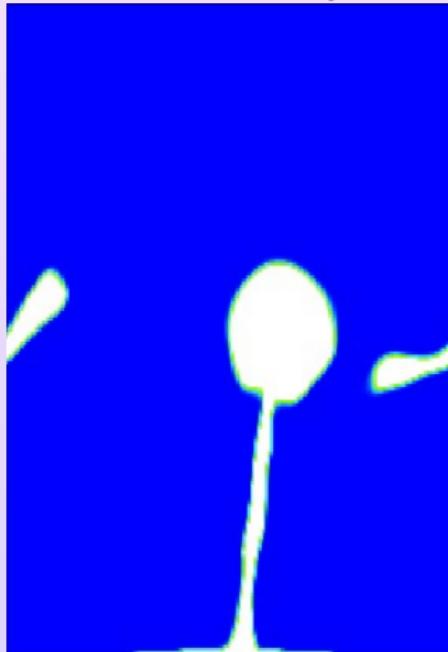
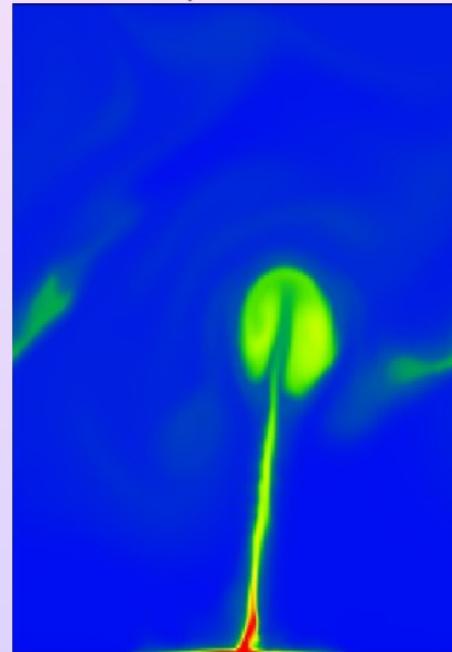
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Nucleating Bubble

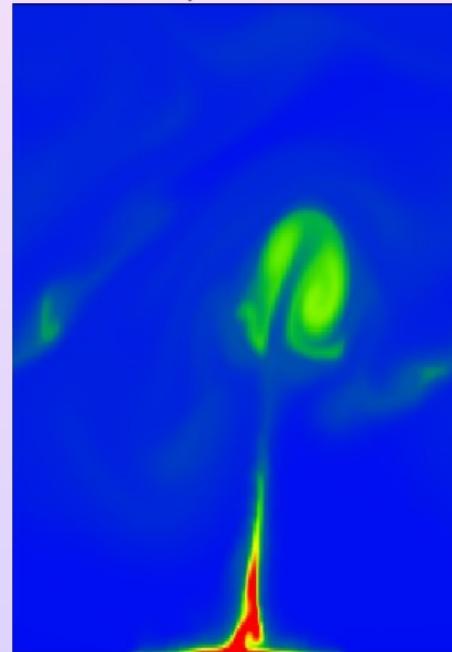
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◀ Geometry

▶ Play

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Nucleating Bubble

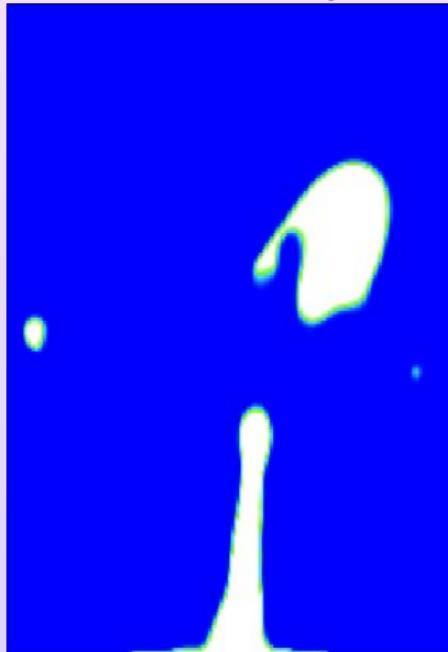
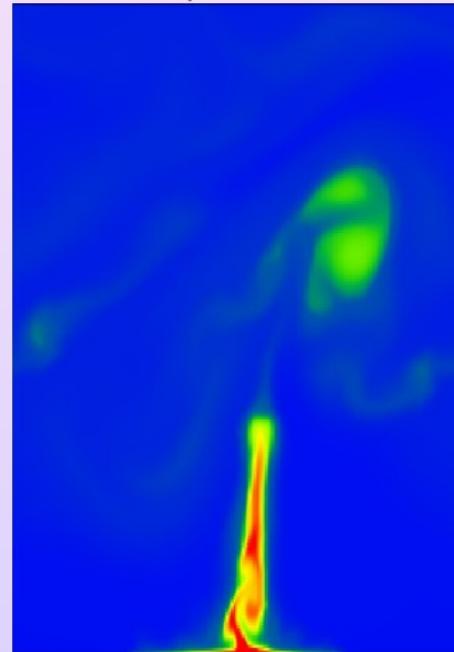
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

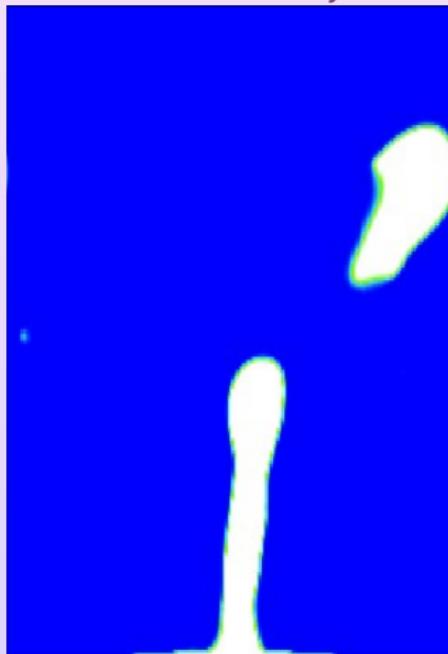
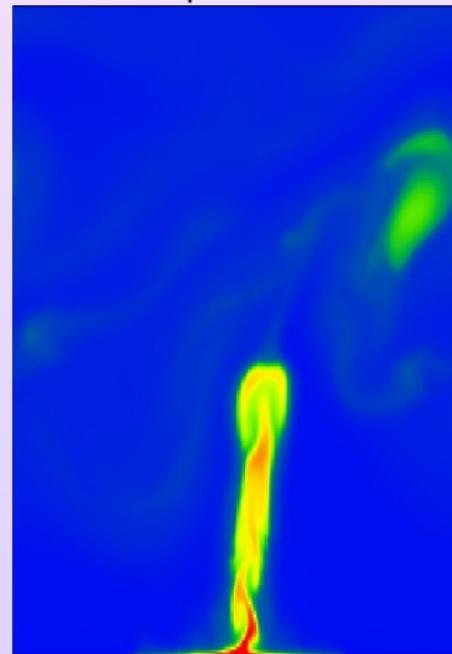
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

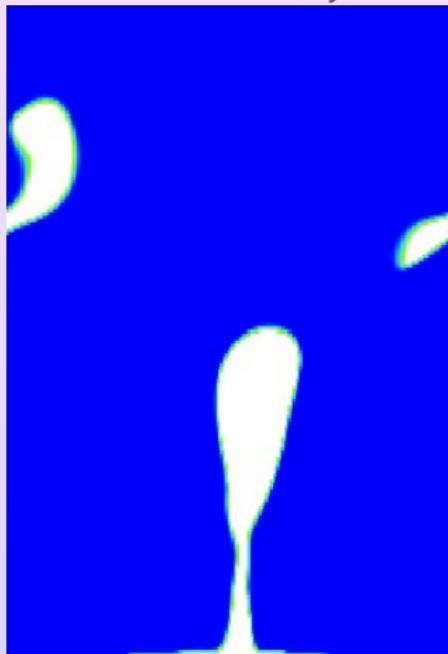
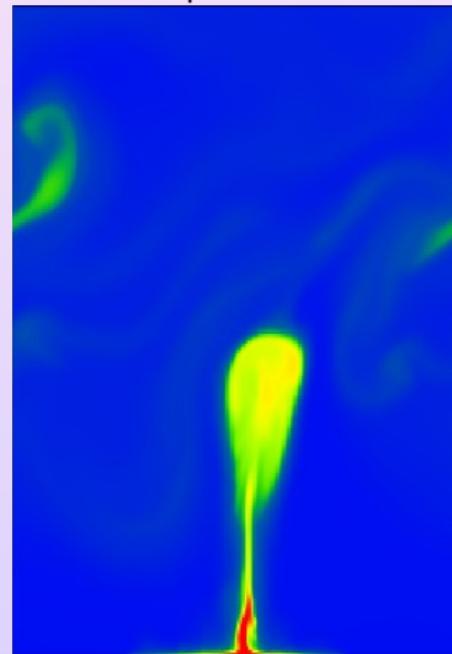
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◀ Geometry

▶ Play

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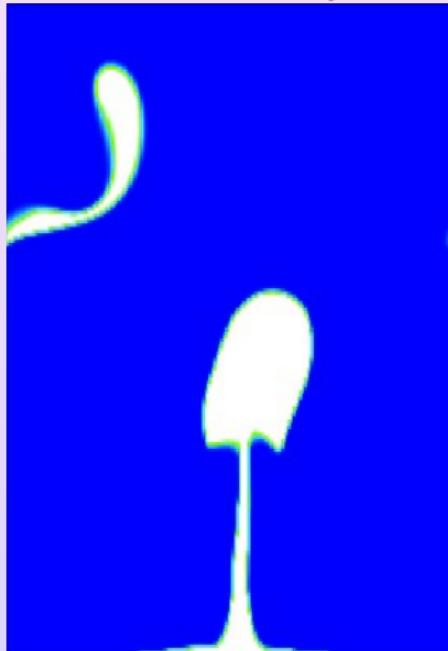
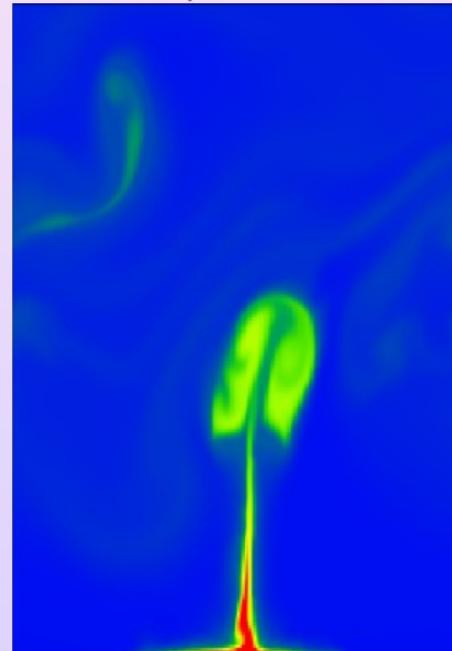
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◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

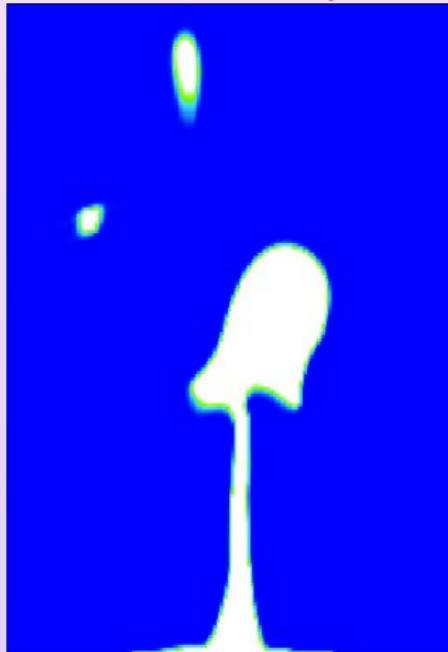
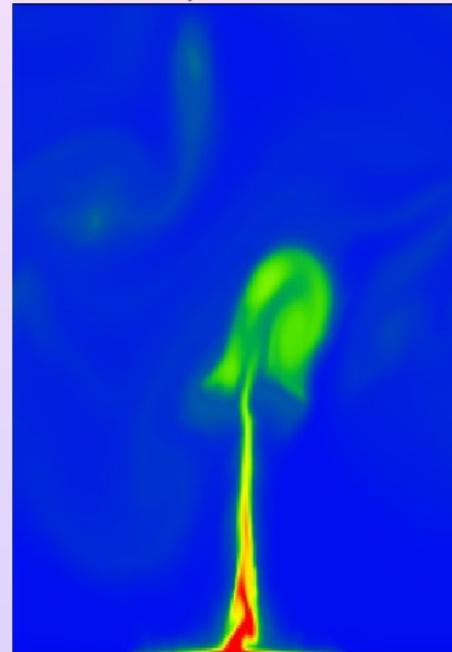
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

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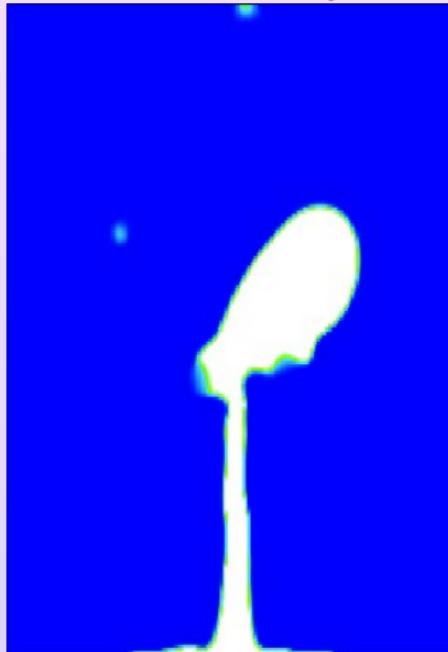
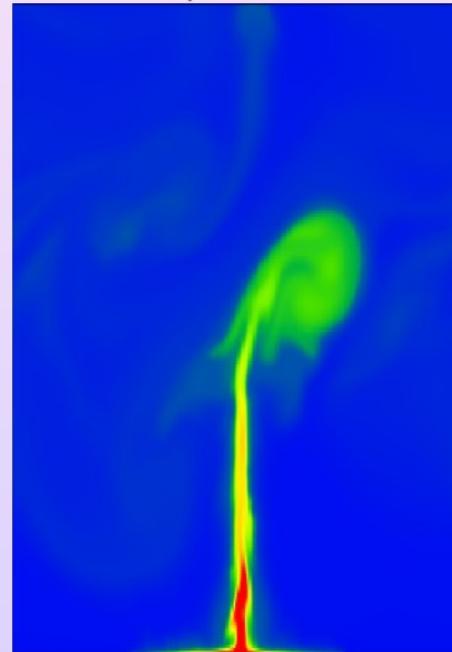
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

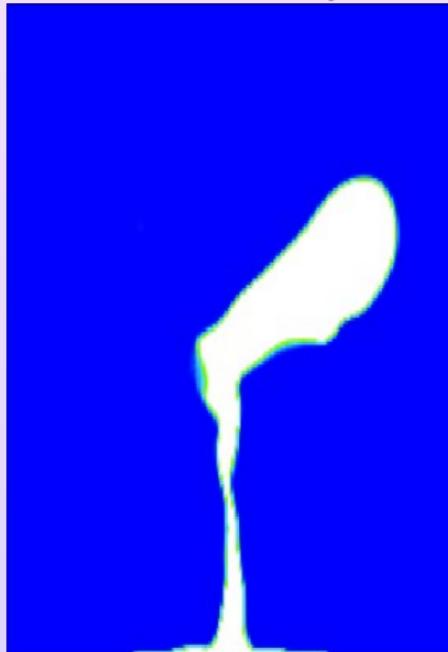
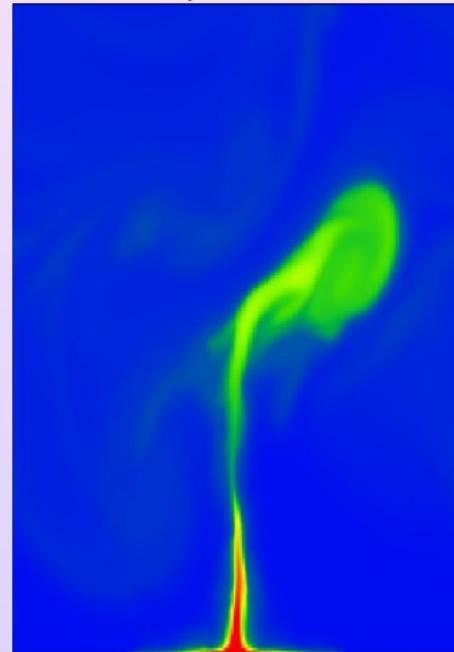
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

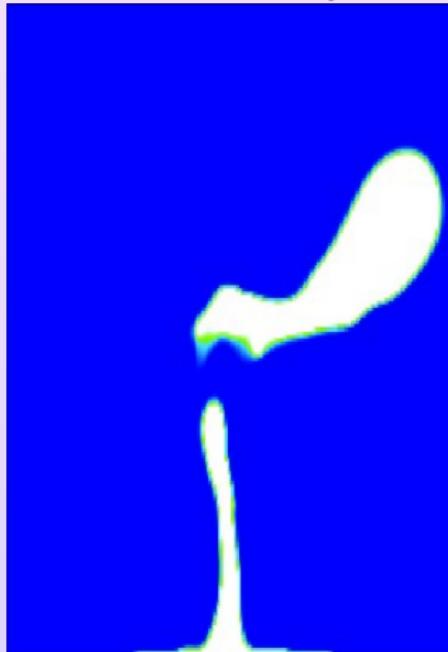
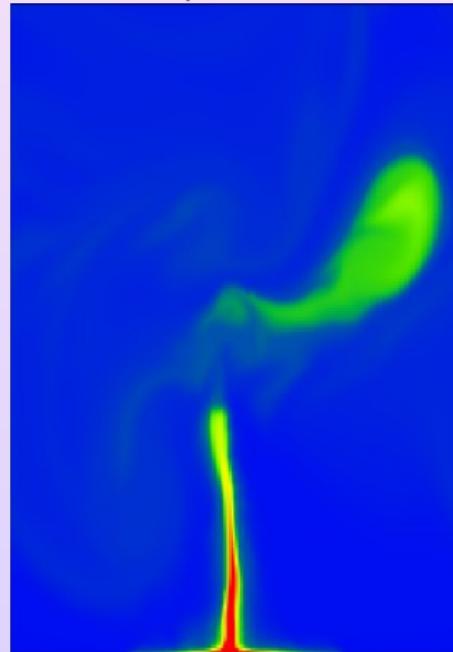
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

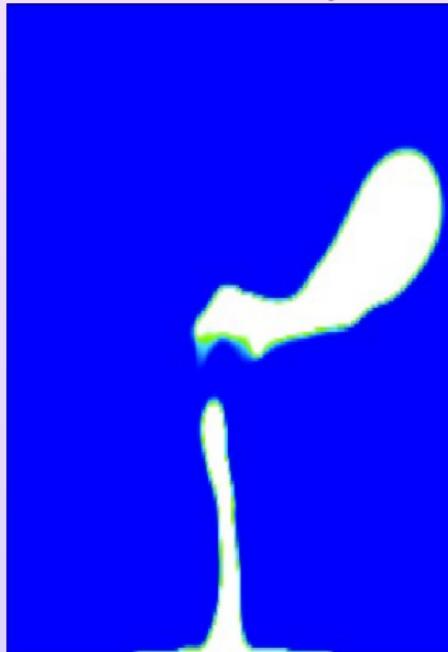
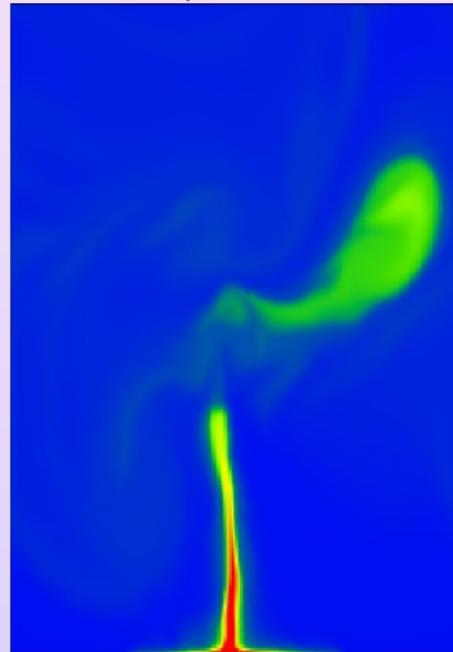
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Nucleating Bubble

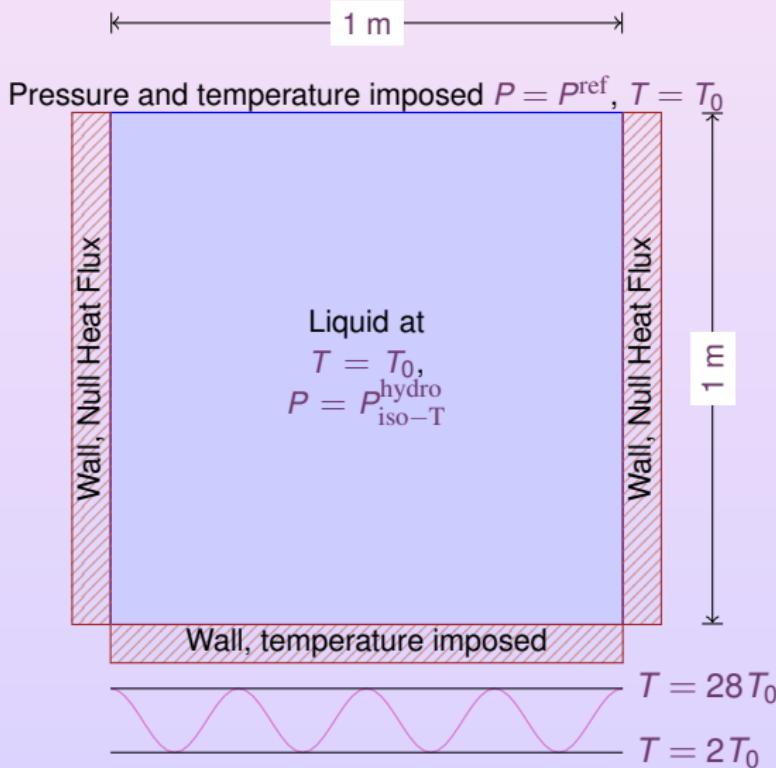
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film



Film

Mass Fraction y



Temperature T



◀ Geometry

▶ Play

▶ Skip

Film

Mass Fraction y



Temperature T

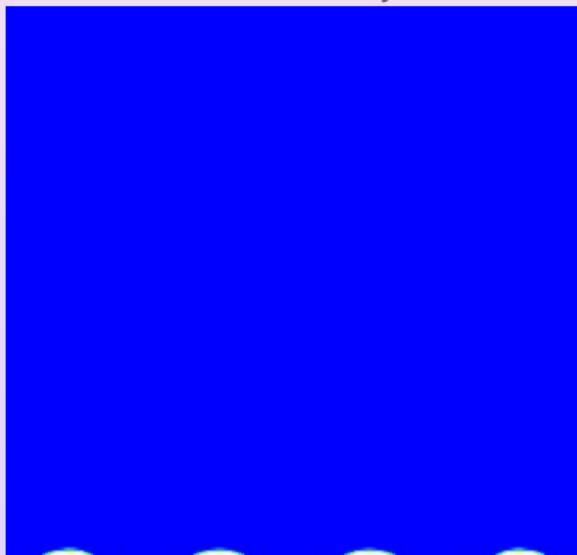
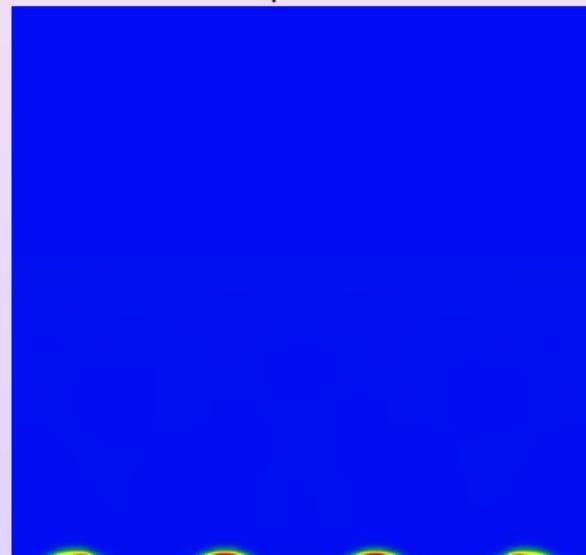


◀ Geometry

▶ Play

▶ Skip

Film

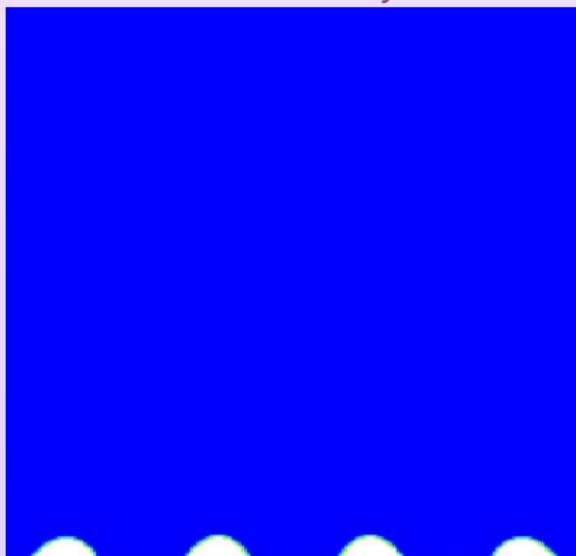
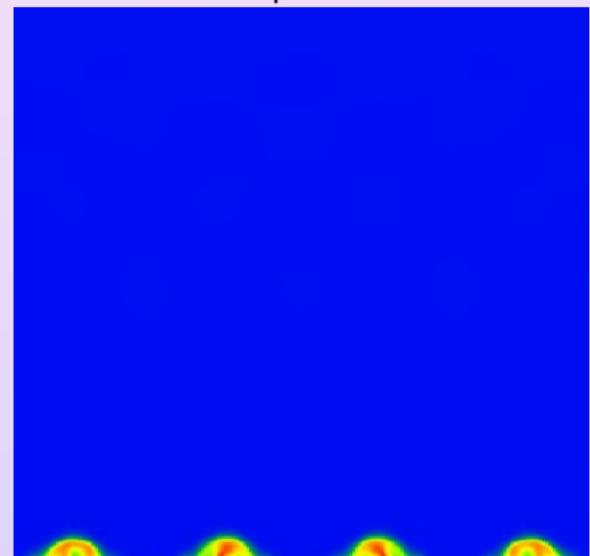
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

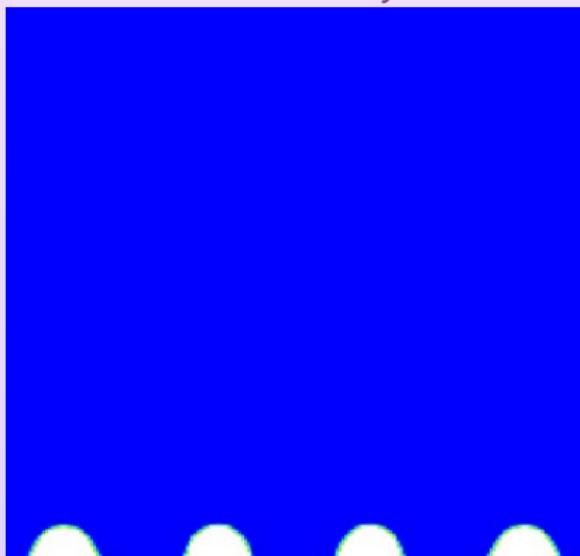
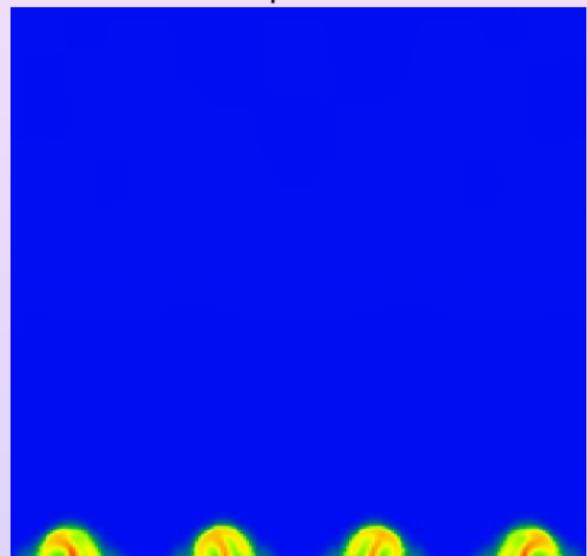
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

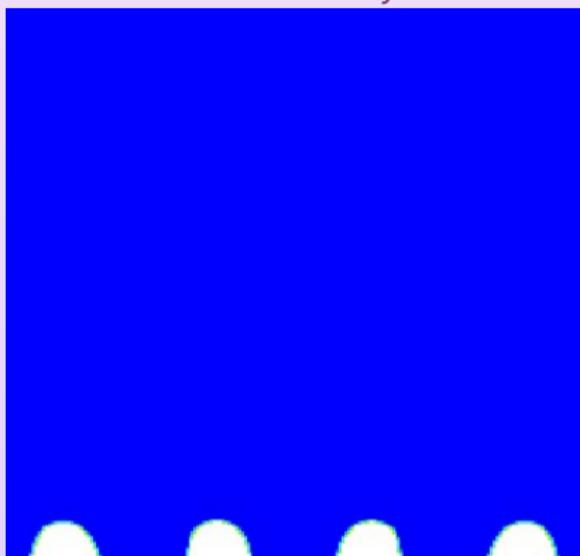
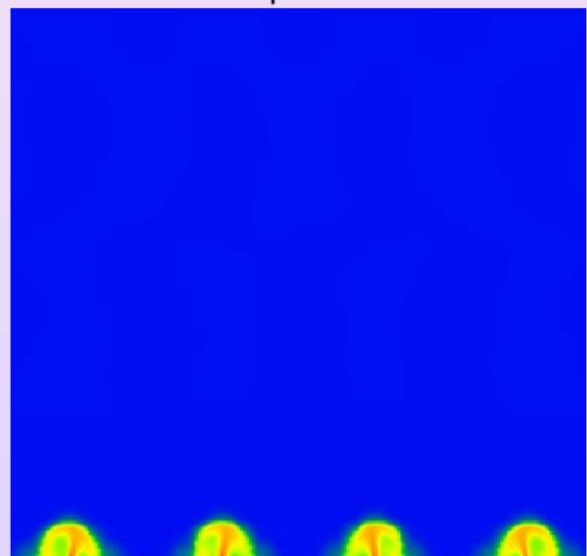
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

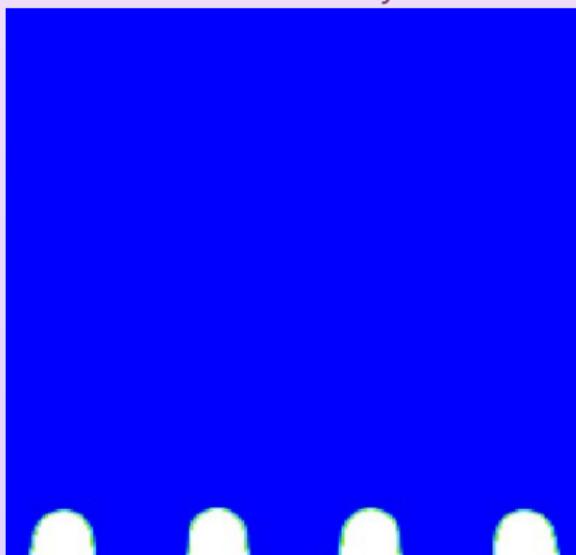
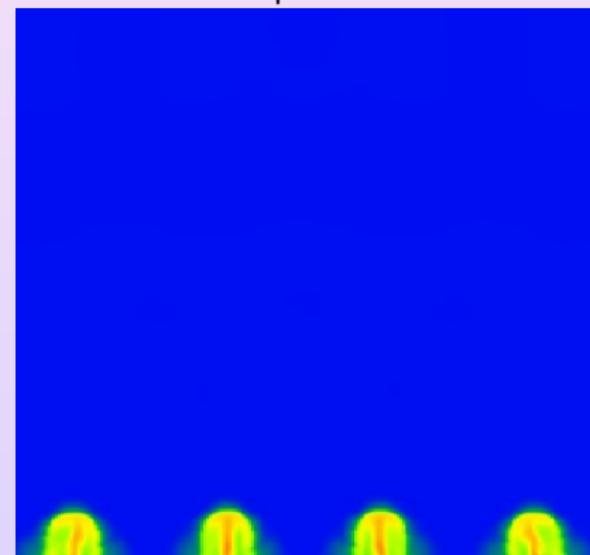
Mass Fraction y Temperature T 

◀ Geometry

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▶ Skip

Film

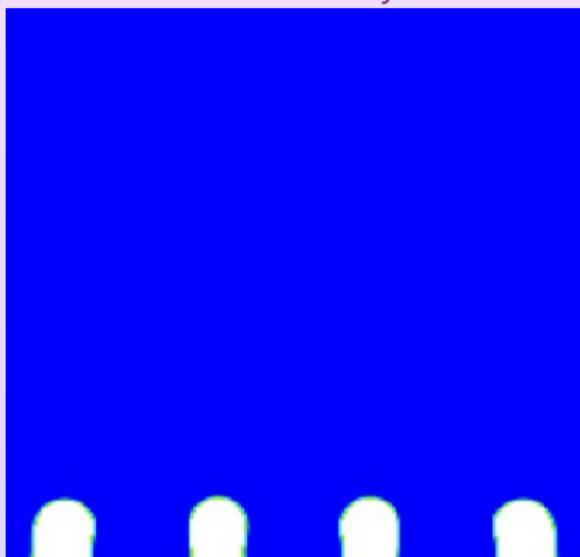
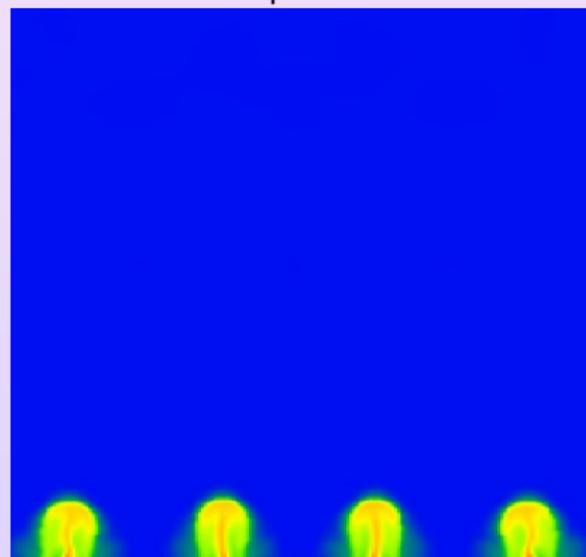
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

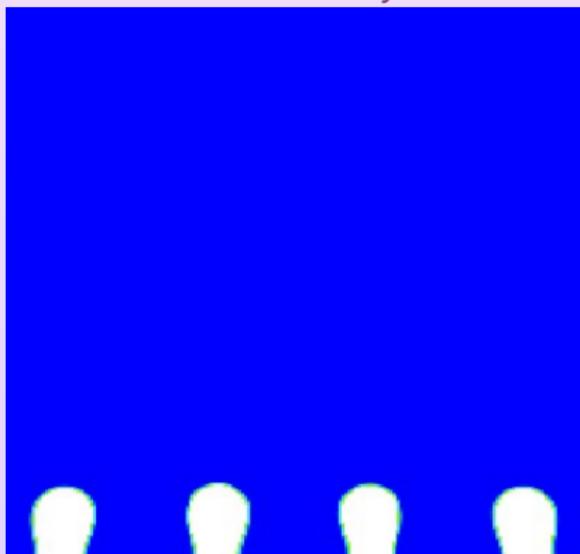
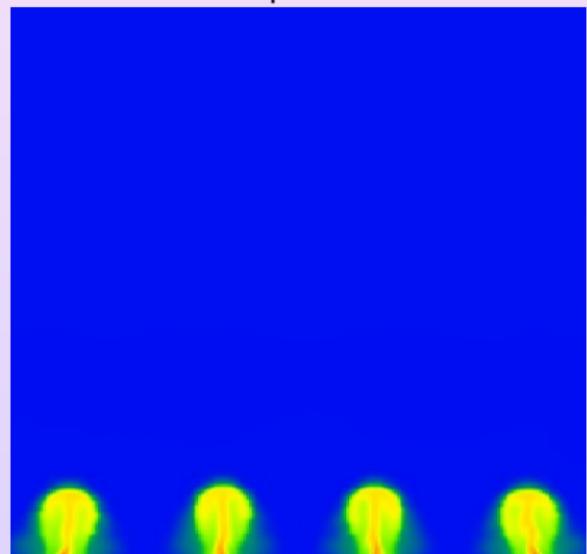
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

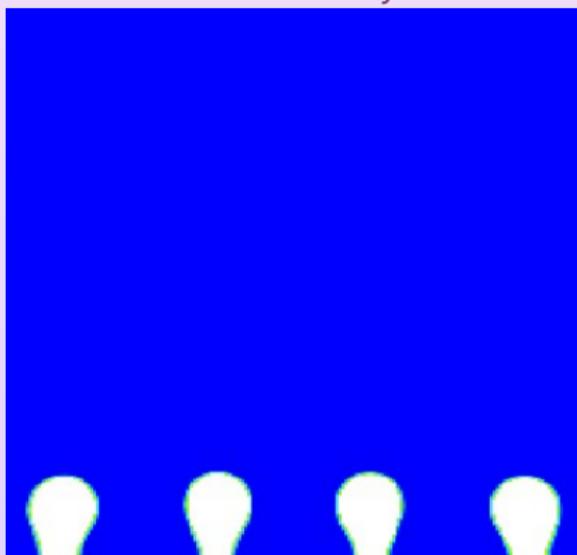
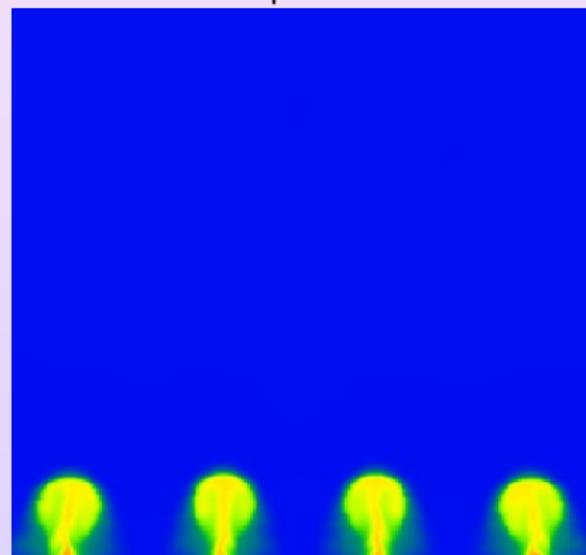
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

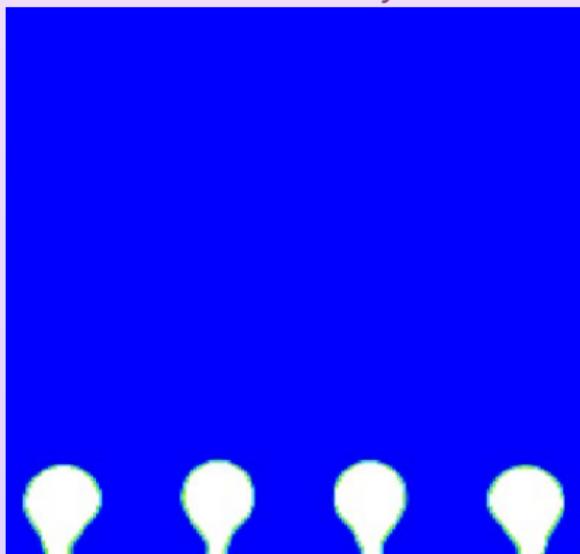
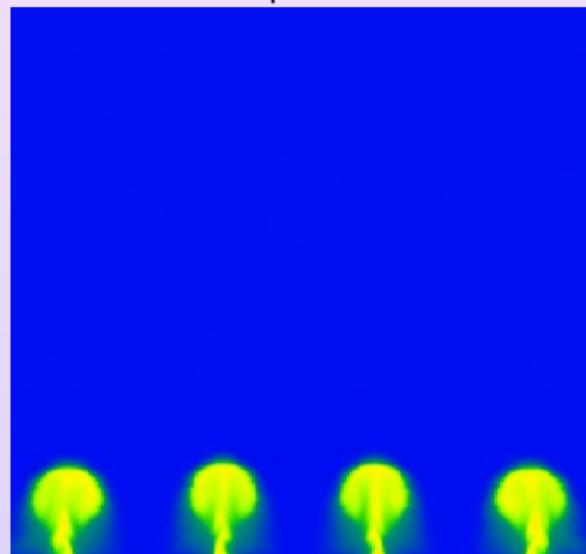
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

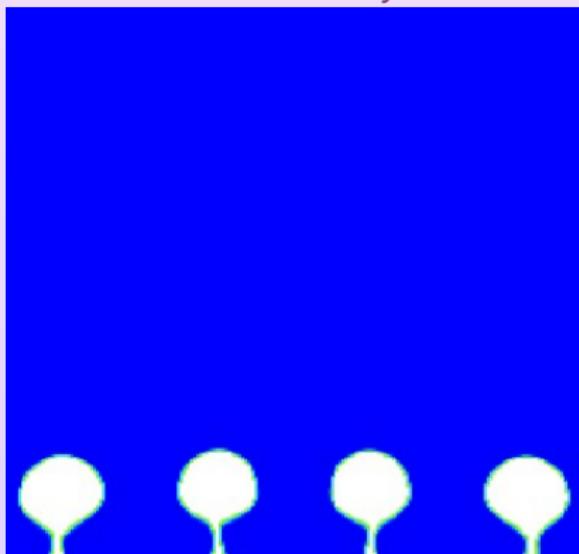
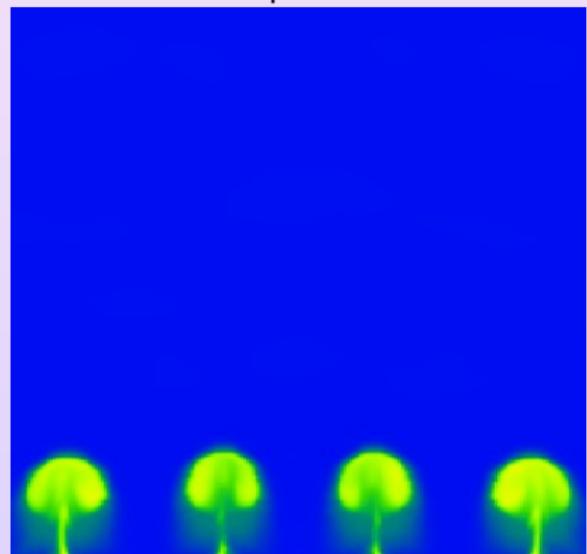
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

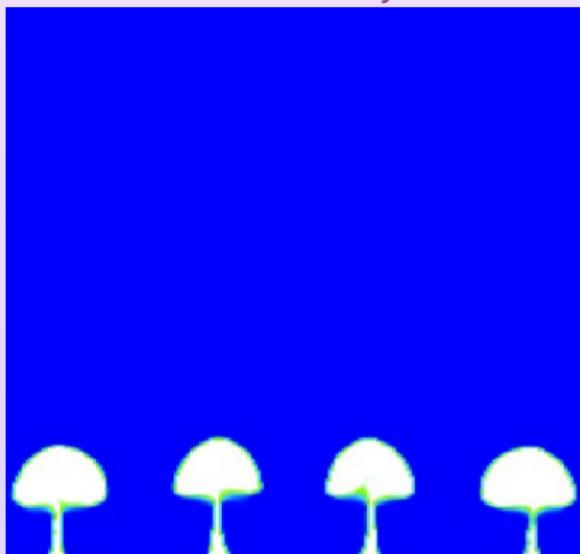
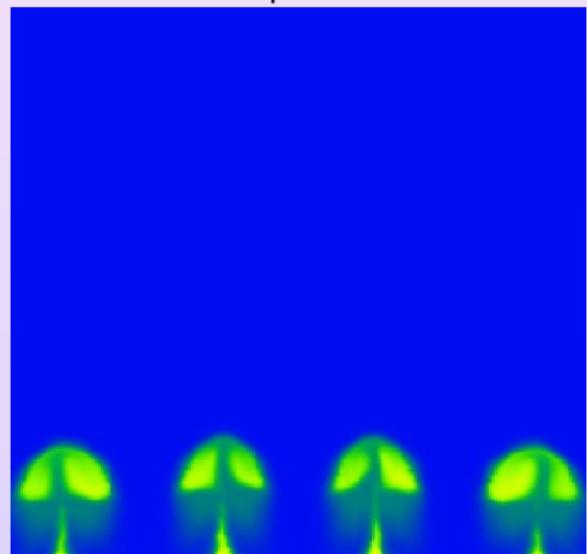
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

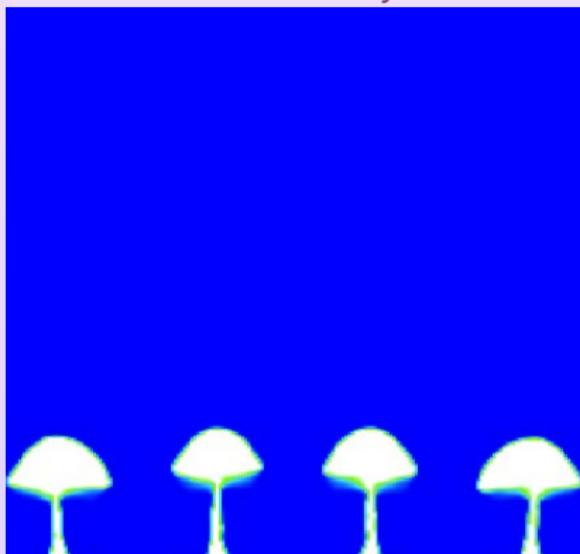
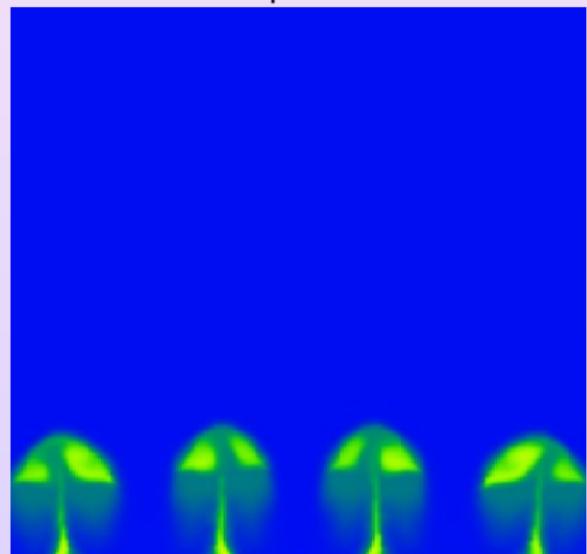
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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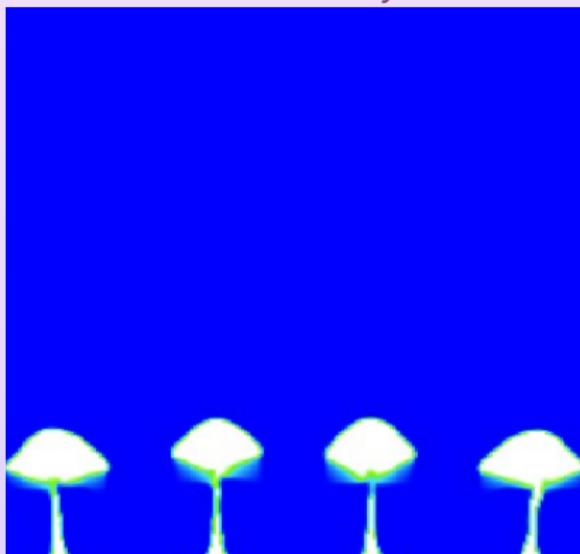
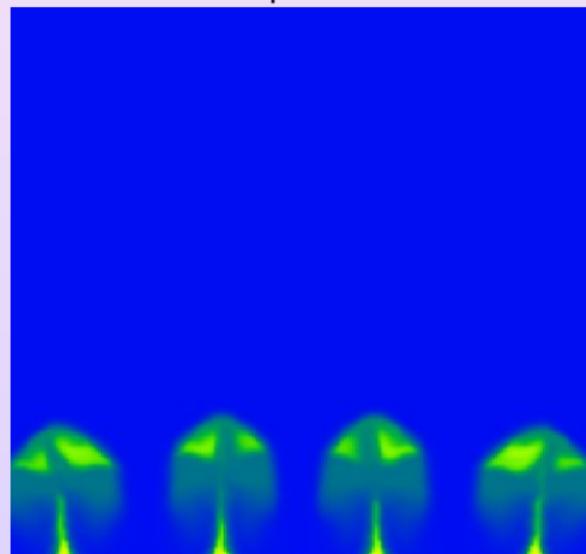
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

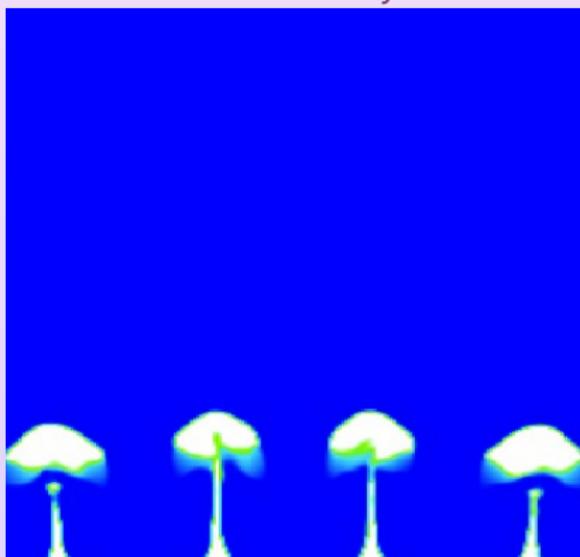
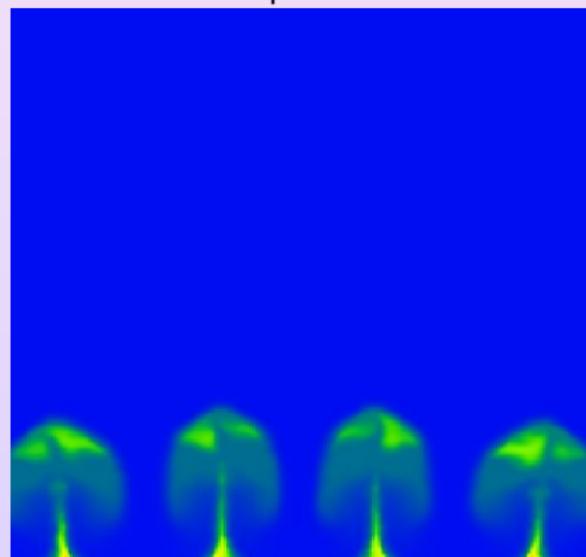
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

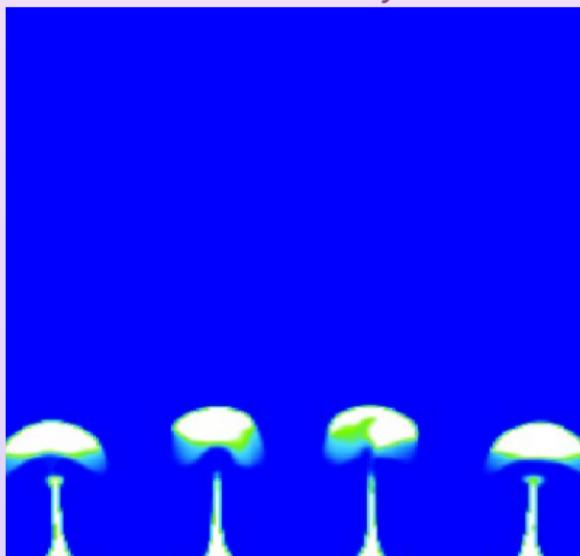
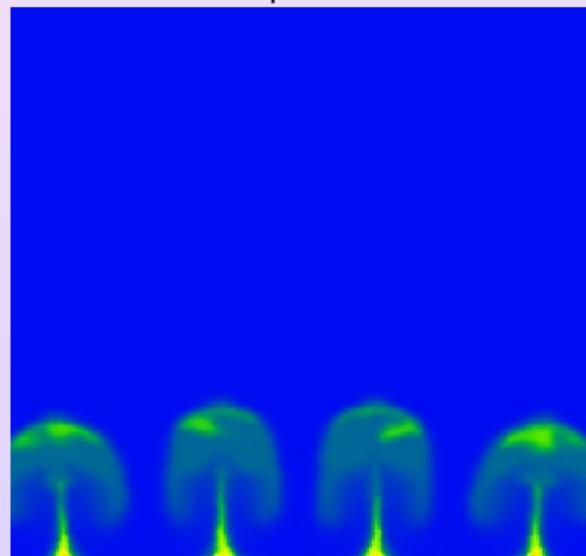
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

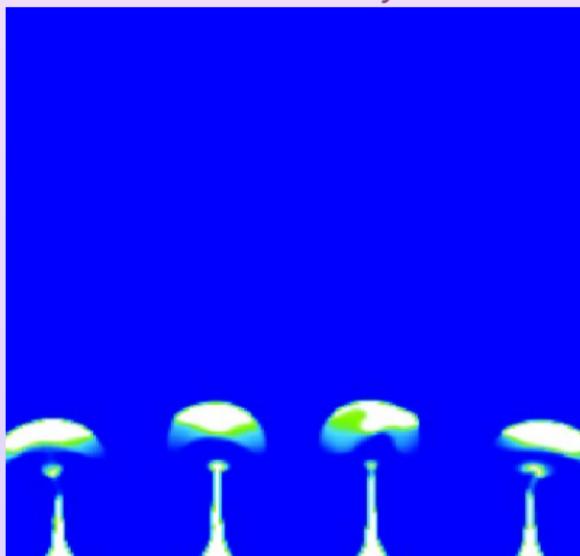
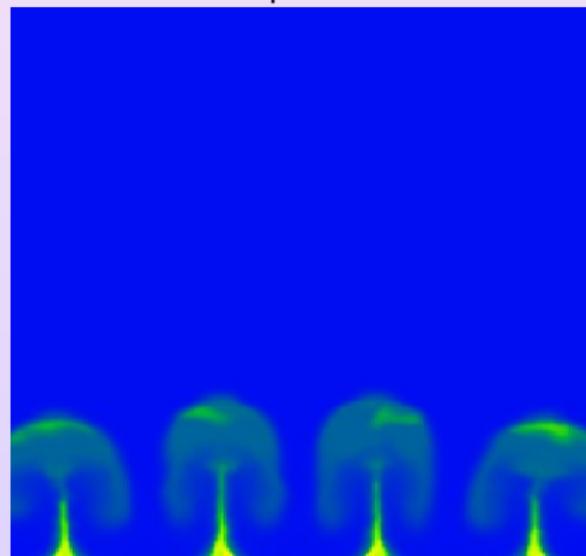
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

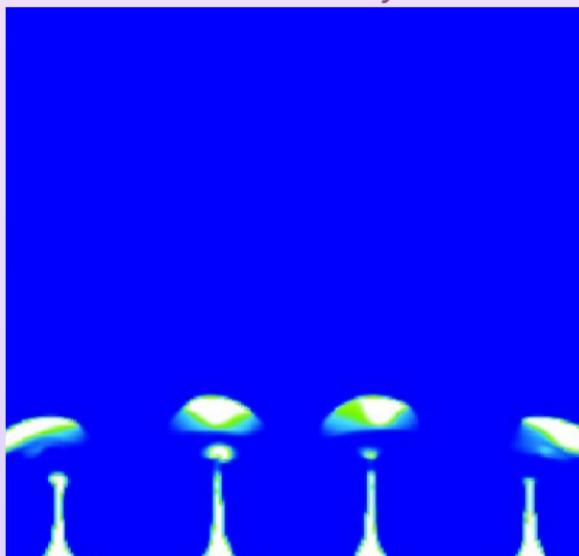
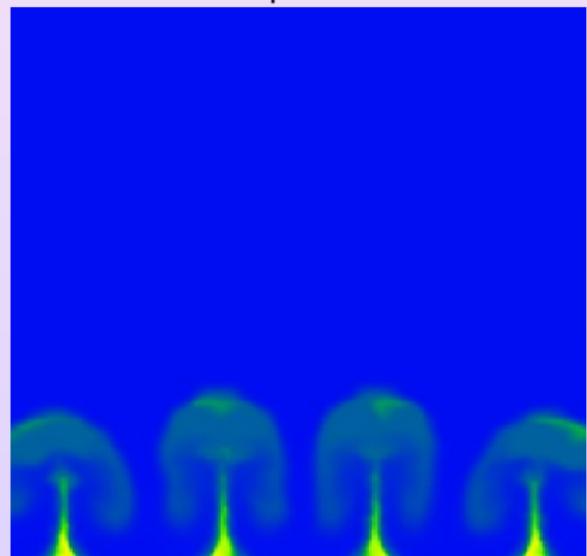
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

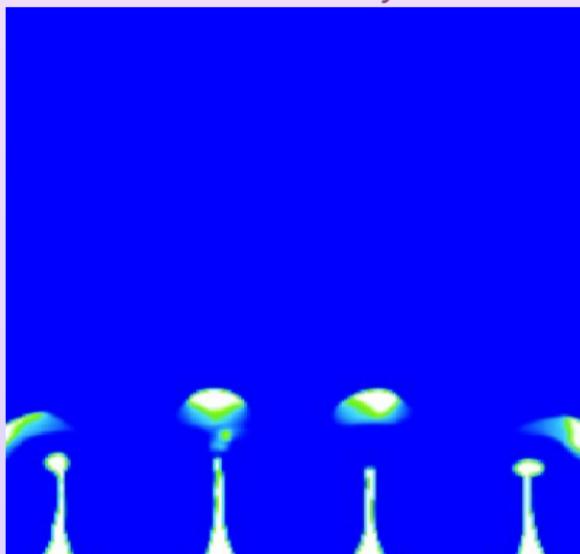
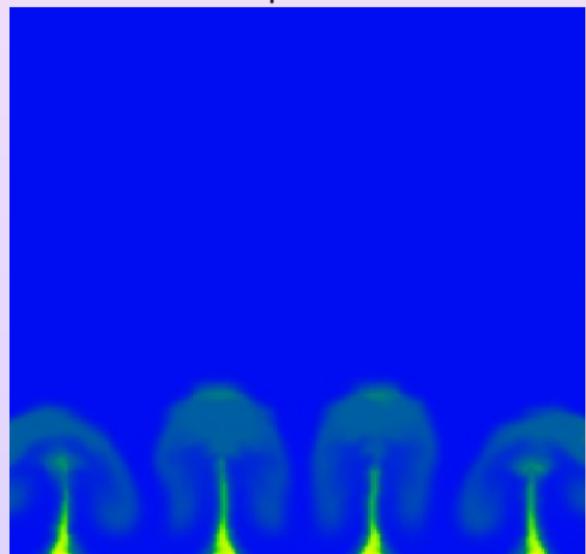
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

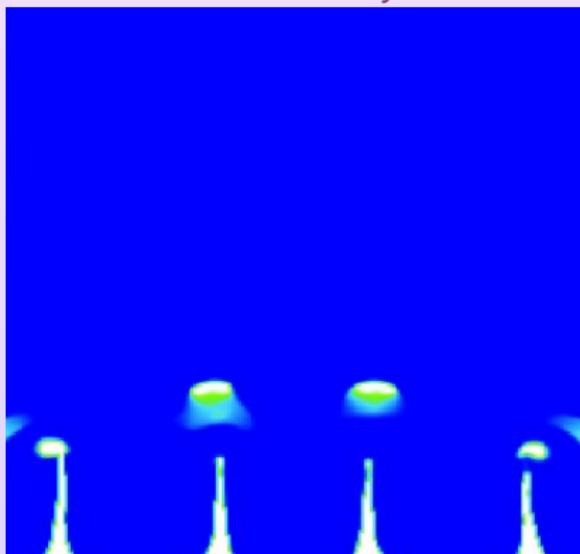
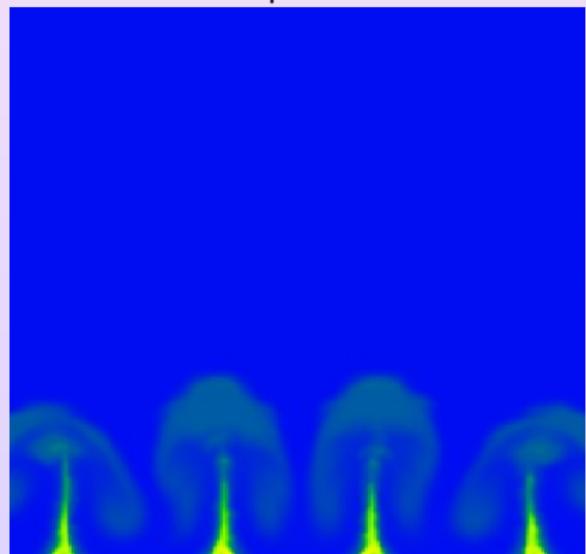
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

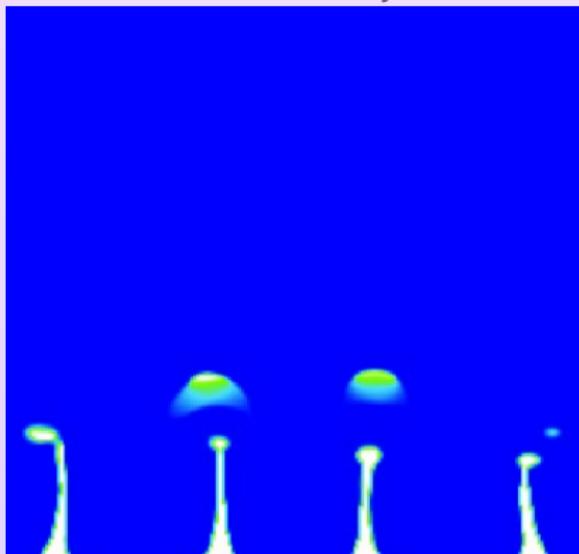
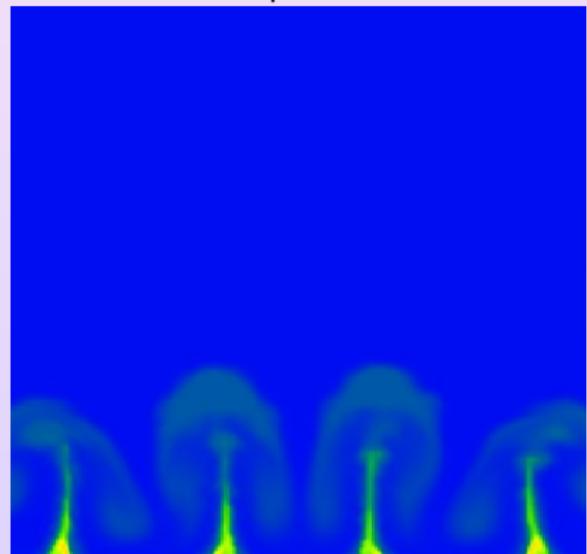
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

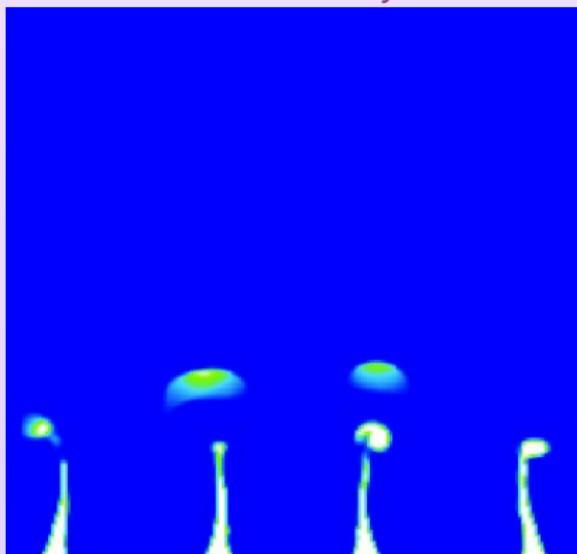
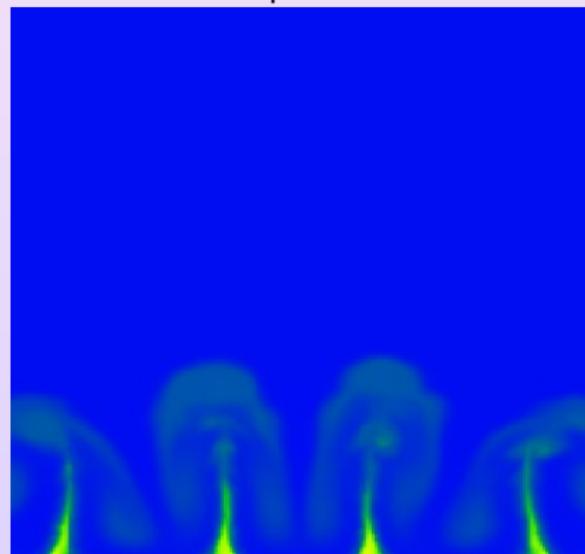
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

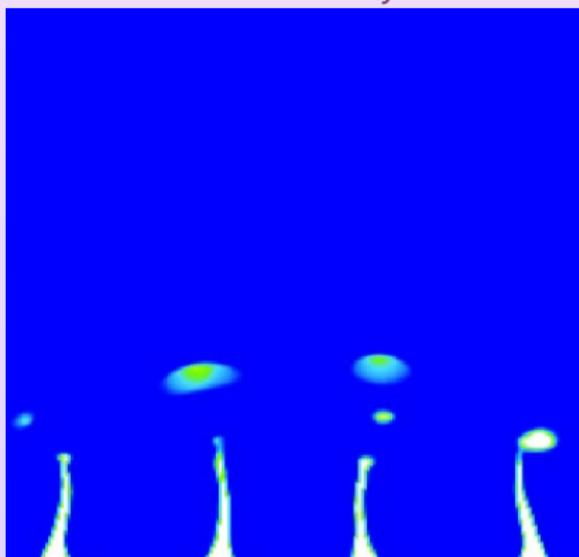
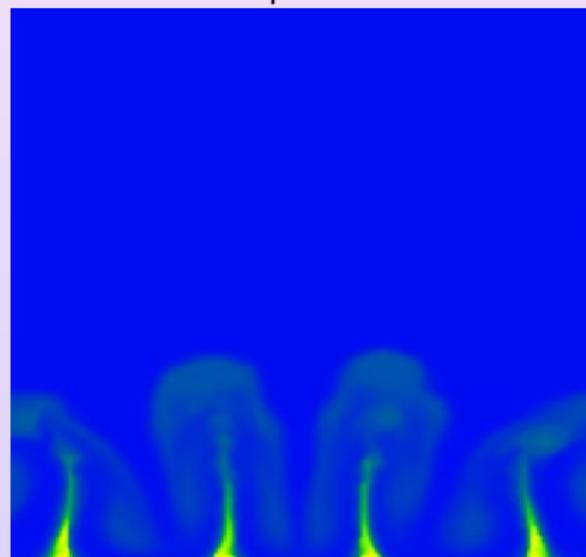
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

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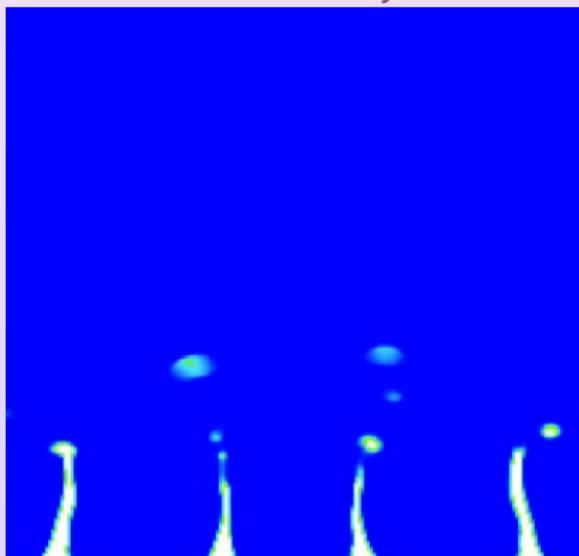
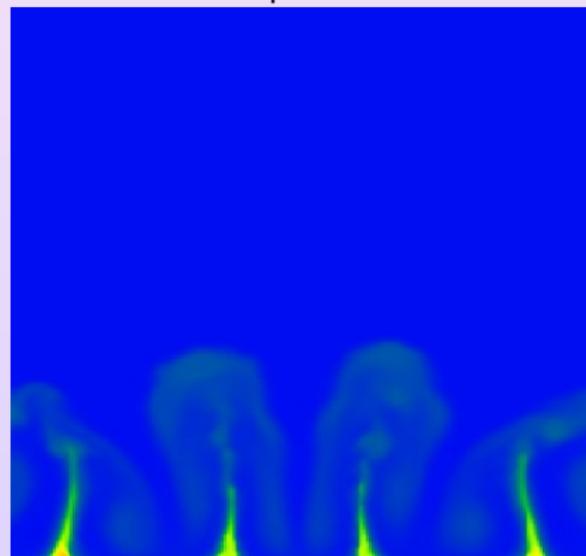
Mass Fraction y Temperature T 

◀ Geometry

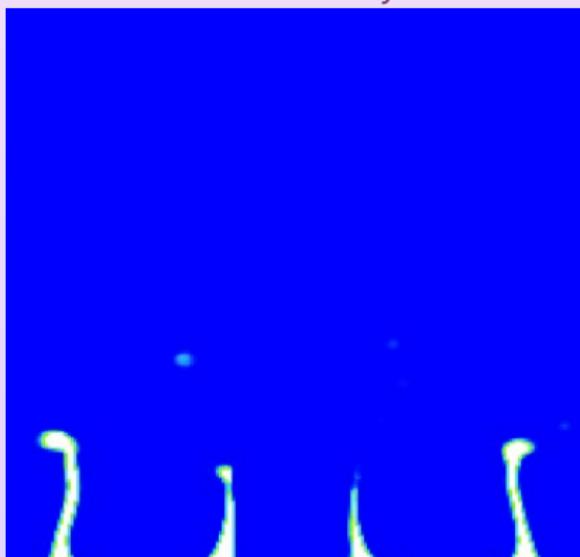
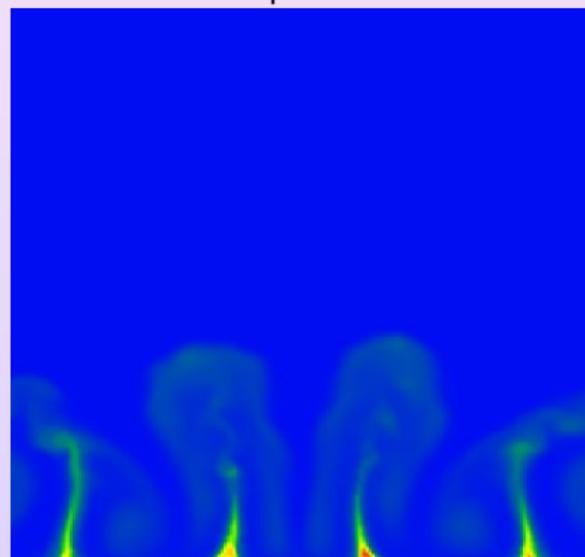
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Film

Mass Fraction y Temperature T [◀ Geometry](#)[▶ Play](#)[▶ Skip](#)

Film

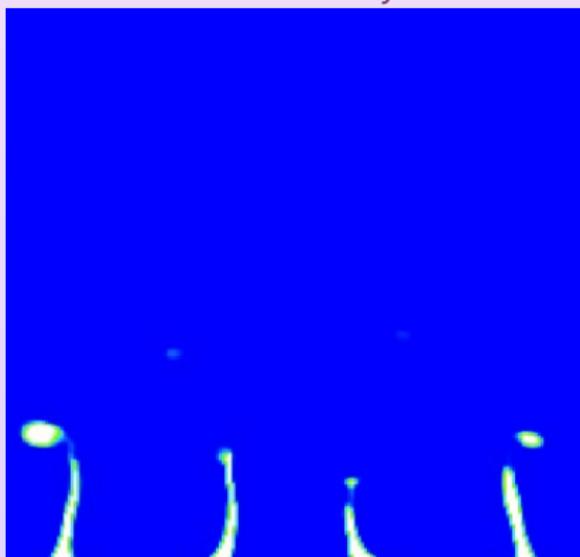
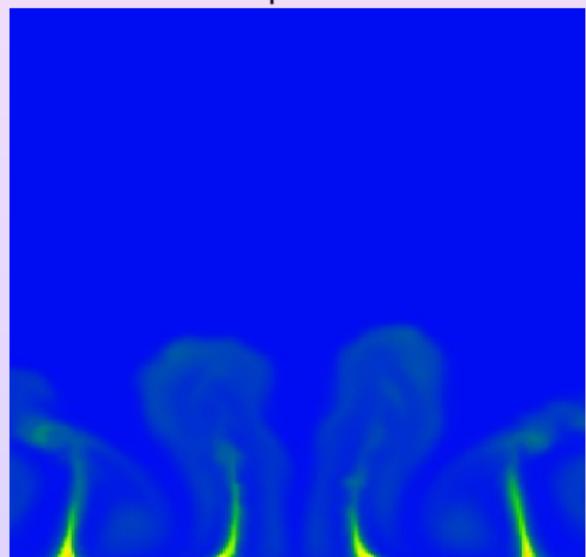
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

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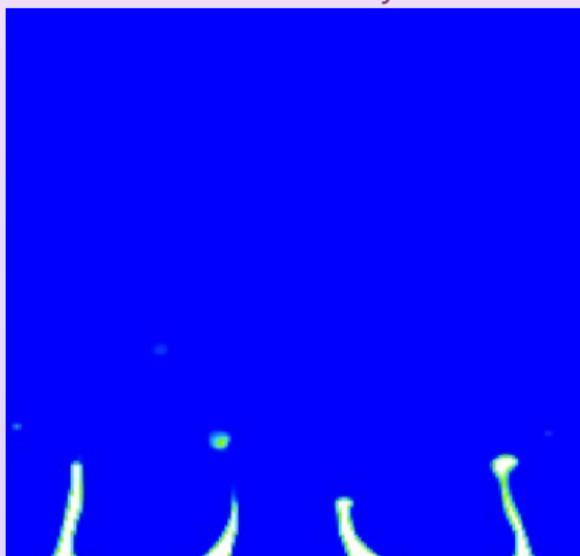
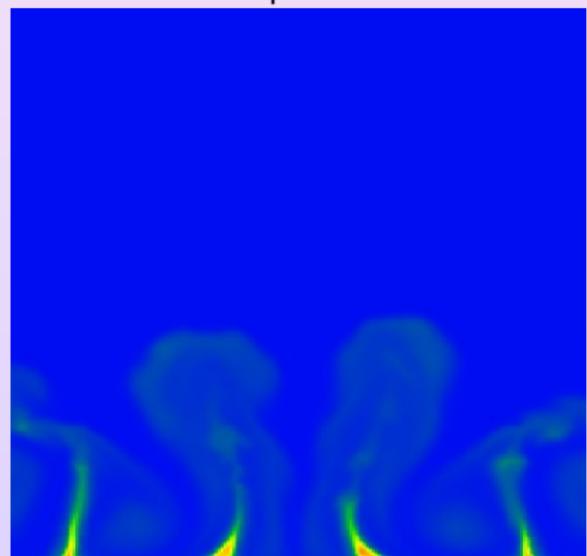
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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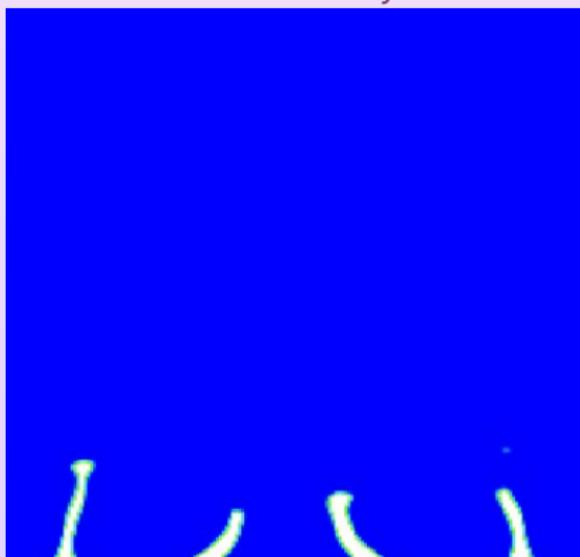
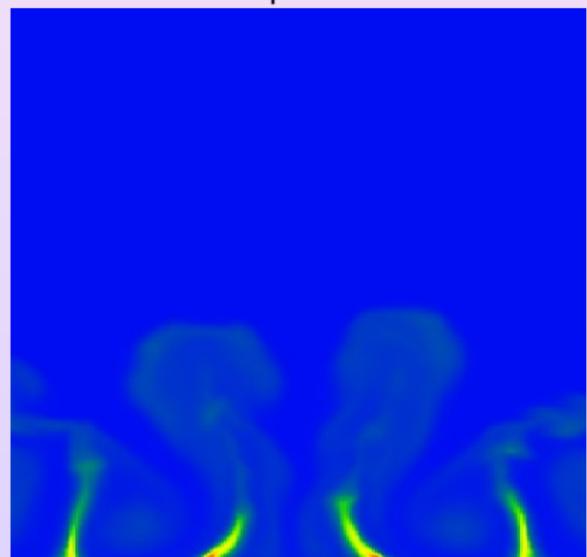
Mass Fraction y Temperature T 

◀ Geometry

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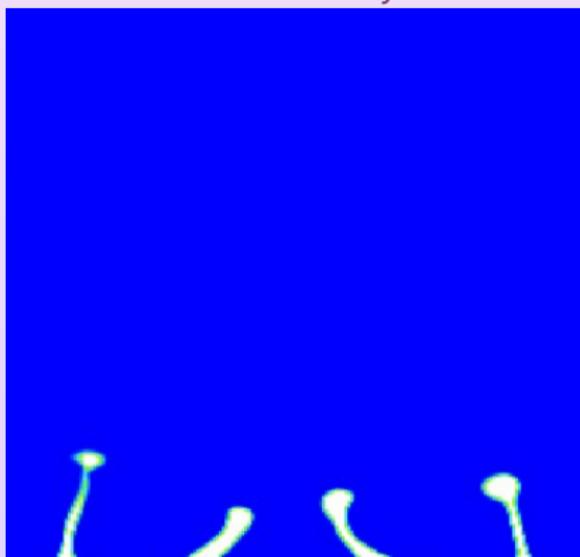
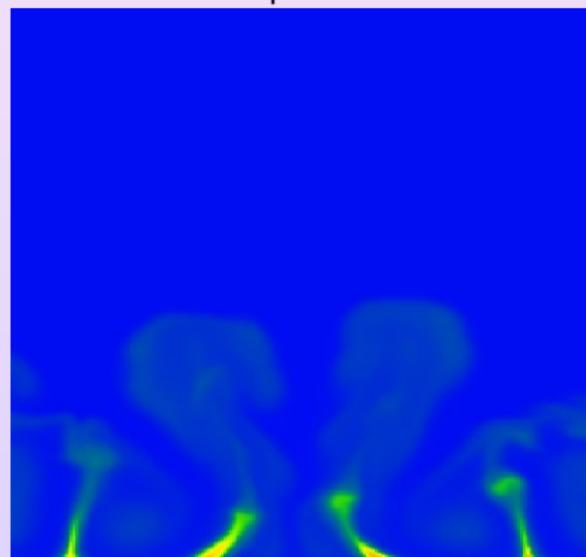
Mass Fraction y Temperature T 

◀ Geometry

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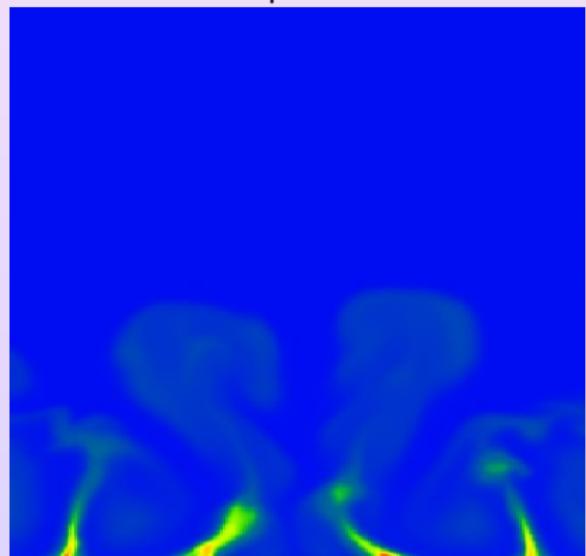
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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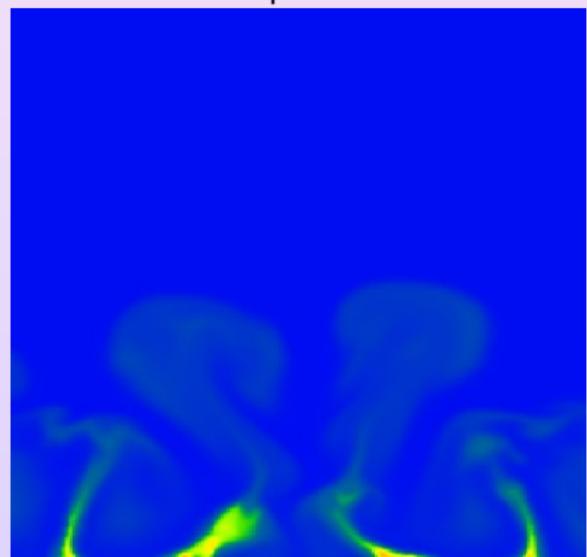
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◀ Geometry

▶ Play

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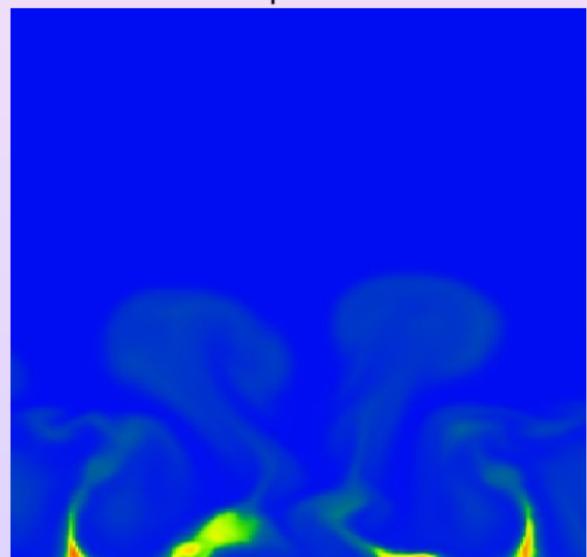
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

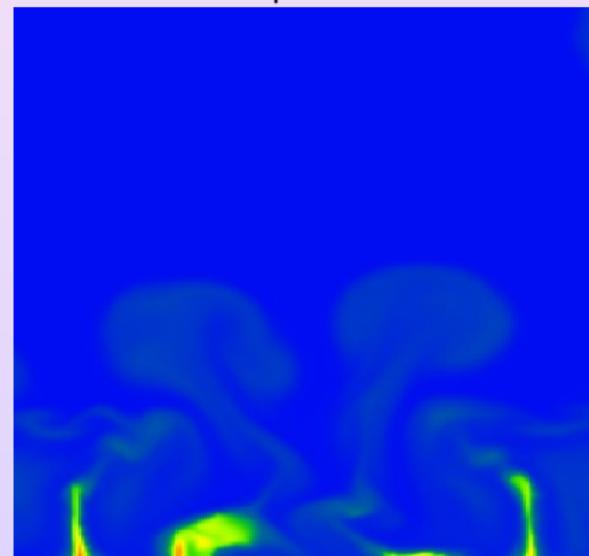
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◀ Geometry

▶ Play

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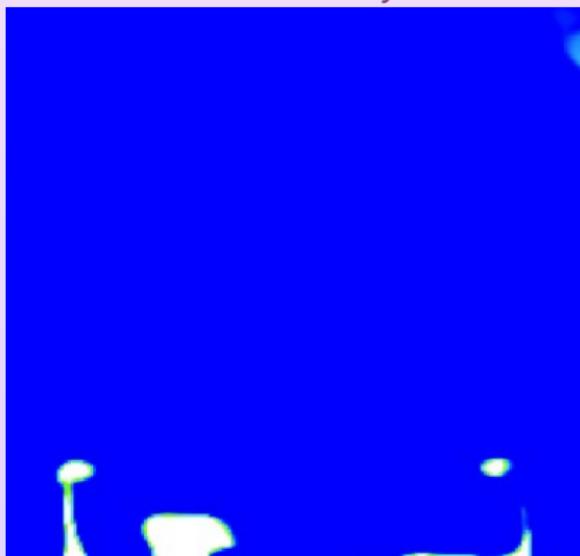
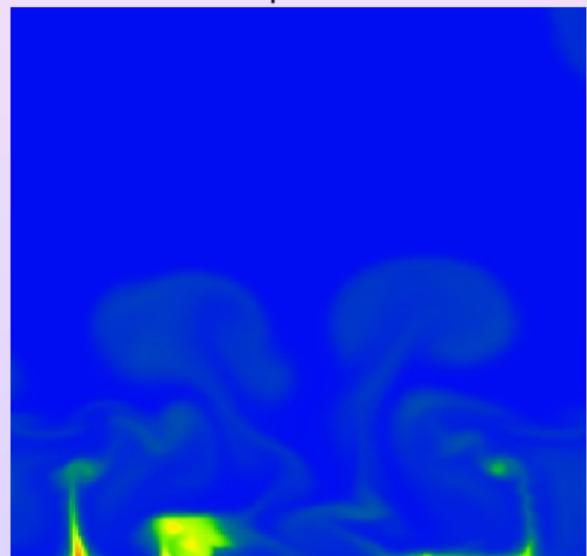
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◀ Geometry

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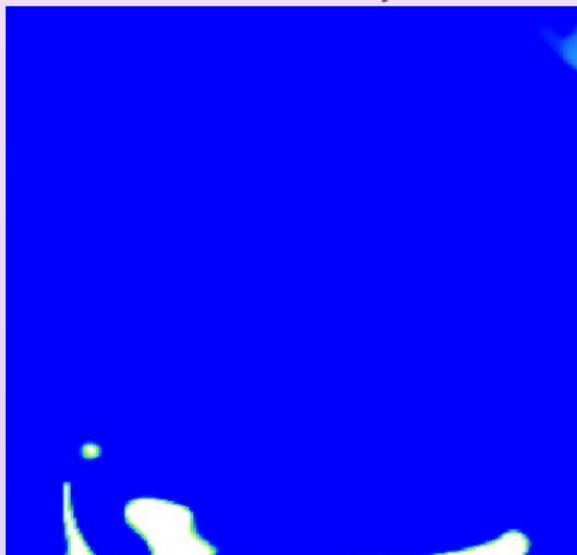
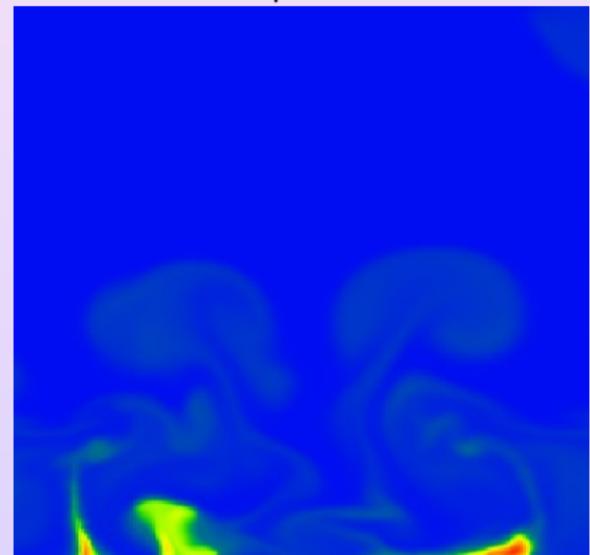
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◀ Geometry

▶ Play

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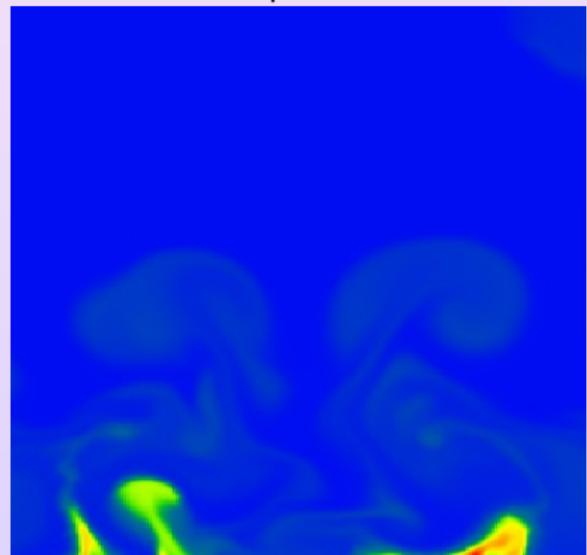
Mass Fraction y Temperature T 

◀ Geometry

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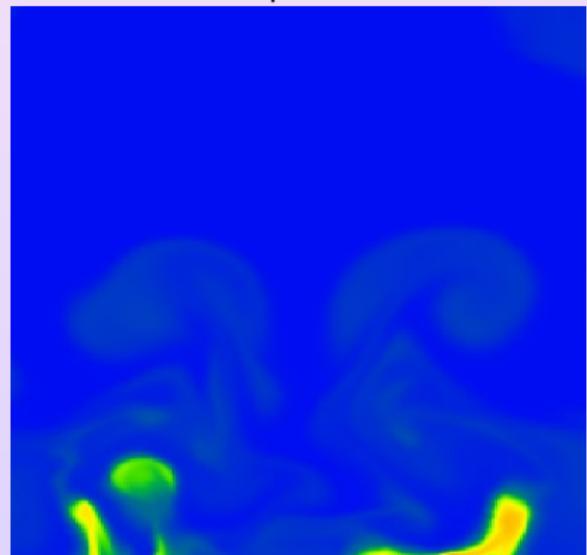
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◀ Geometry

▶ Play

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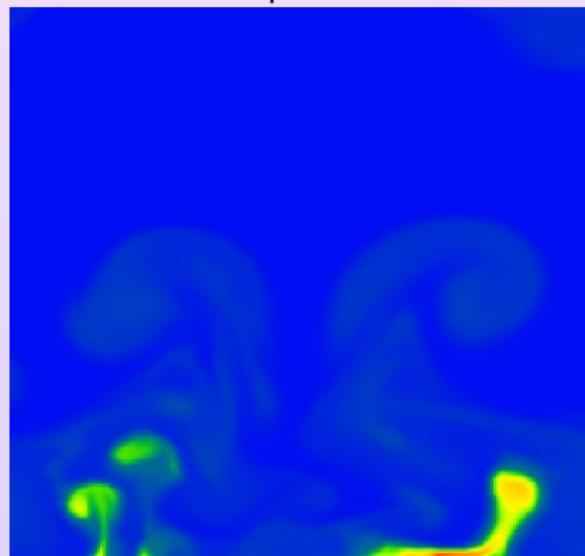
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◀ Geometry

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Film

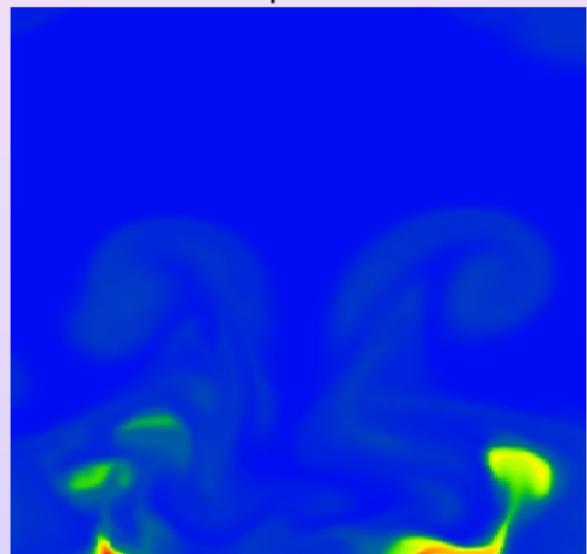
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

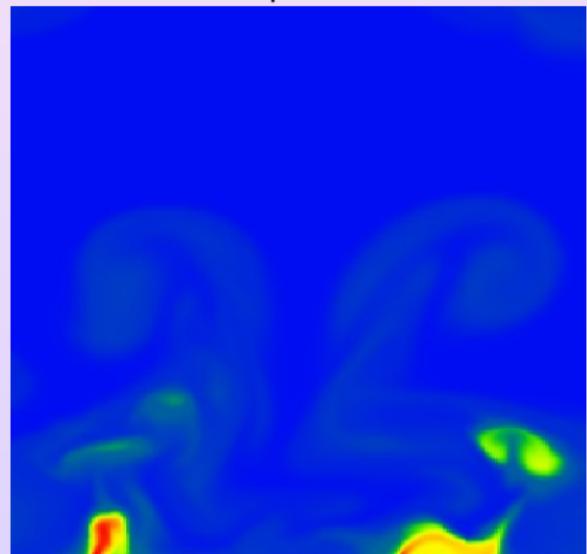
Mass Fraction y Temperature T 

◀ Geometry

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Film

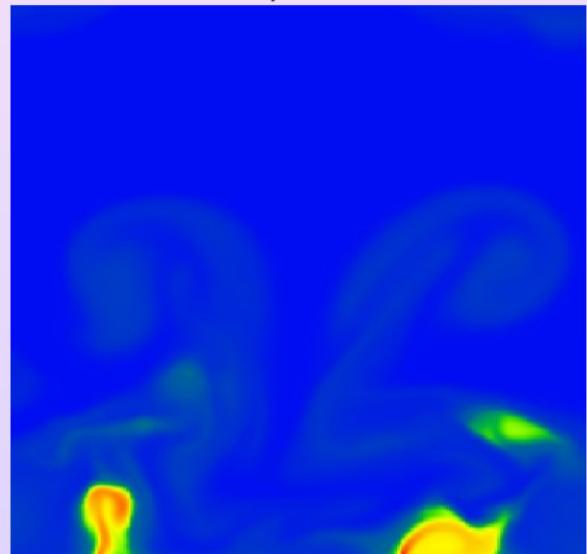
Mass Fraction y Temperature T 

◀ Geometry

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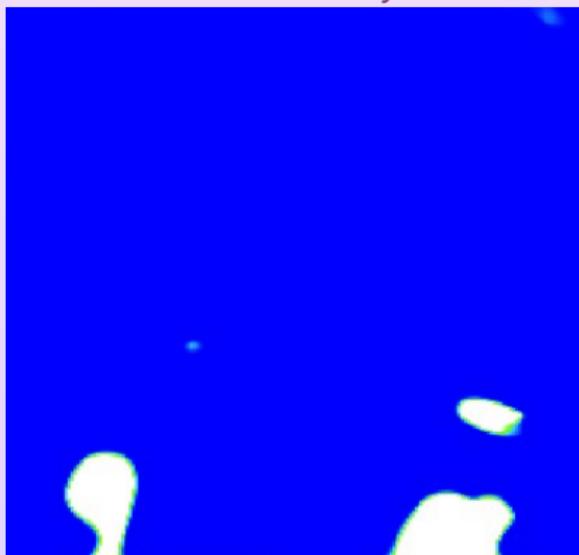
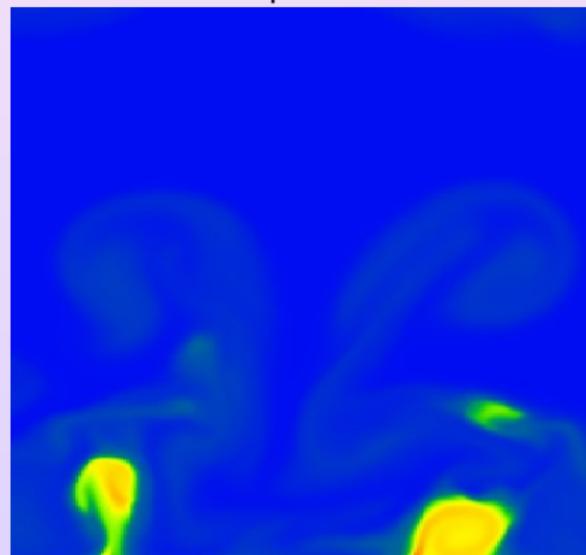
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◀ Geometry

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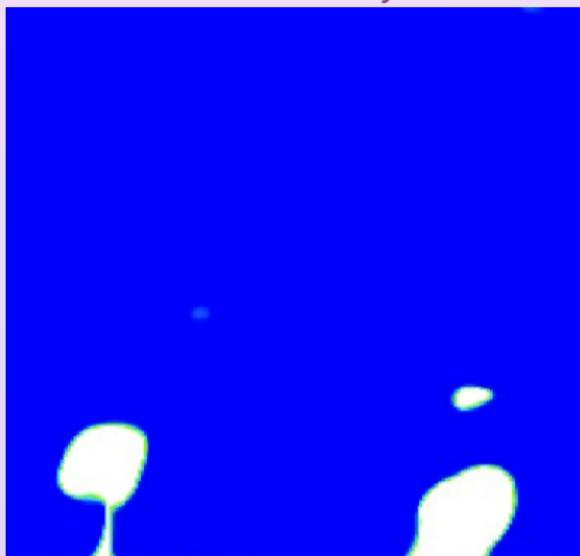
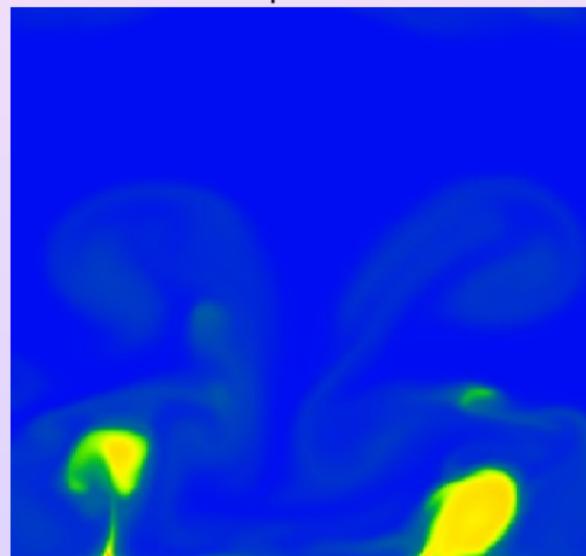
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◀ Geometry

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Film

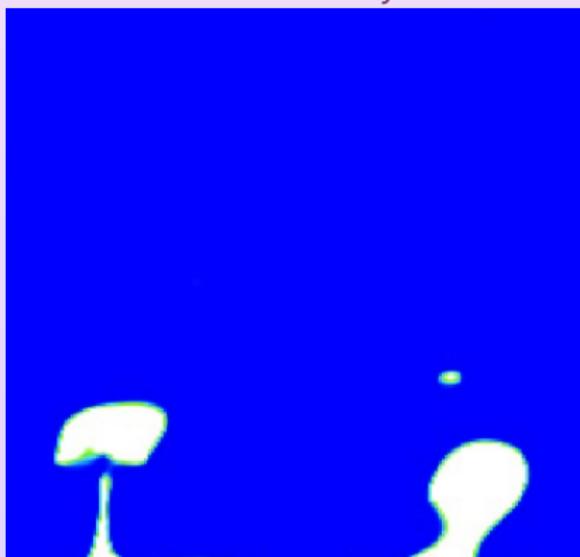
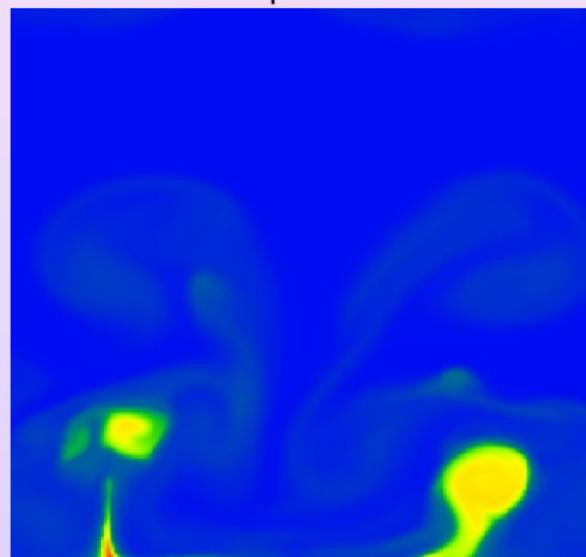
Mass Fraction y Temperature T 

◀ Geometry

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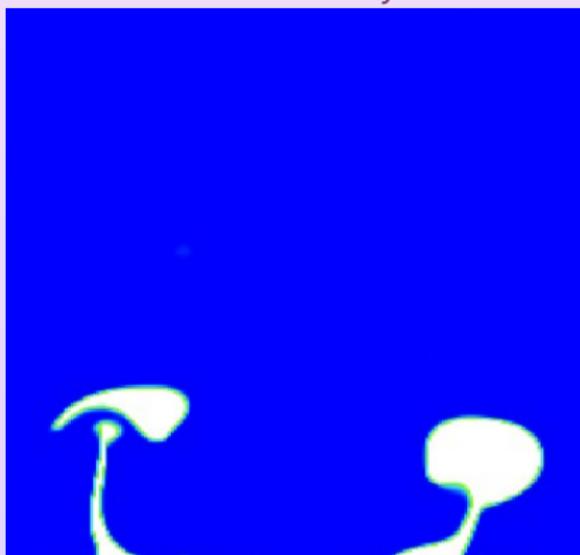
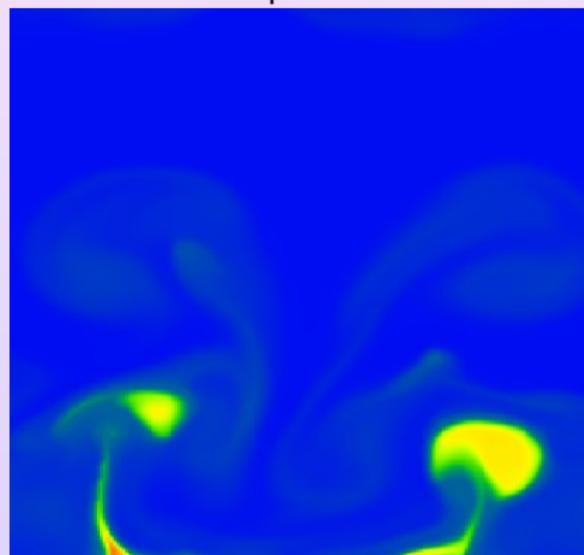
Mass Fraction y Temperature T 

◀ Geometry

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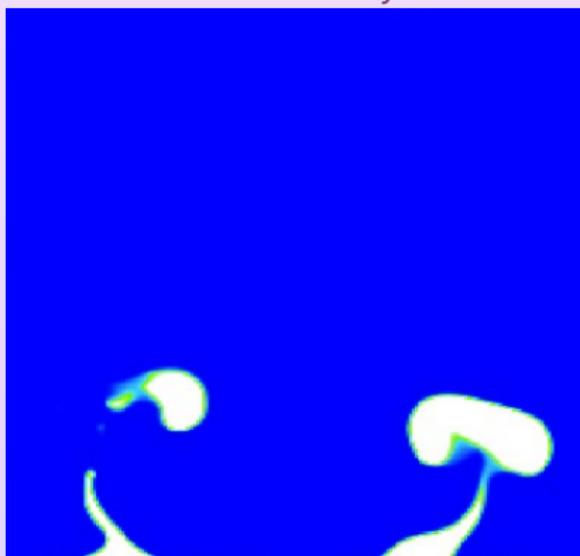
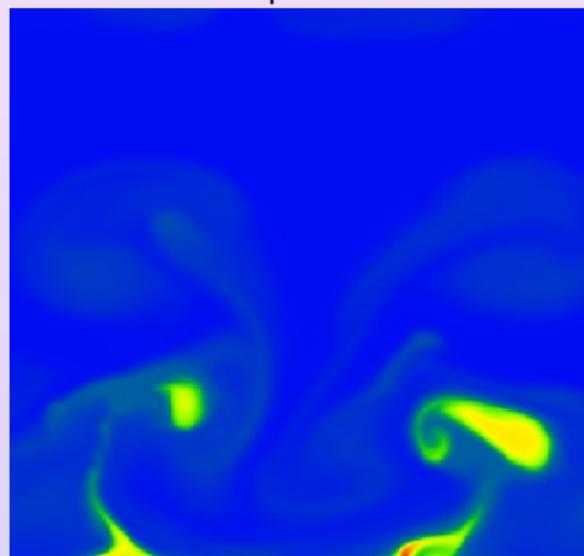
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◀ Geometry

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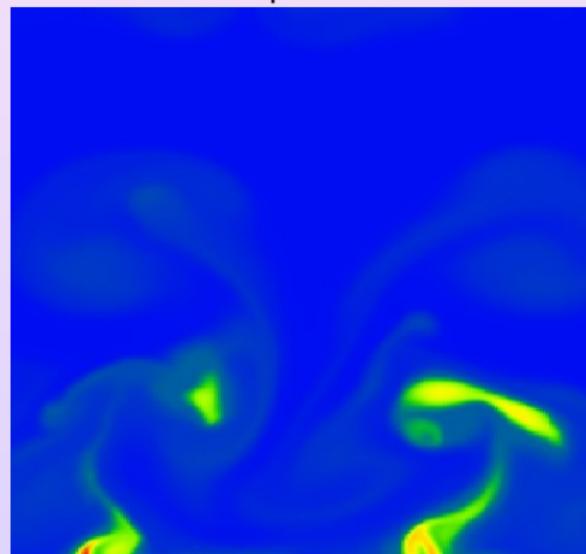
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◀ Geometry

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Film

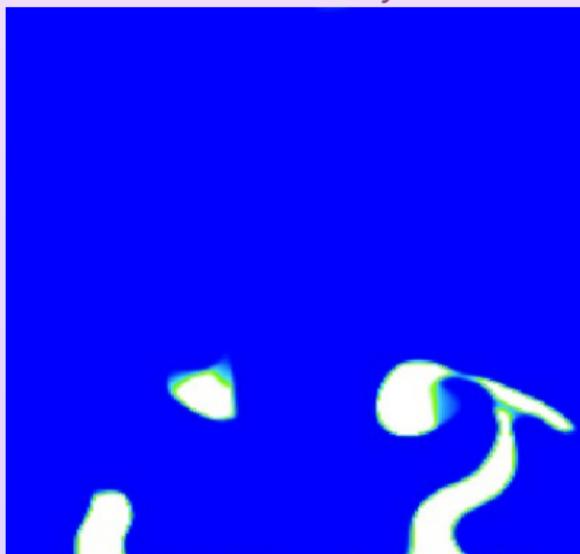
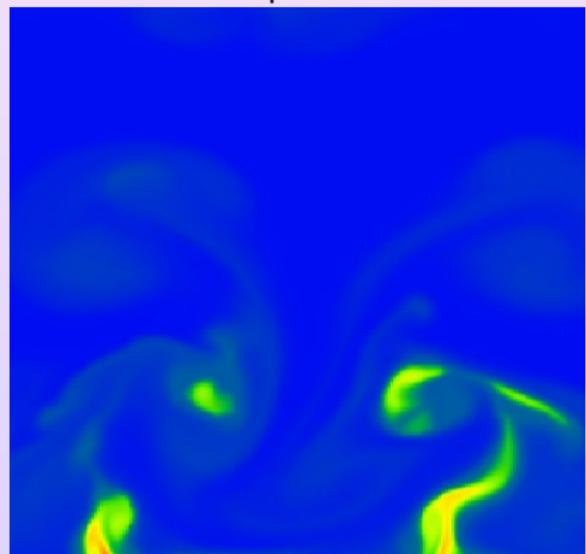
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◀ Geometry

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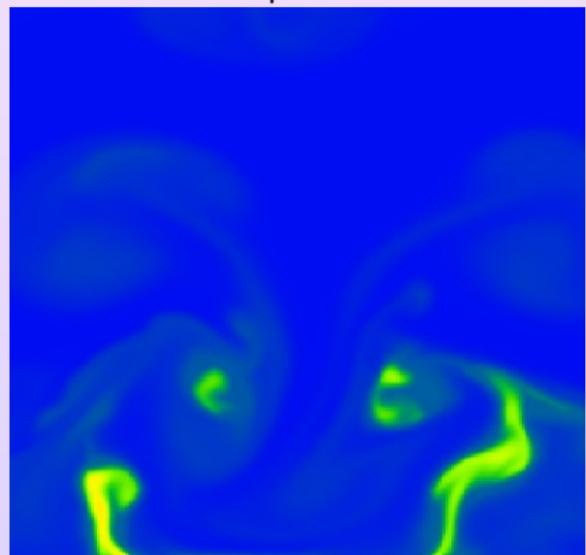
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◀ Geometry

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Film

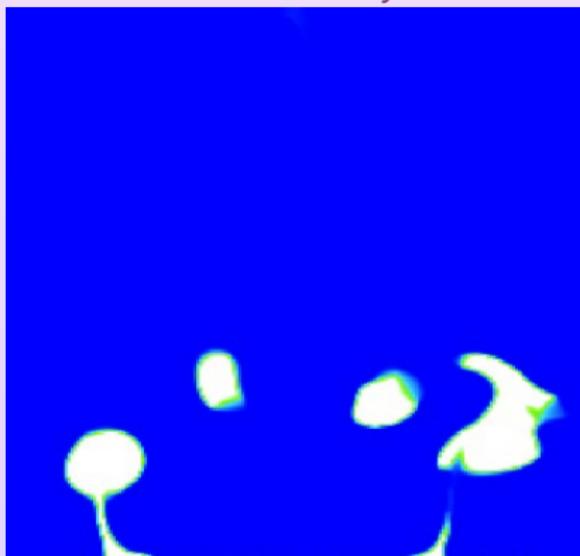
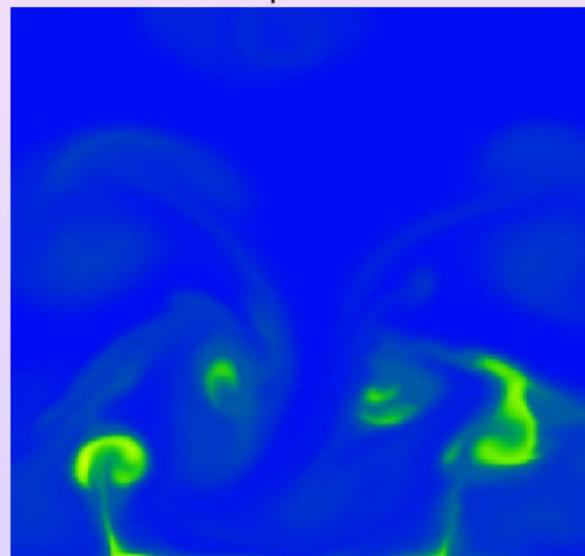
Mass Fraction y Temperature T 

◀ Geometry

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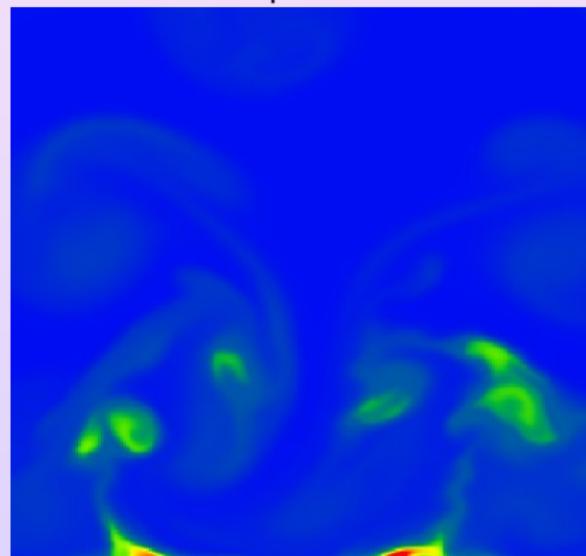
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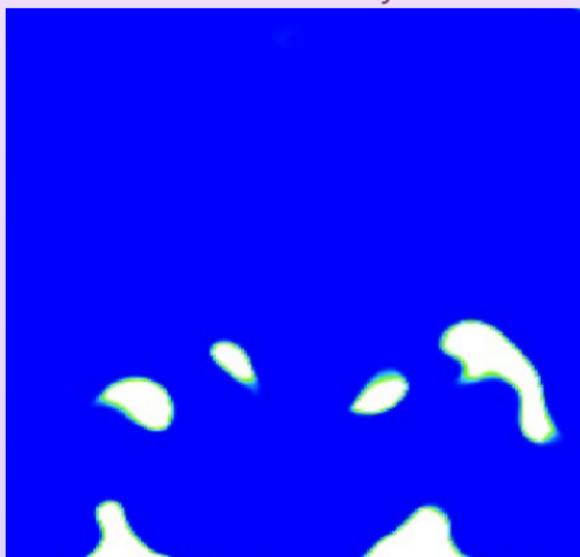
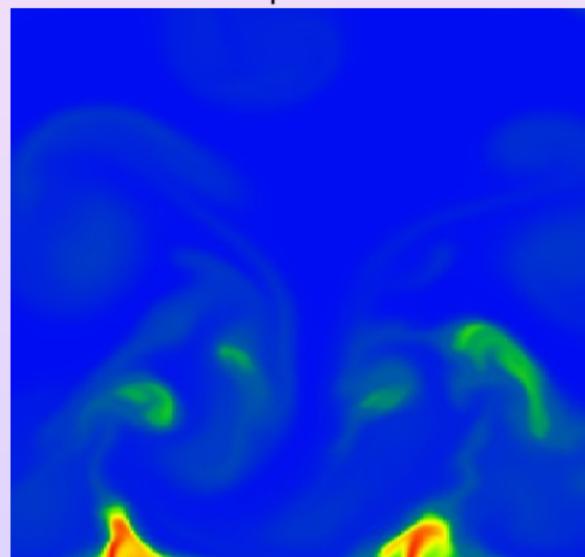
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

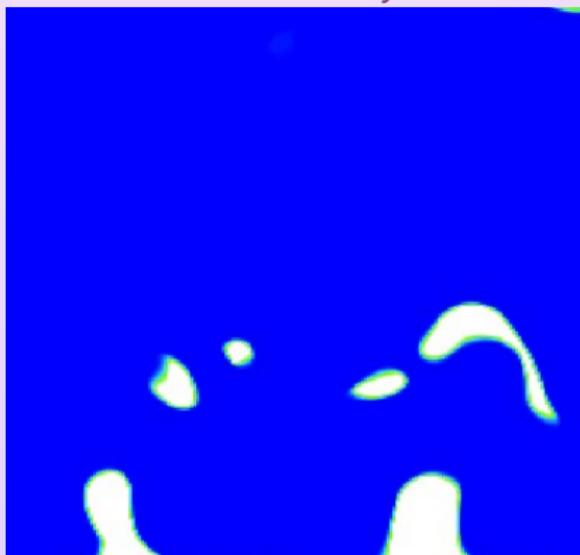
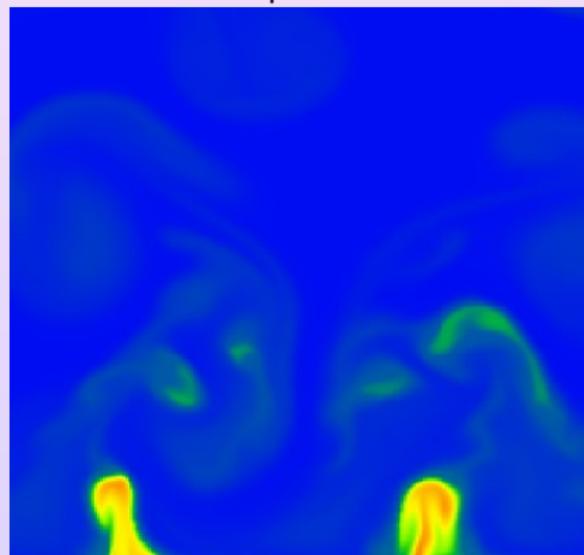
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

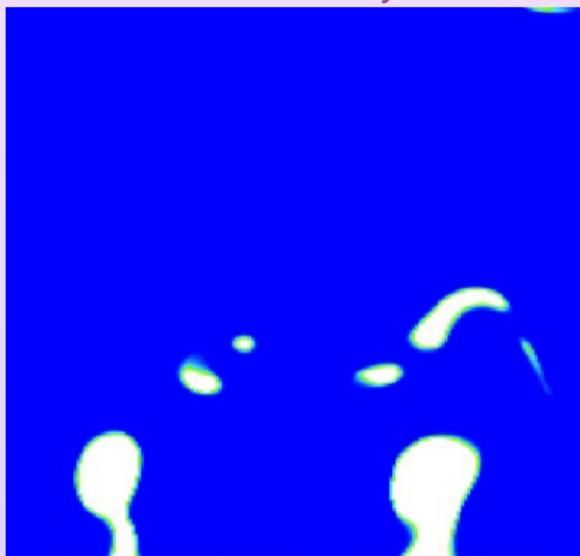
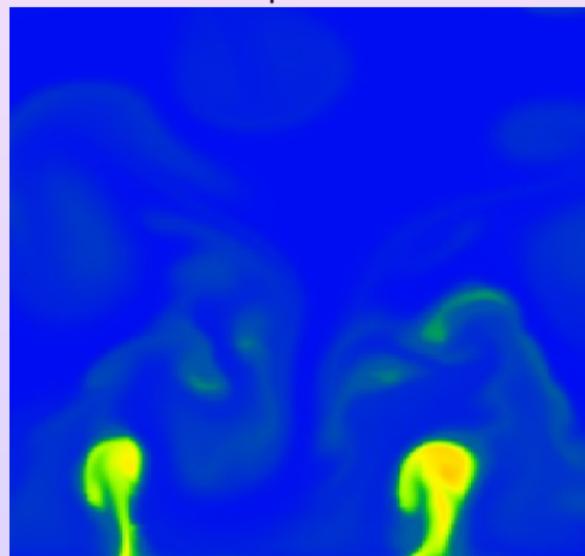
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

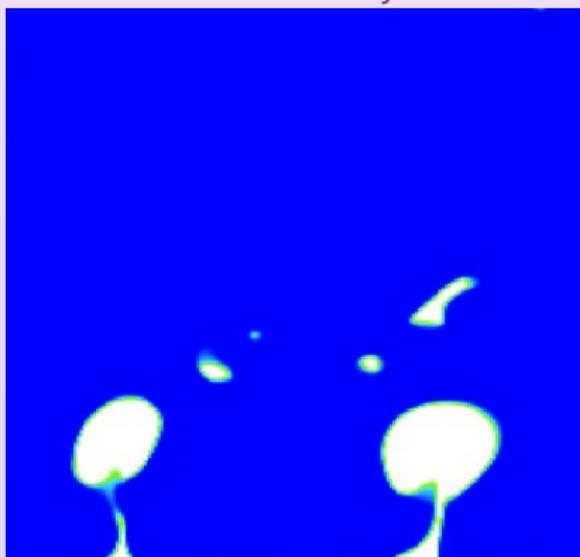
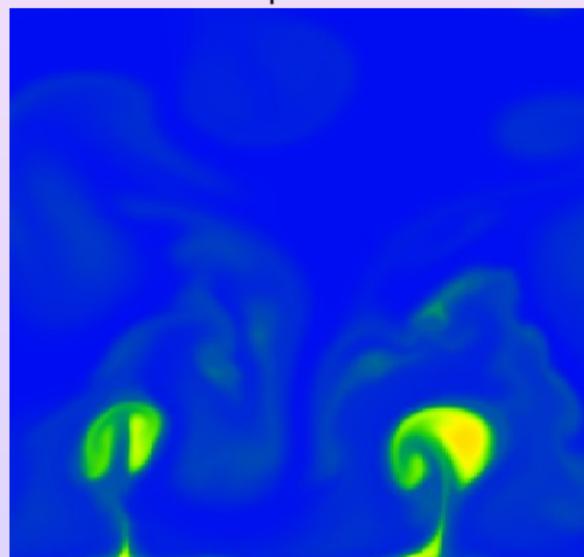
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

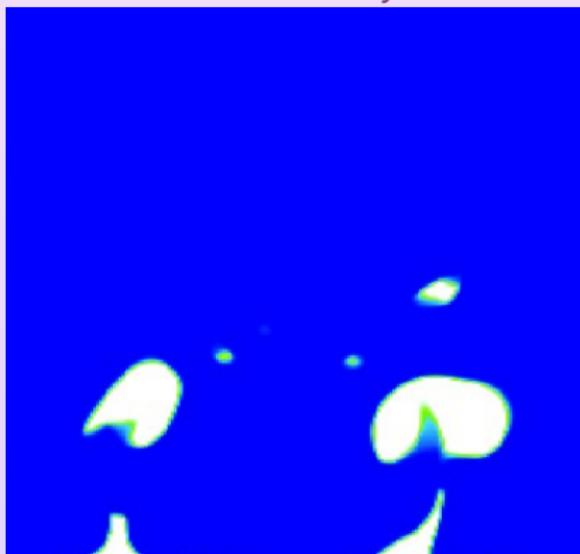
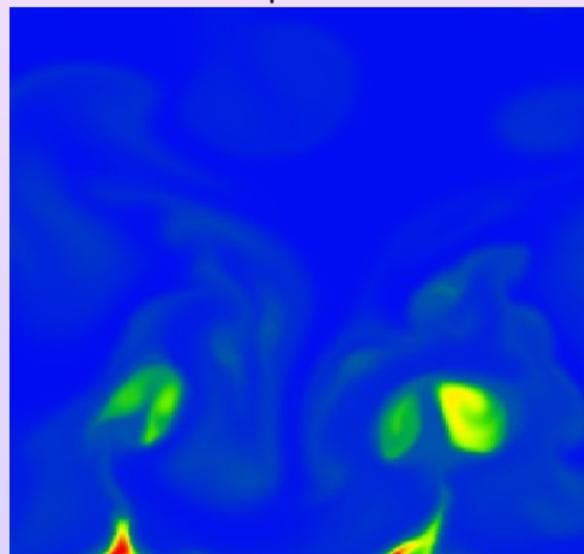
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

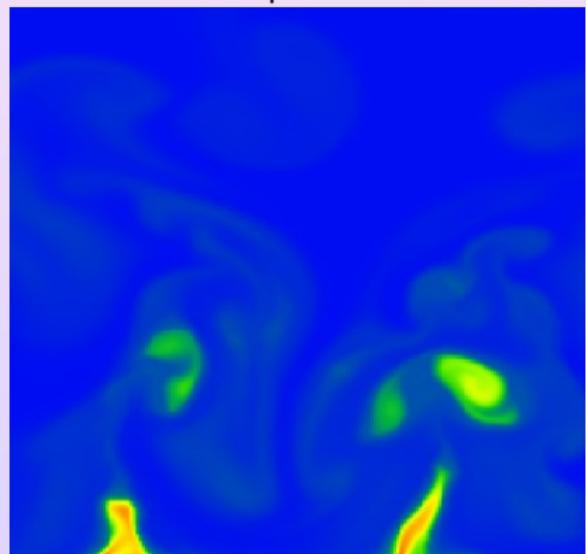
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

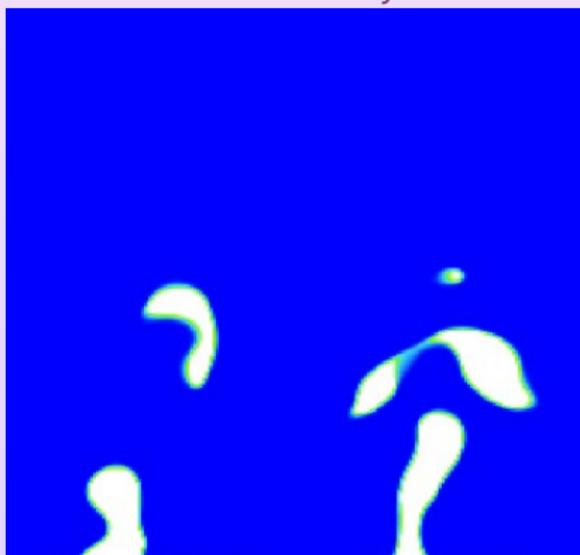
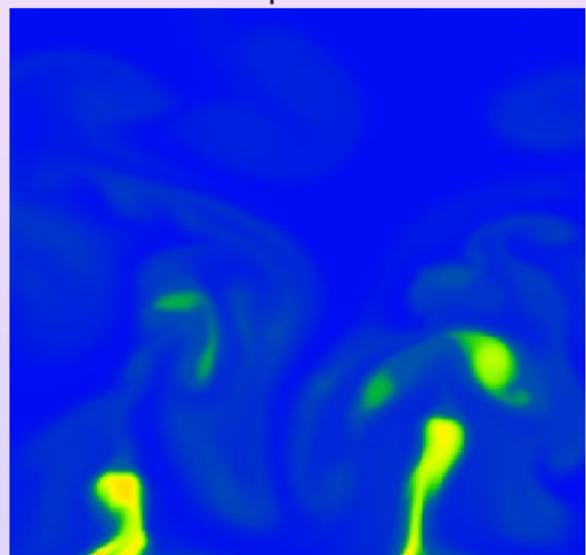
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

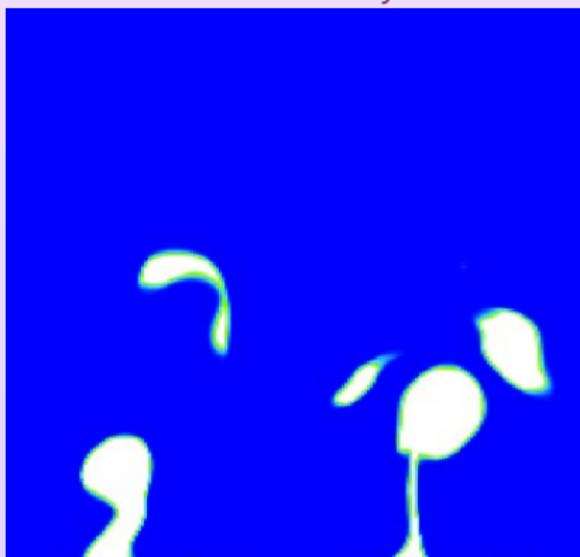
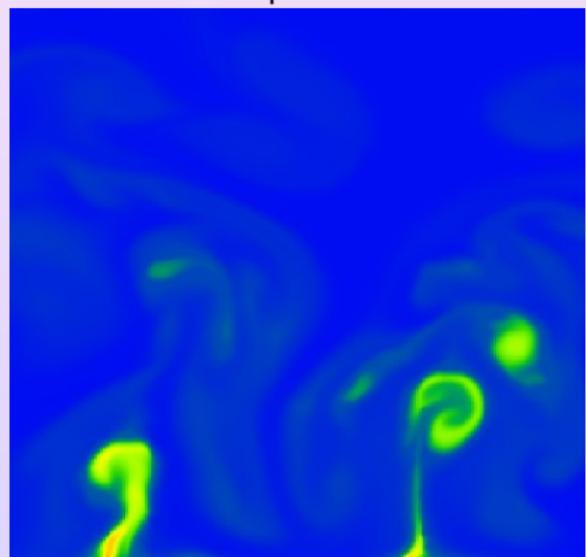
Mass Fraction y Temperature T 

◀ Geometry

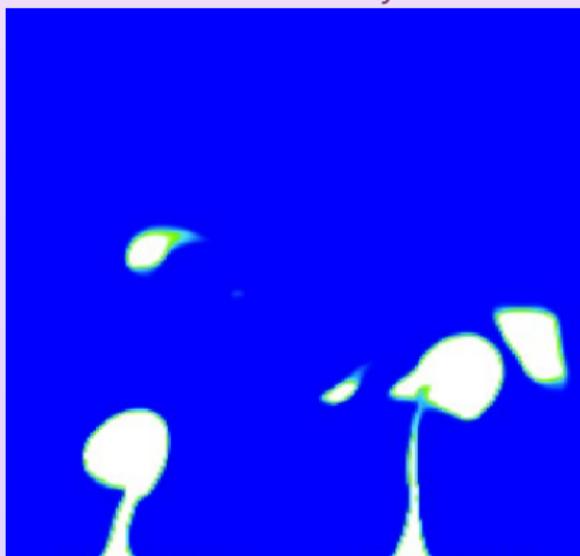
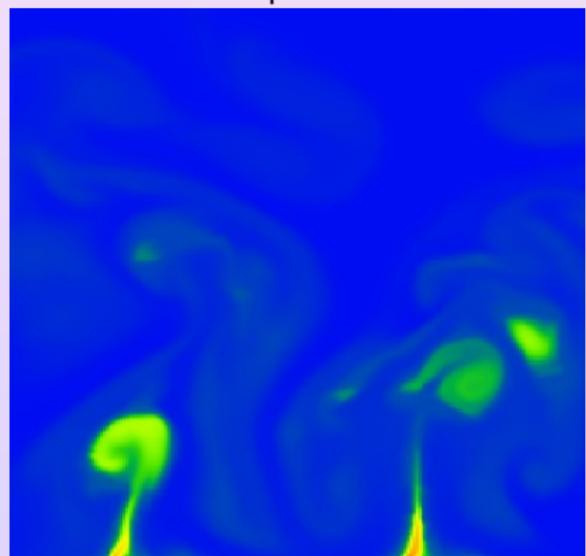
▶ Play

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Film

Mass Fraction y Temperature T [◀ Geometry](#)[▶ Play](#)[▶ Skip](#)

Film

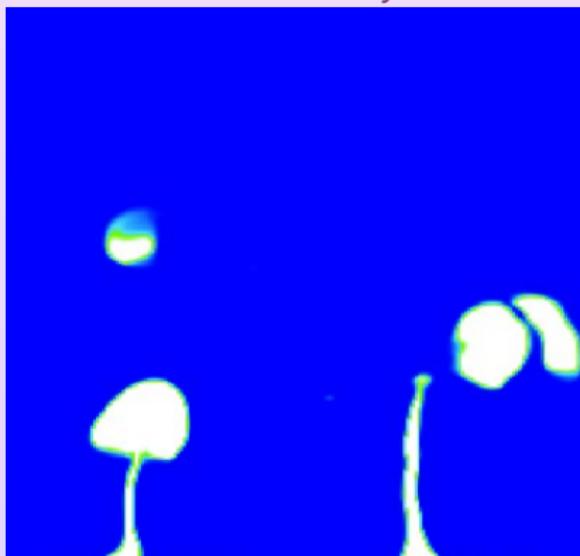
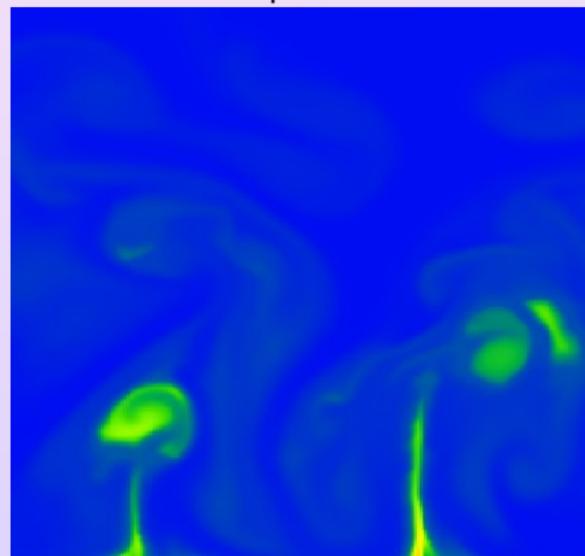
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

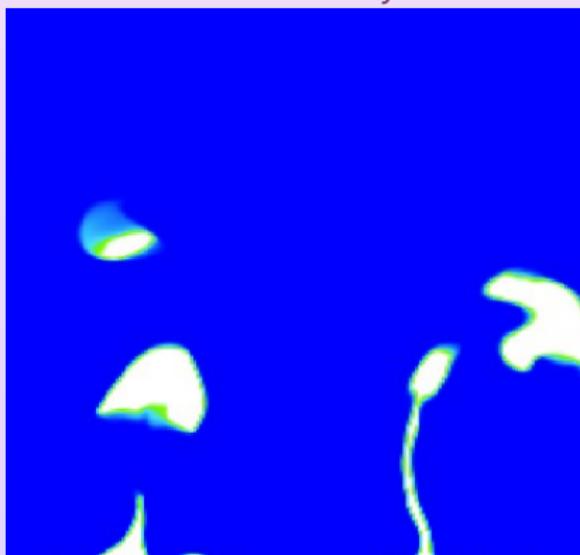
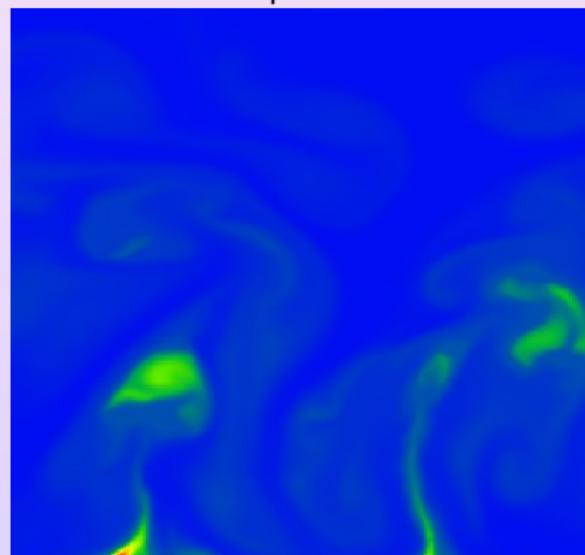
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

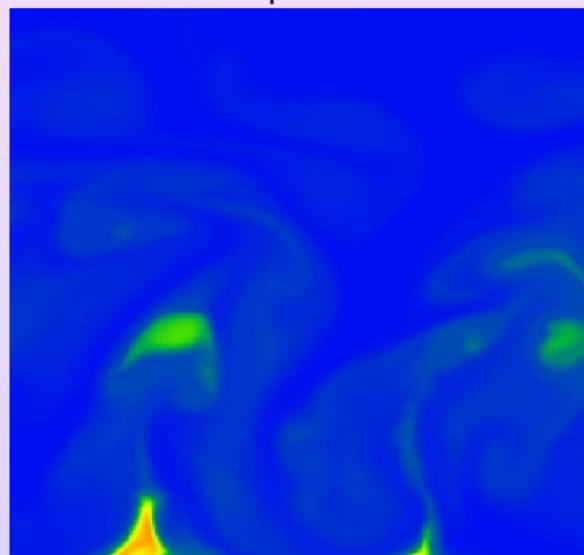
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

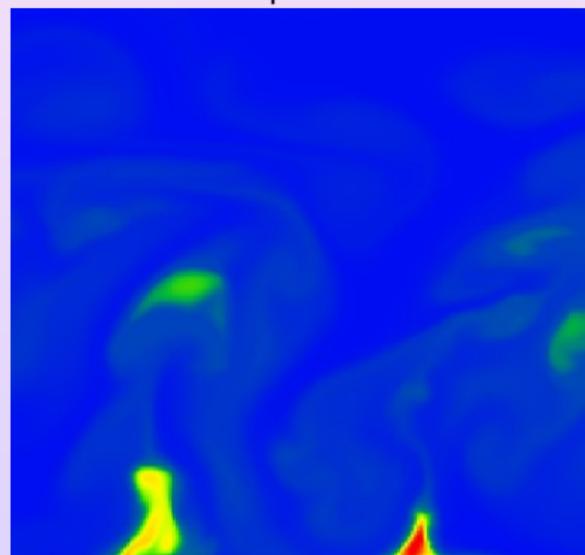
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

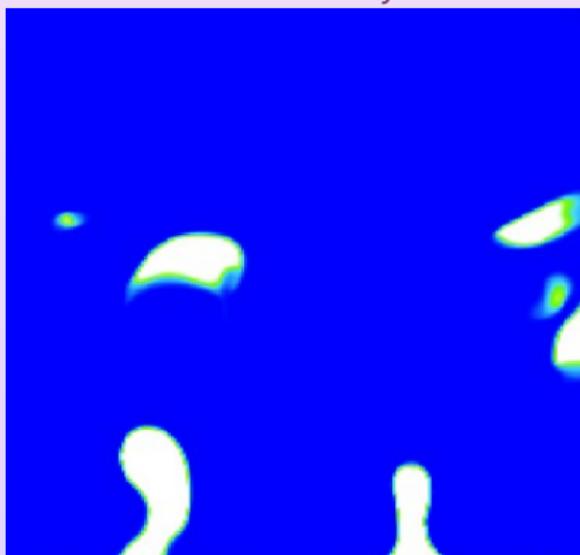
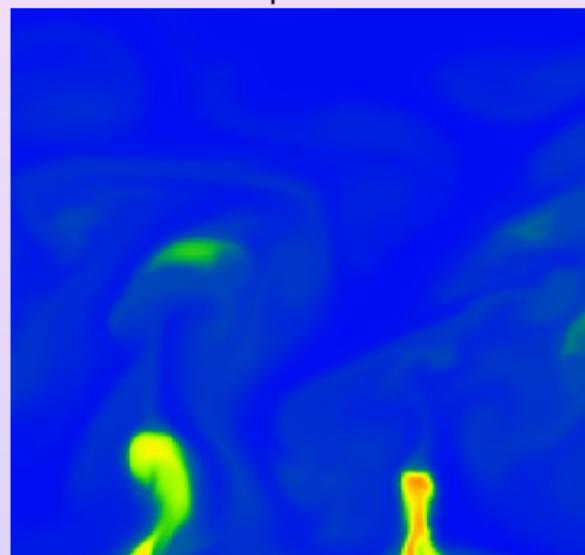
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

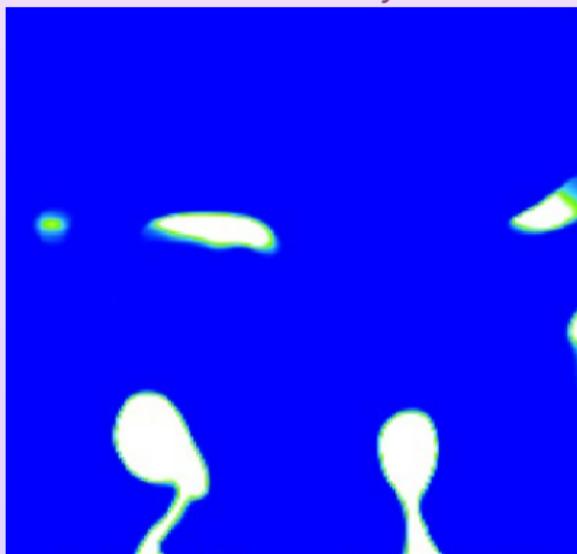
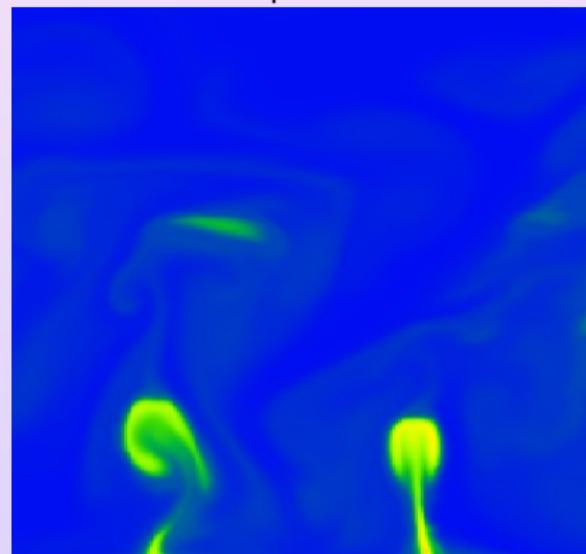
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

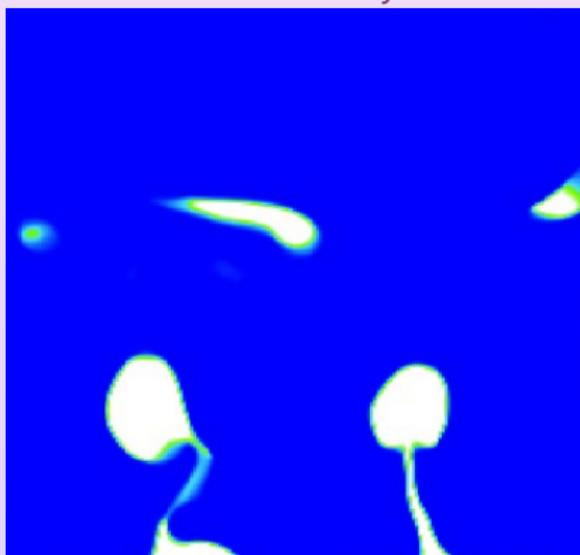
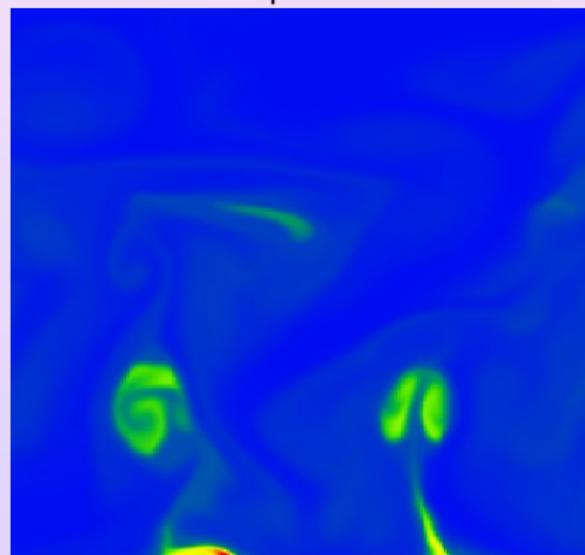
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

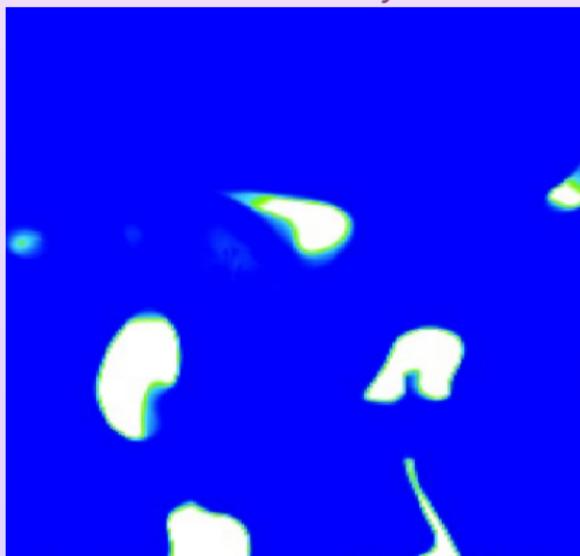
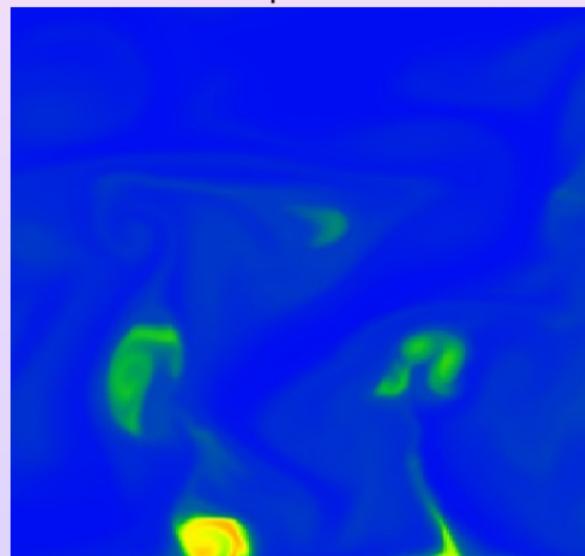
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

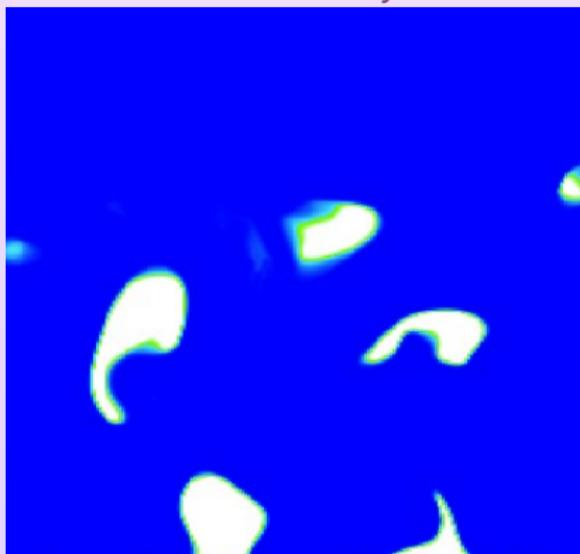
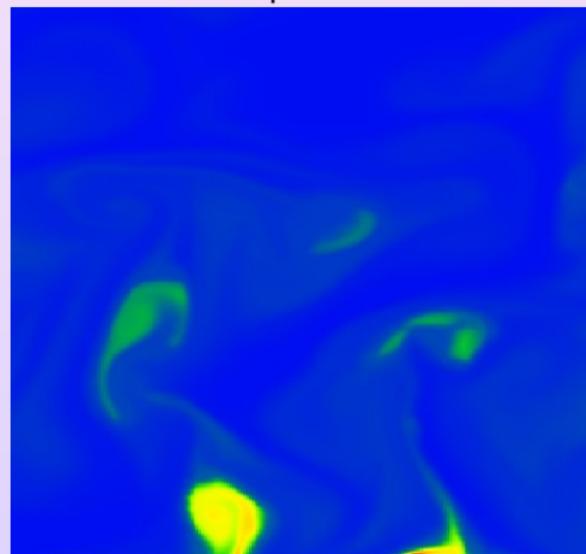
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

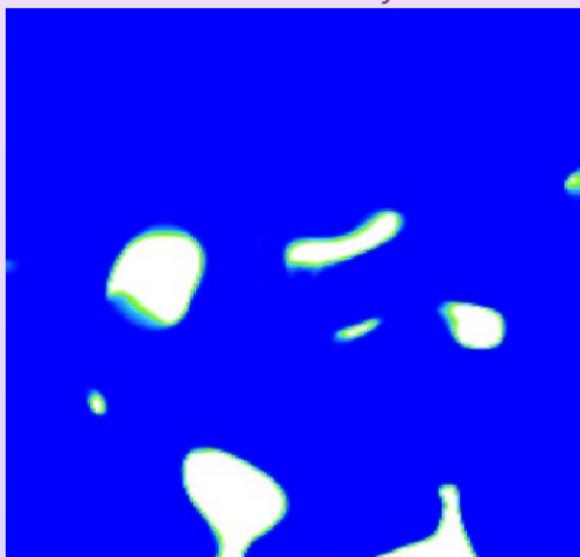
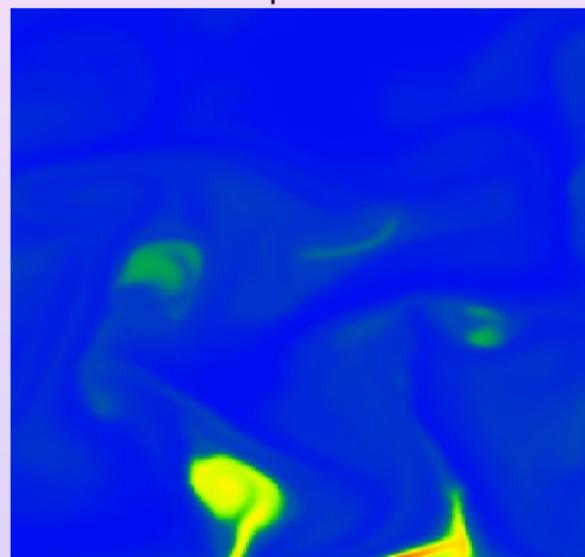
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

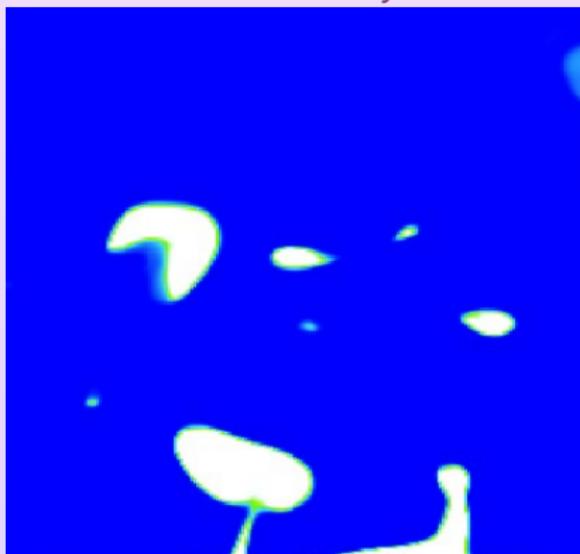
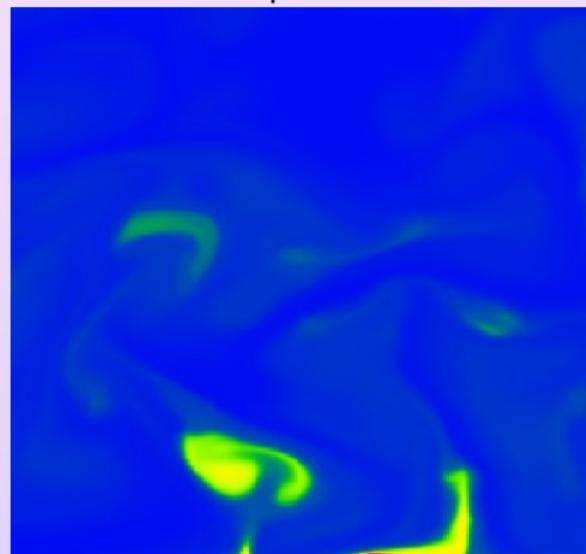
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

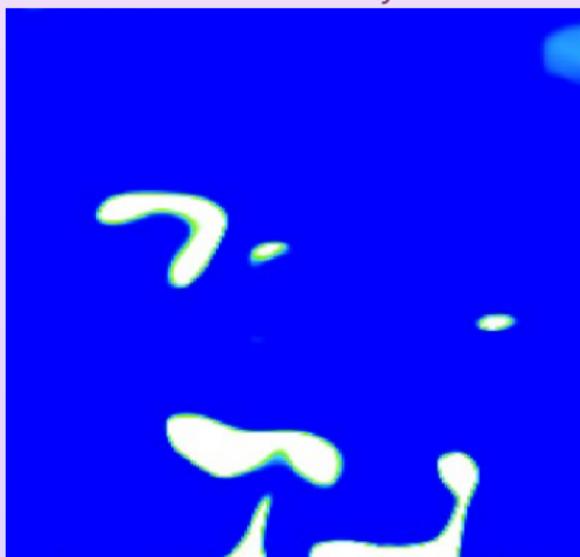
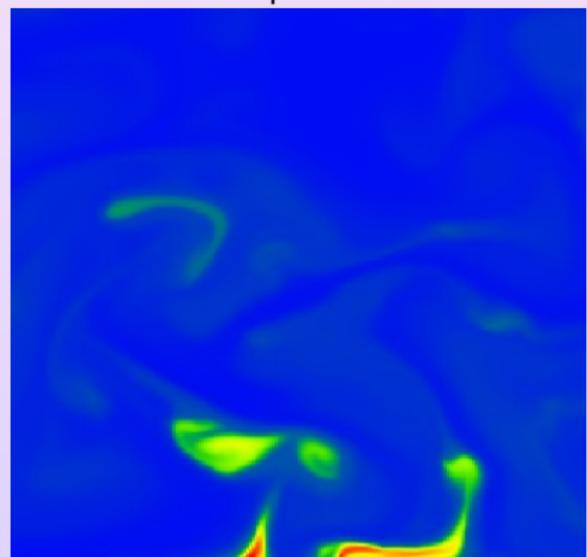
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

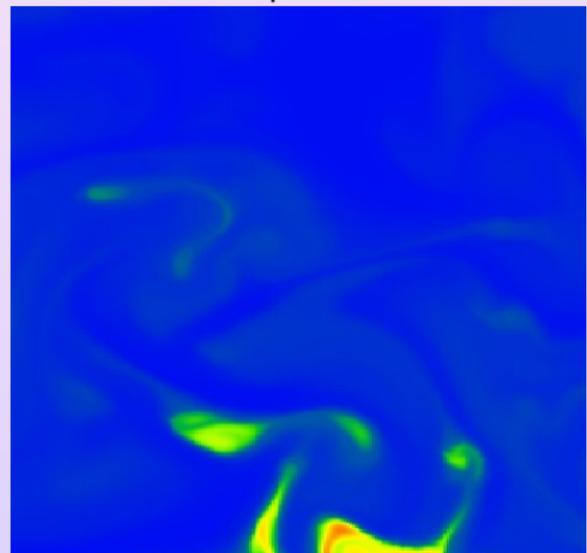
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

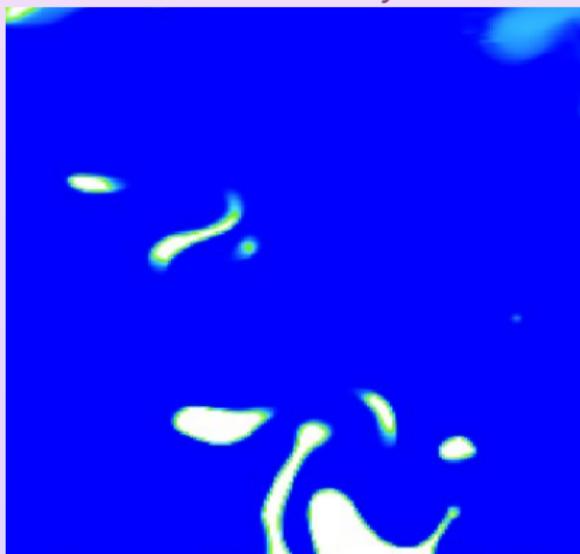
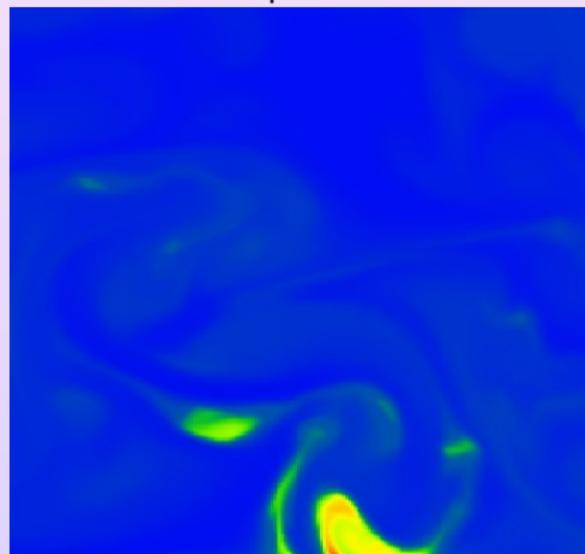
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

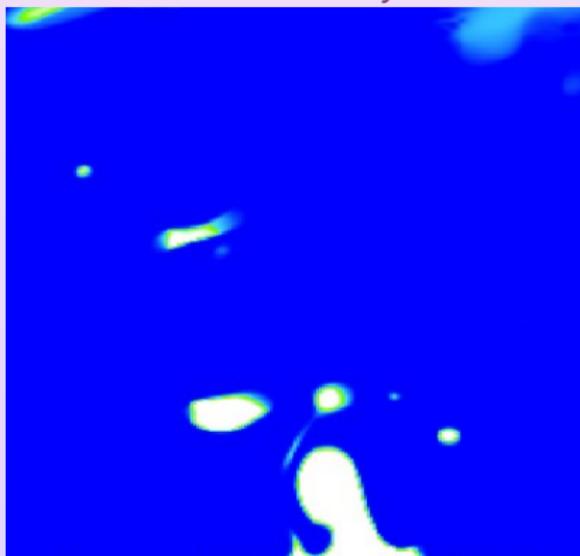
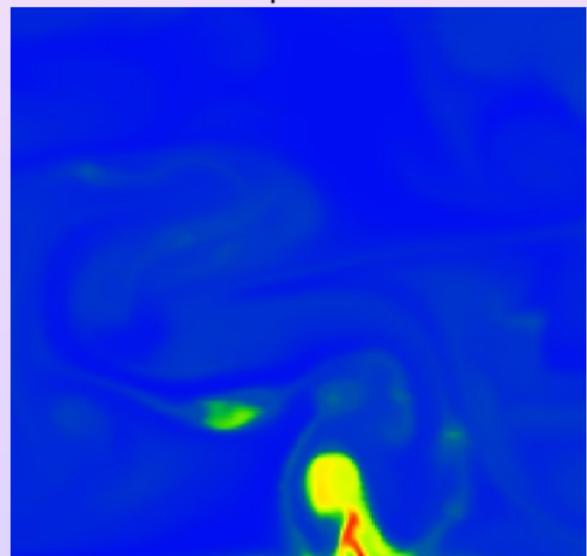
Mass Fraction y Temperature T 

◀ Geometry

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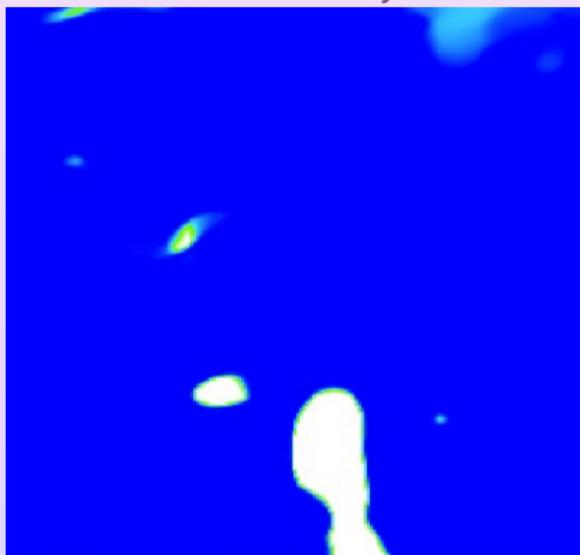
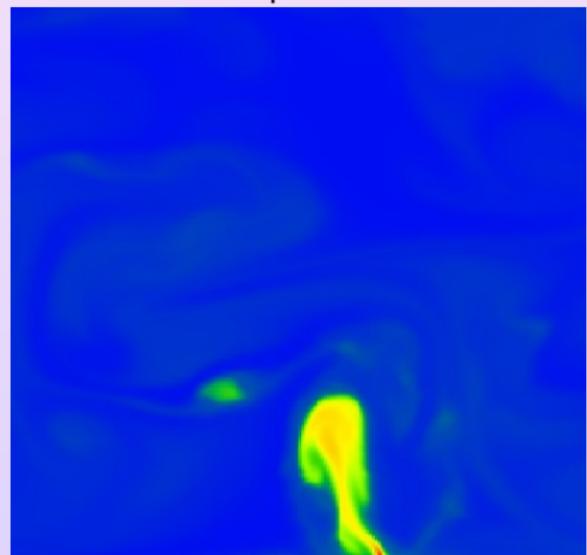
Mass Fraction y Temperature T 

◀ Geometry

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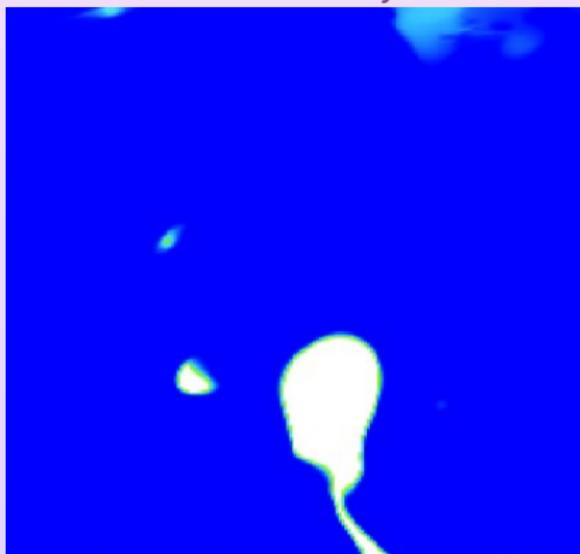
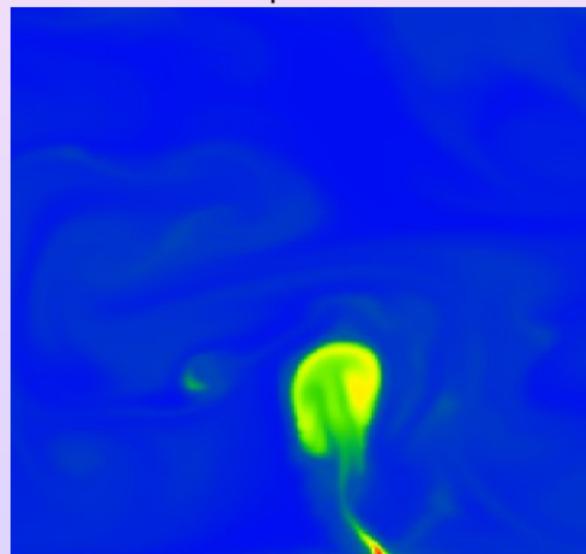
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

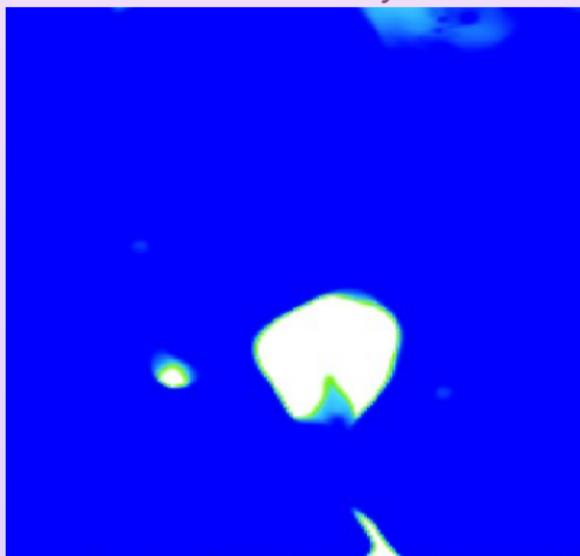
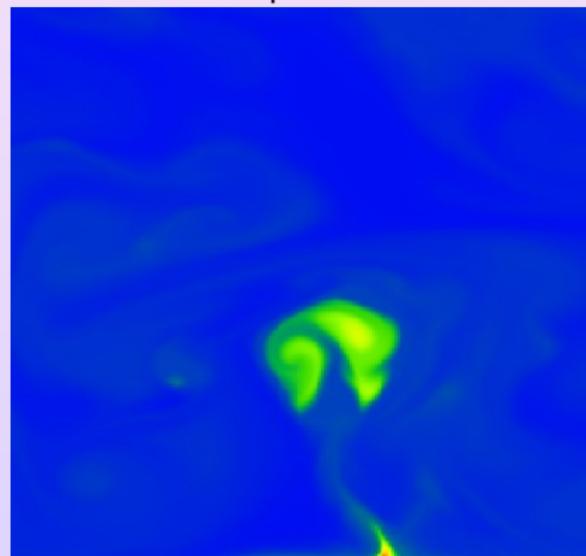
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

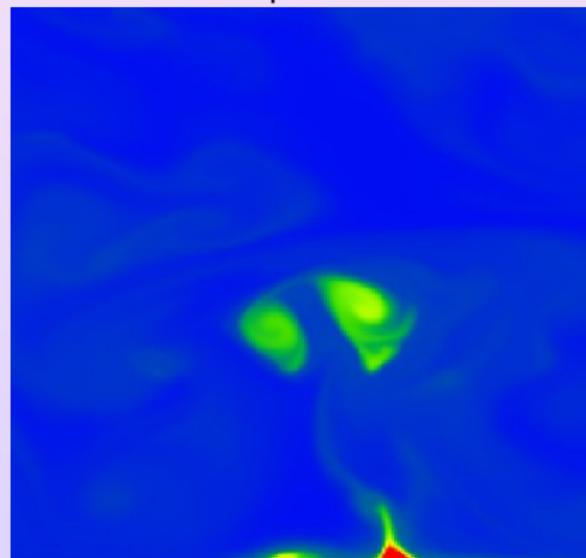
Mass Fraction y Temperature T 

◀ Geometry

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Film

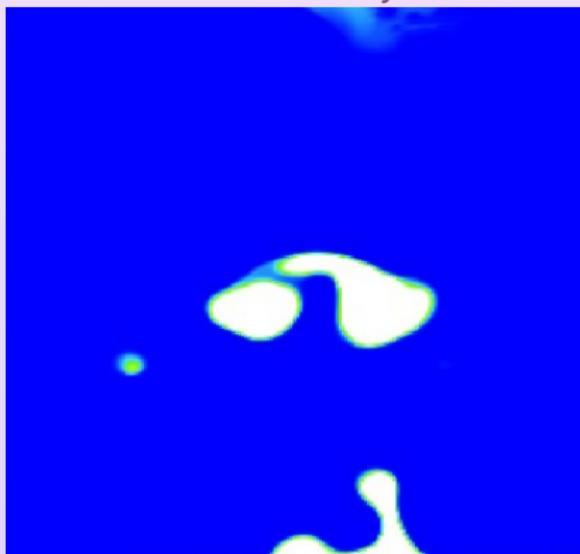
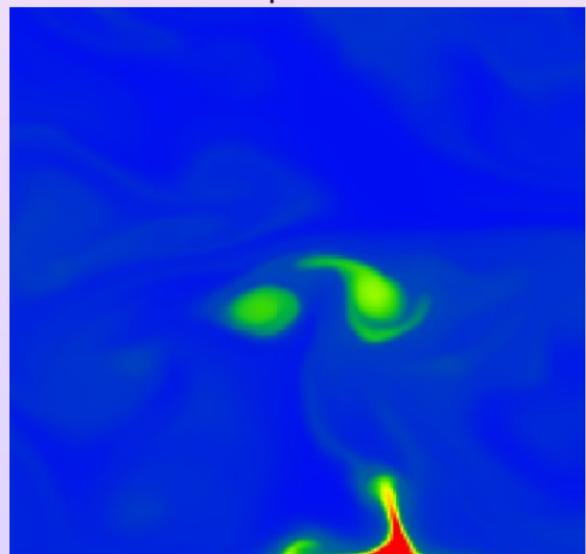
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

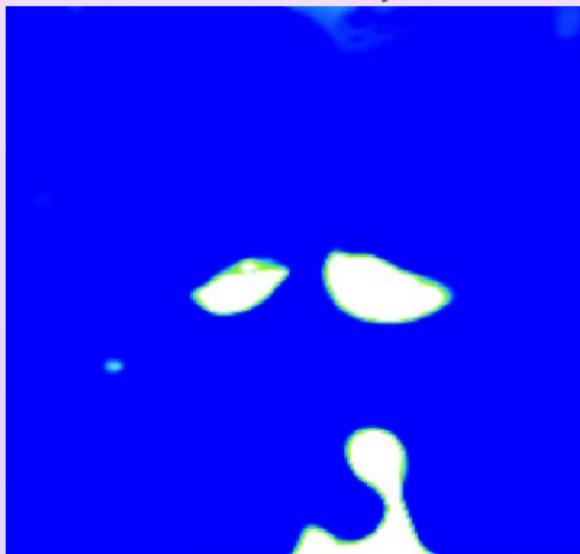
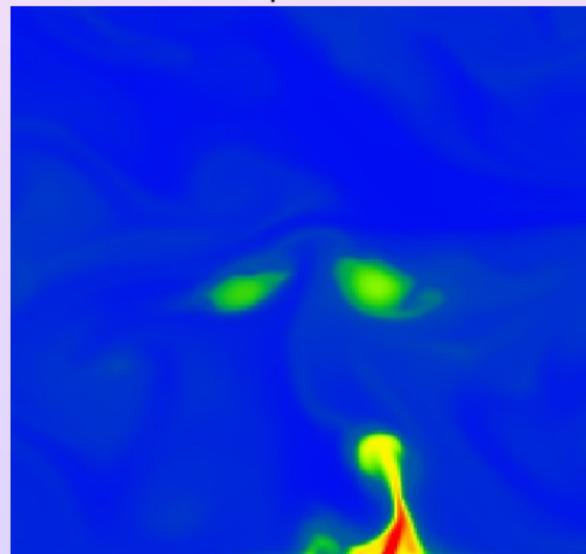
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

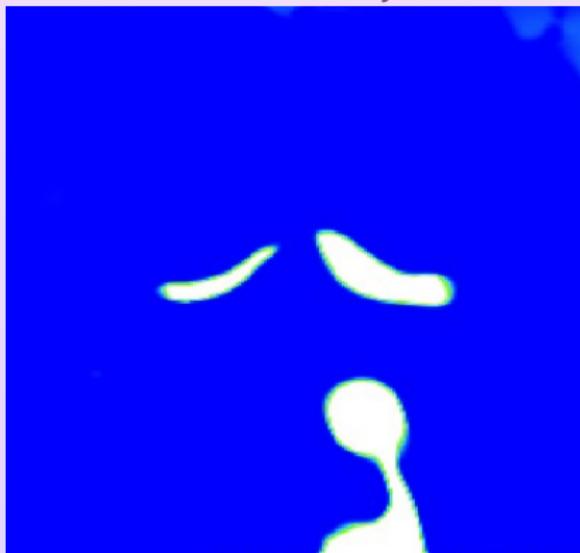
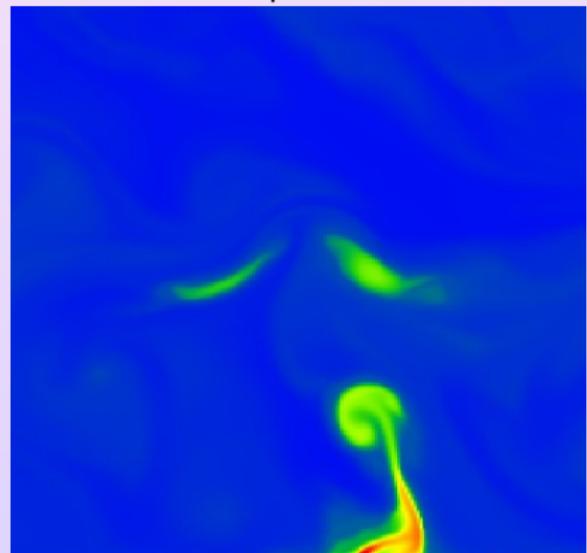
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

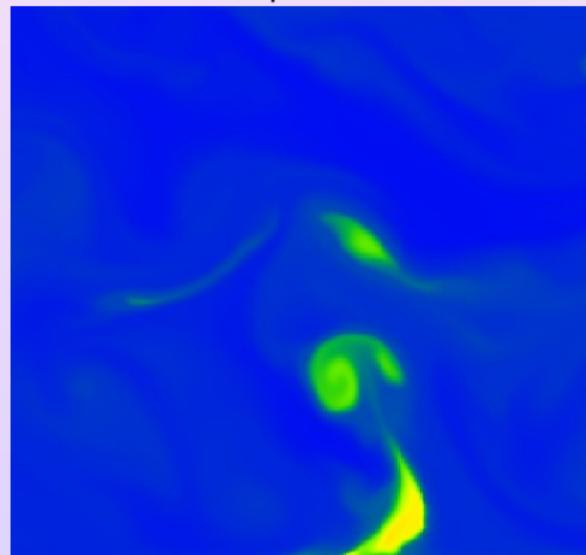
Mass Fraction y Temperature T 

◀ Geometry

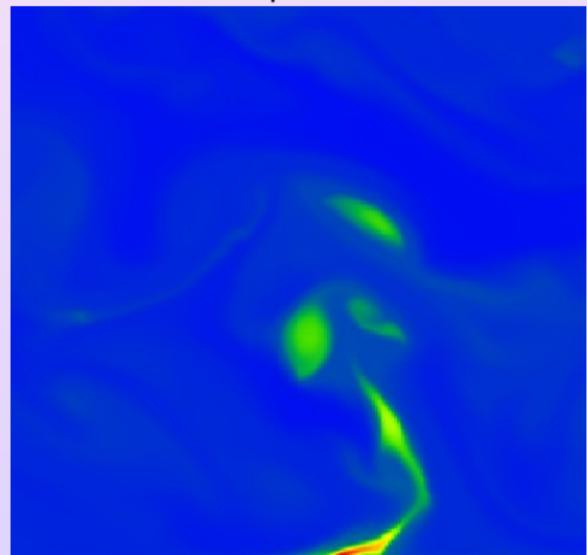
▶ Play

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Film

Mass Fraction y Temperature T [◀ Geometry](#)[▶ Play](#)[▶ Skip](#)

Film

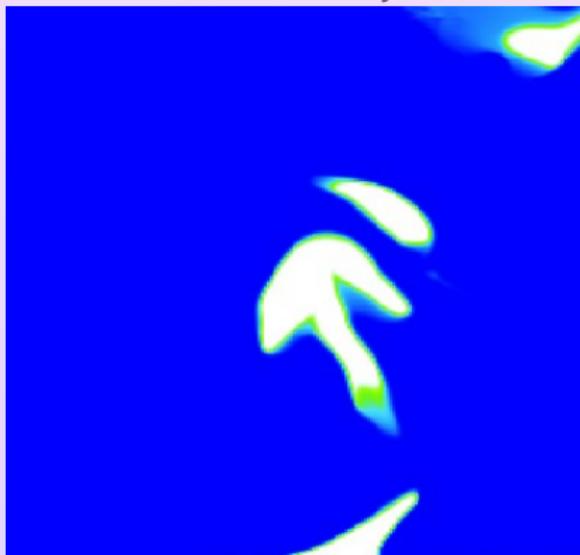
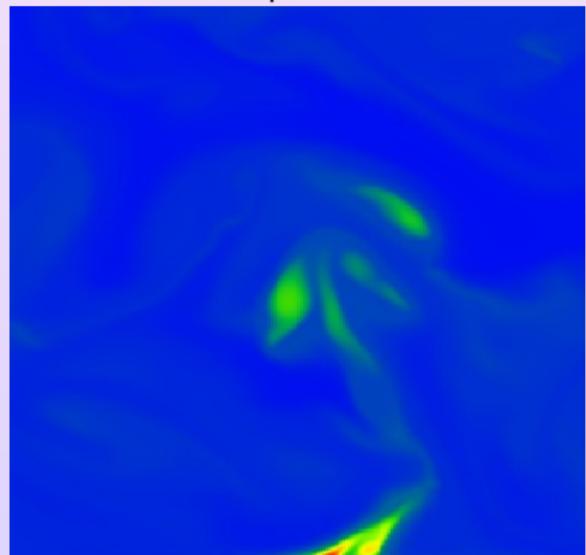
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

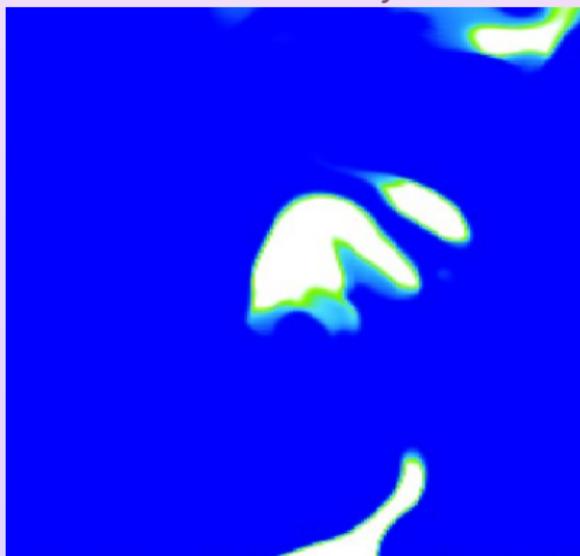
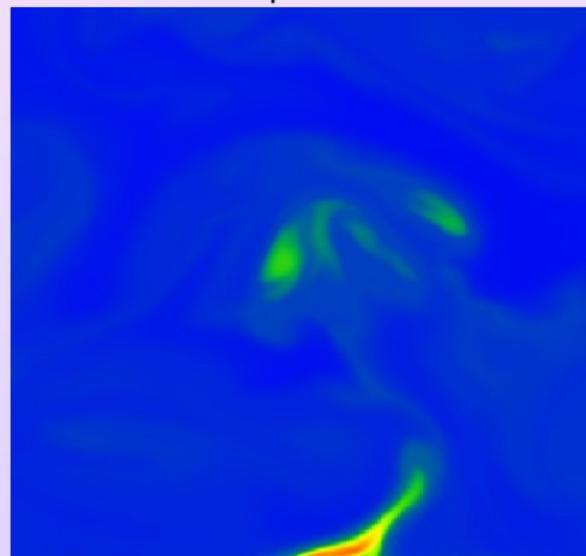
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

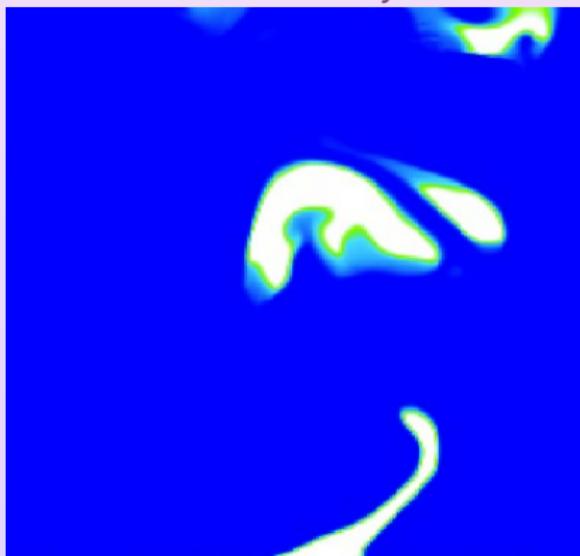
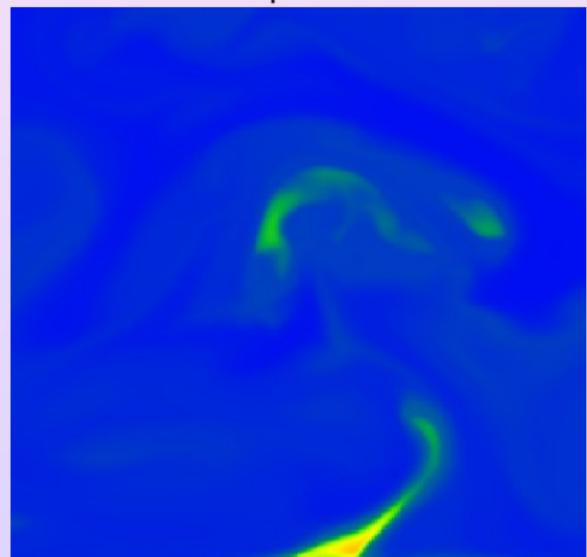
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

▶ Skip

Film

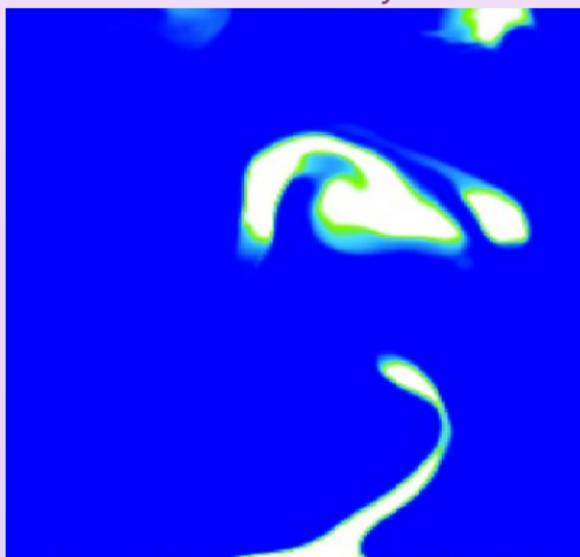
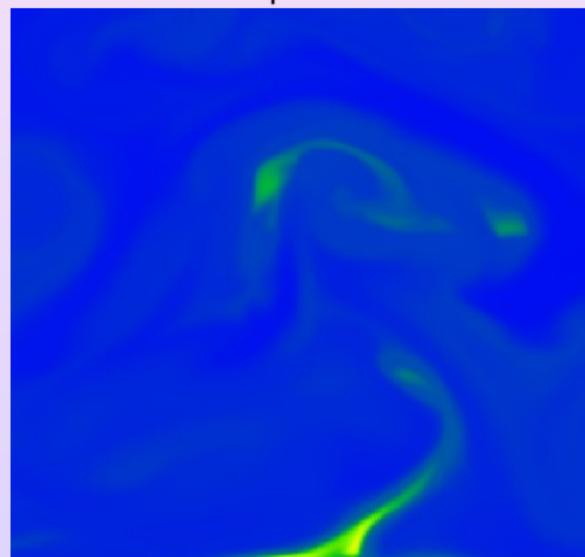
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

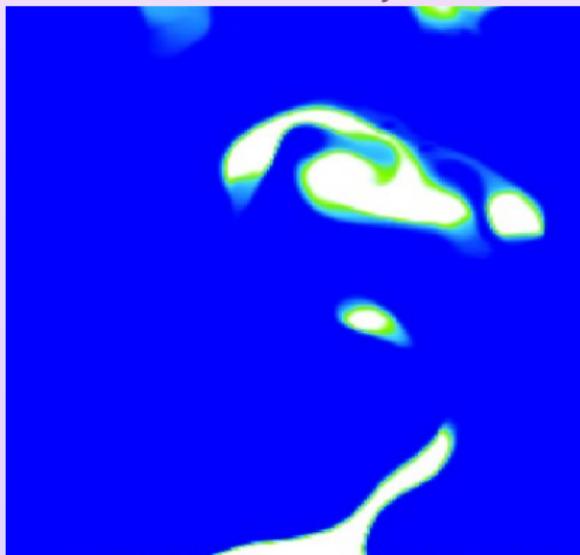
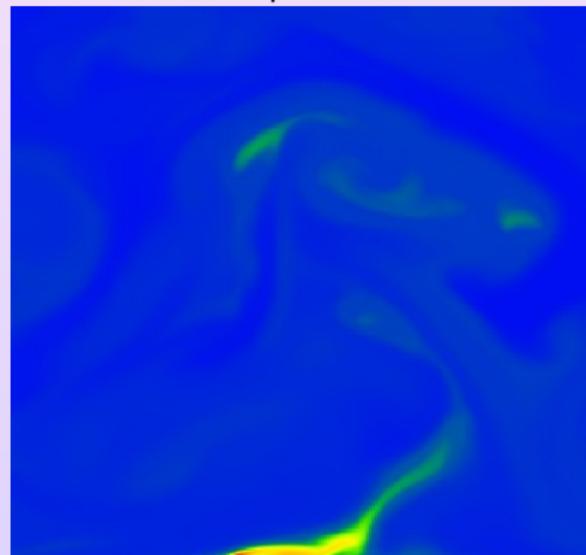
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

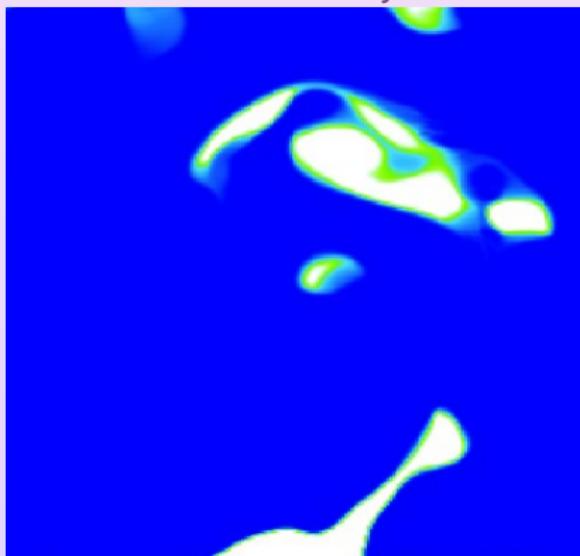
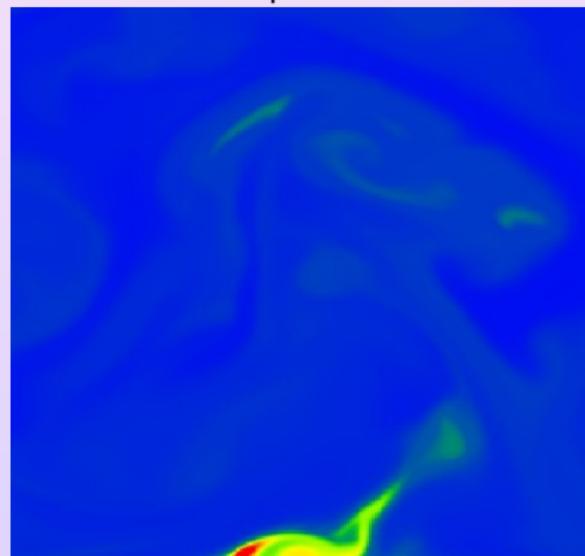
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

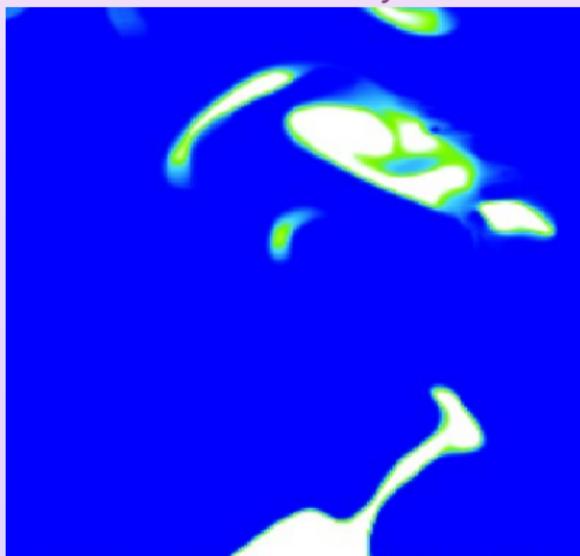
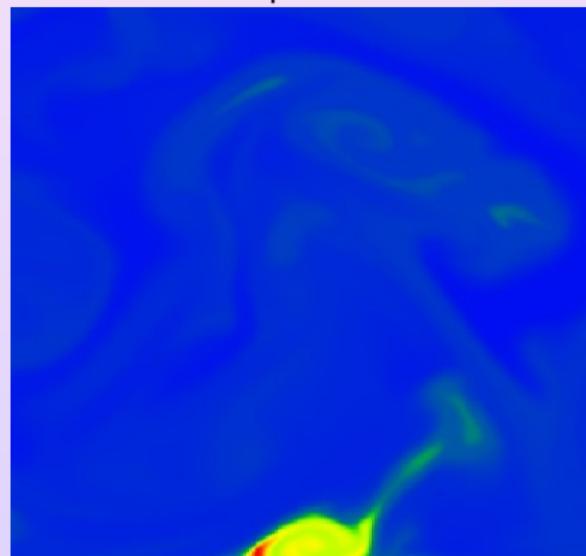
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

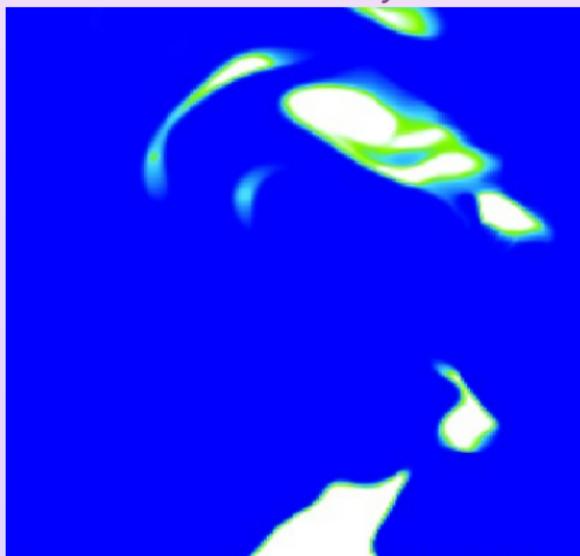
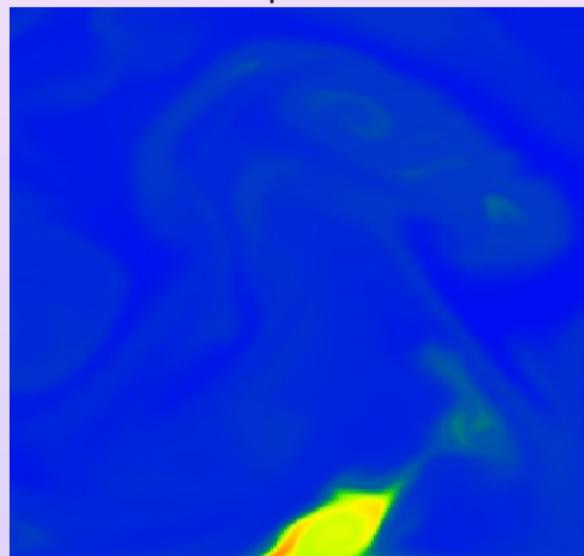
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

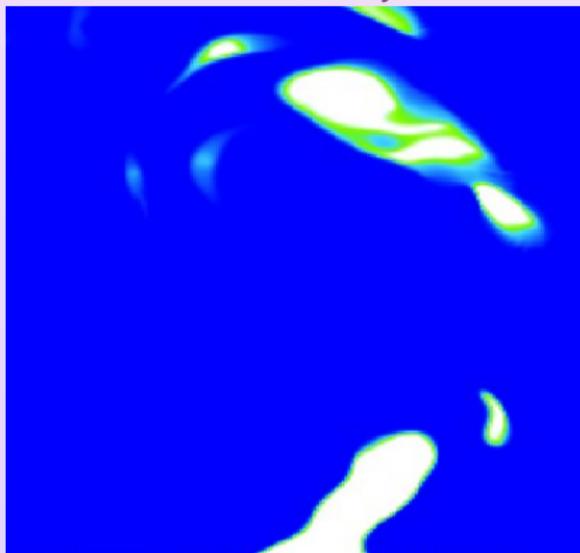
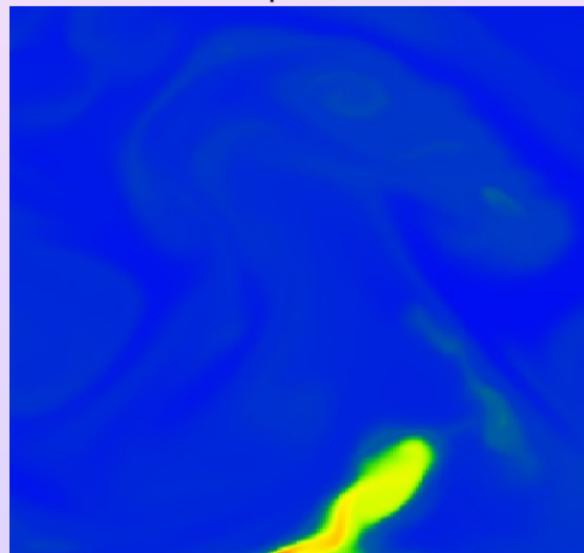
Mass Fraction y Temperature T 

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Film

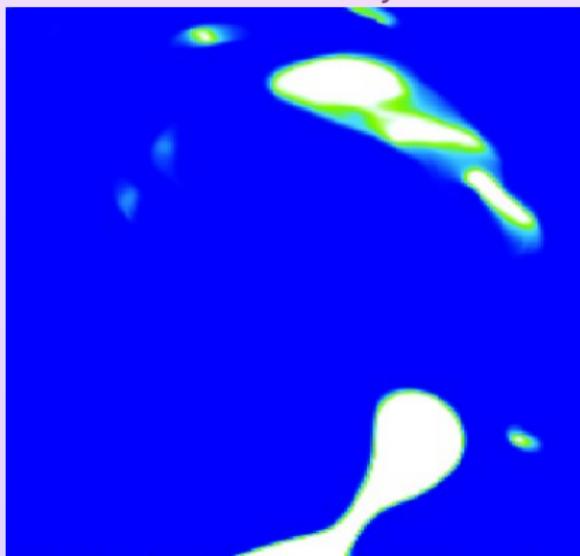
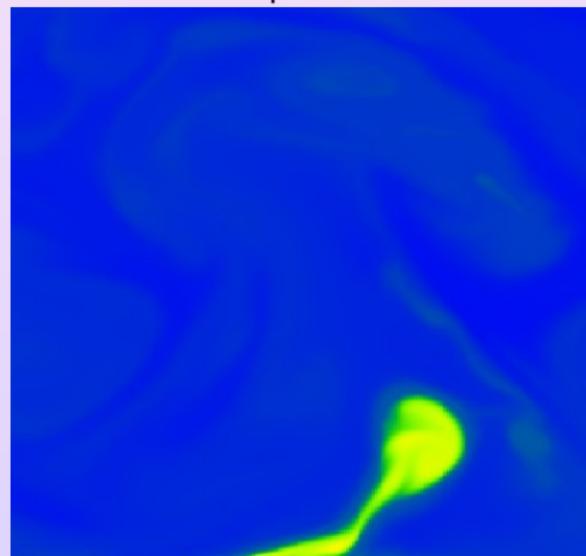
Mass Fraction y Temperature T 

◀ Geometry

▶ Play

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Film

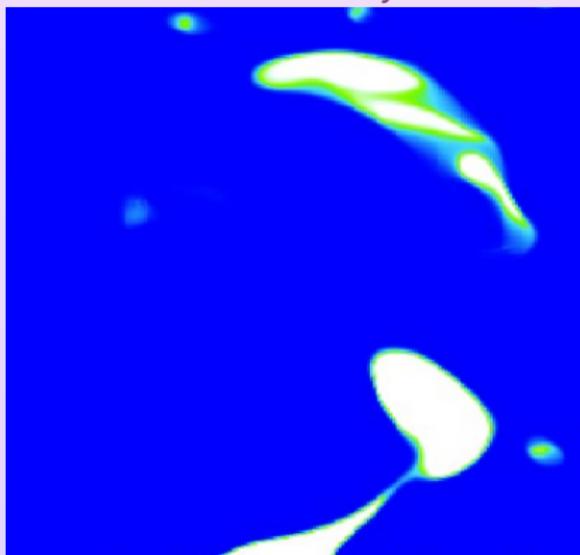
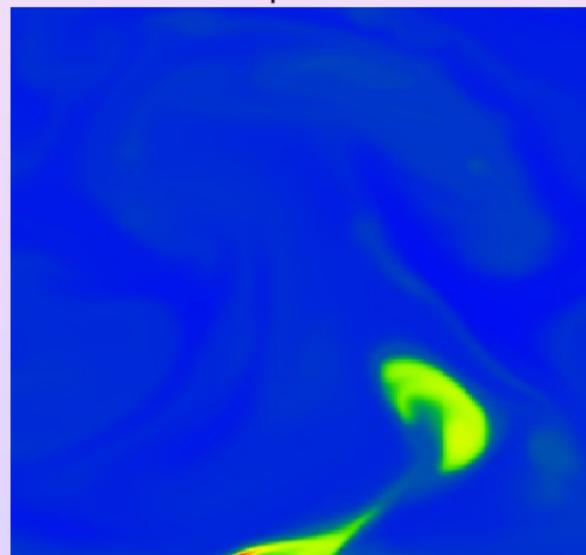
Mass Fraction y Temperature T 

◀ Geometry

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Film

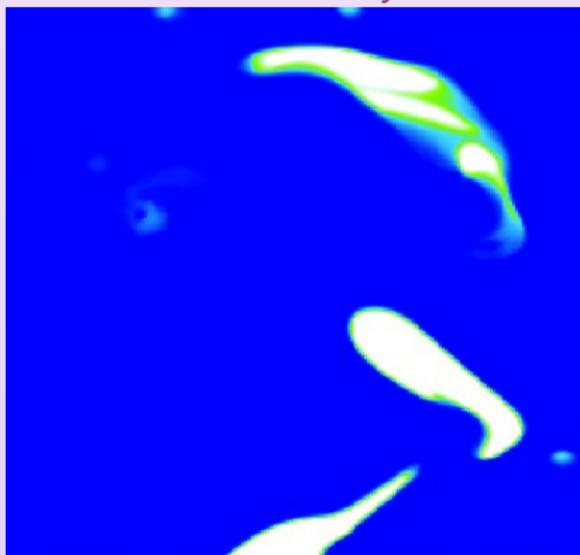
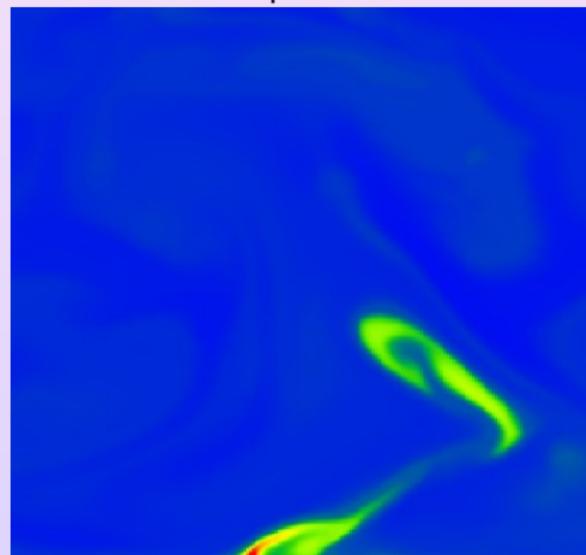
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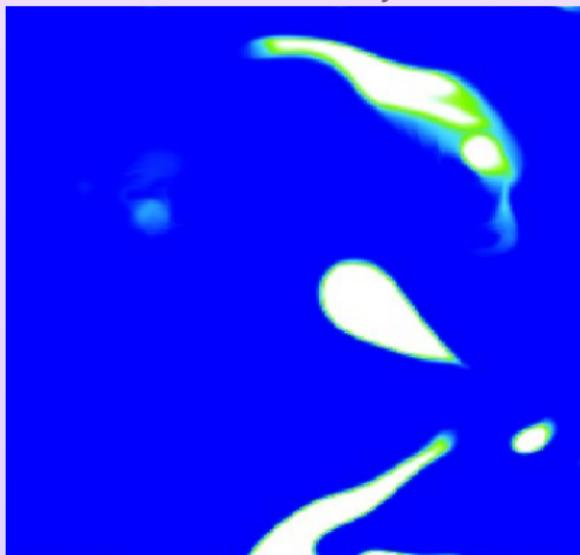
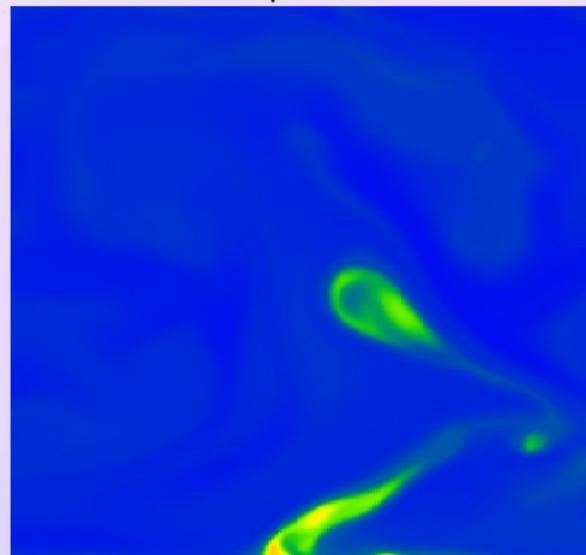
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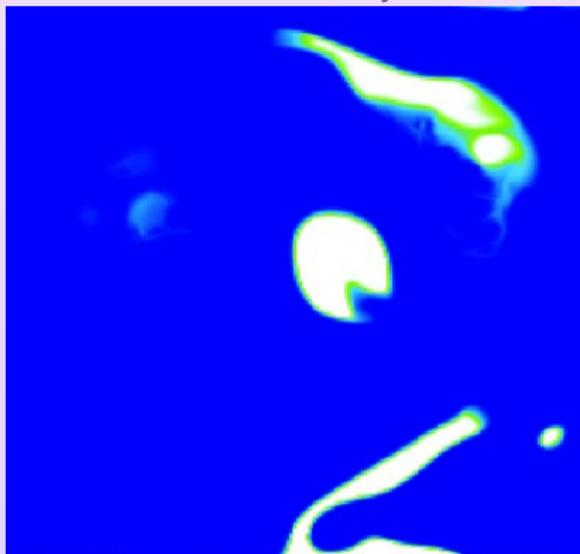
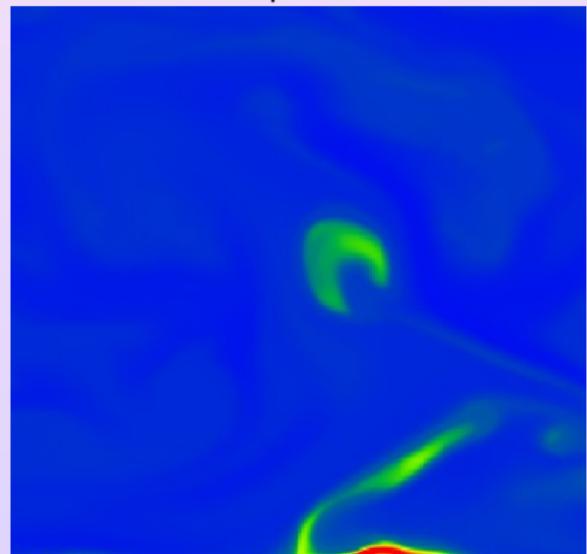
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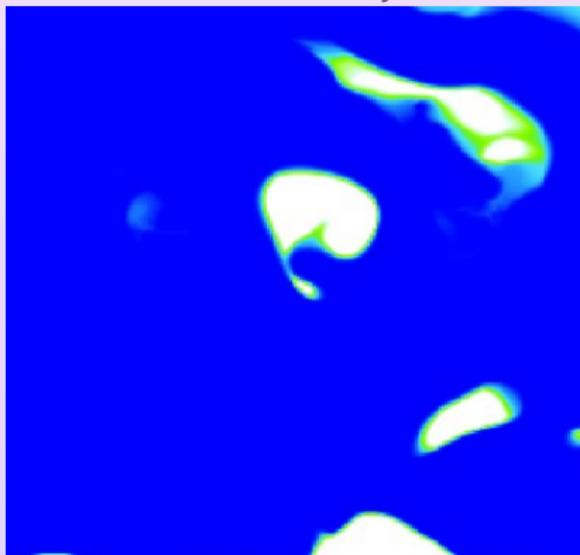
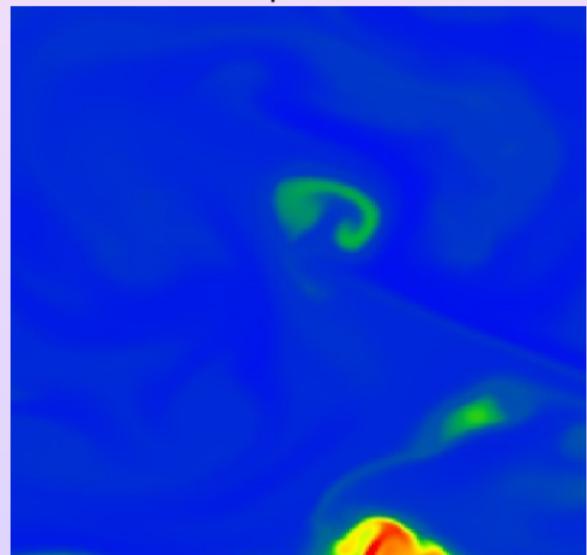
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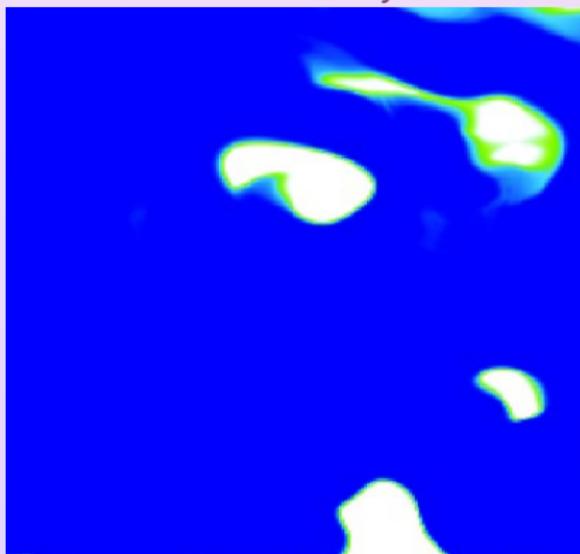
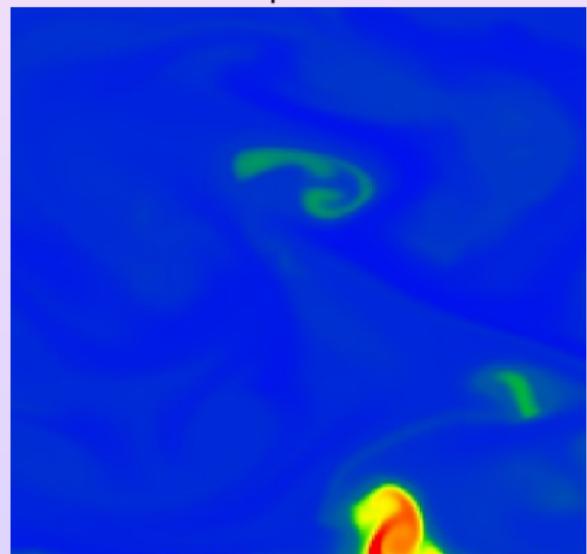
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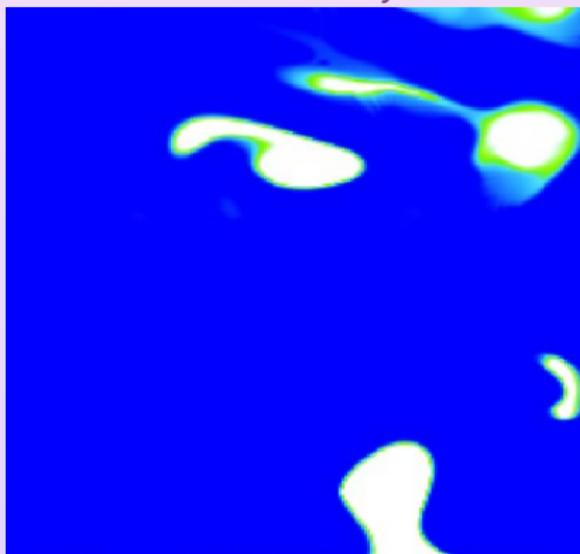
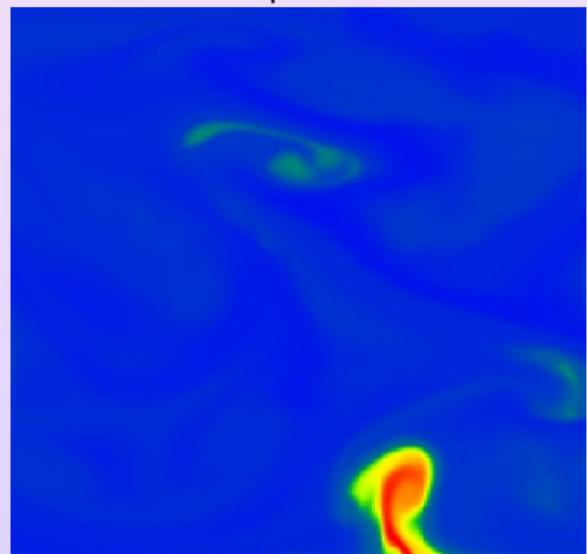
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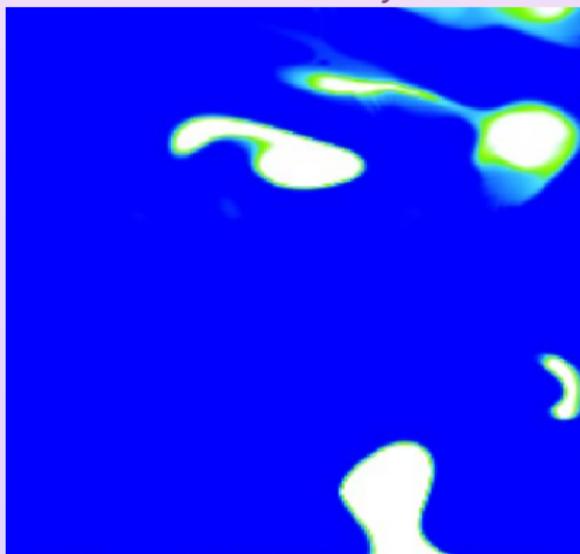
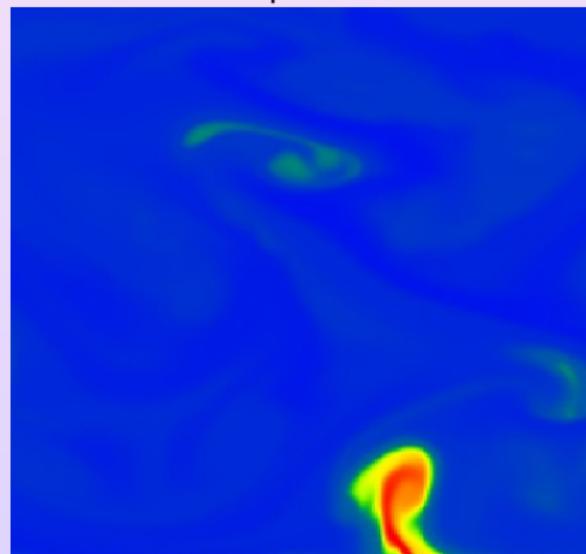
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Outline

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

4 Numerical Examples

5 Conclusion

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- ✓ general construction of the Equilibrium EOS (also for tabulated data),
- ✓ strict hyperbolicity of the Euler system with the Equilibrium EOS,

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- ✓ operator splitting based on the 5-eqs iso-T with a Roe like solver [G. ALLAIRE, S. CLERC, S. KOKH],

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- ✓ 2D with Stiffened Gas EOS for
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Appendix

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

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.

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

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

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

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

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

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Water Tabulated EOS

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

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

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

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

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Speed of sound

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

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

- for all \mathbf{w} pure phase state

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

- for all \mathbf{w} equilibrium mixture state

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

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

- for all \mathbf{w} pure phase state

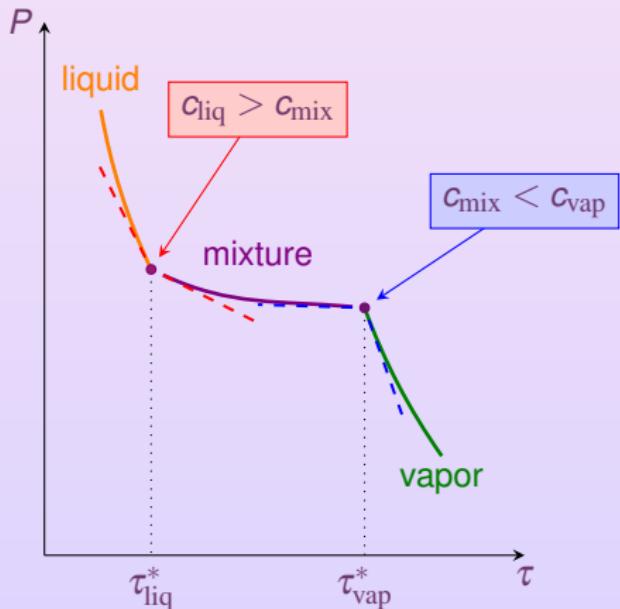
$$\mathbf{v}^T d^2 s^{\text{eq}}(\mathbf{w}) \mathbf{v} < 0 \quad \forall \mathbf{v} \neq 0,$$

- for all \mathbf{w} equilibrium mixture state

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

$\forall \mathbf{w}$ equilibrium mixture state, $\mathbf{v}(\mathbf{w}) \overset{?}{\asymp} [P^{\text{eq}}(\mathbf{w}), -1]$

ISENTROPIC CURVES



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

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

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

• Pure Phases

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

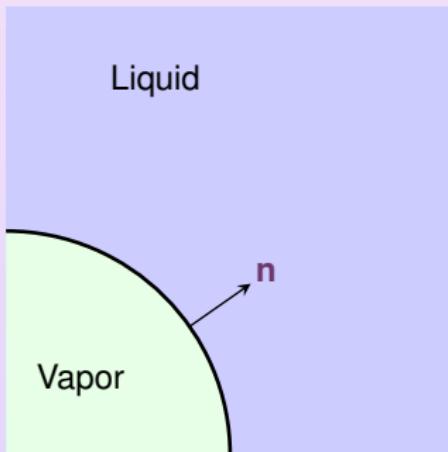
• Mixture

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

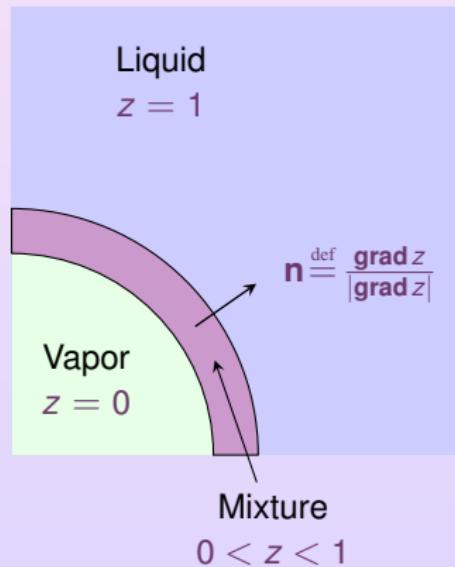
- Regularity: [J. CORREIA, P.G. LEFLOCH, M.D. THANH]
- Loss of convexity: [A. Voss]

Continuum Surface Force (CSF) Approach

Physical Interface

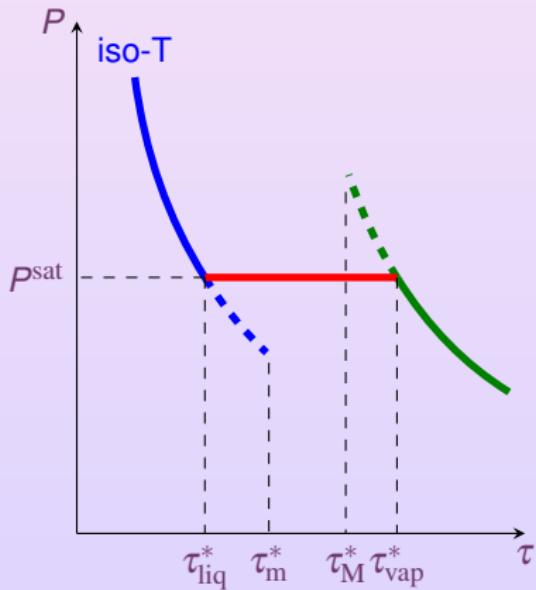


Diffuse Interface



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

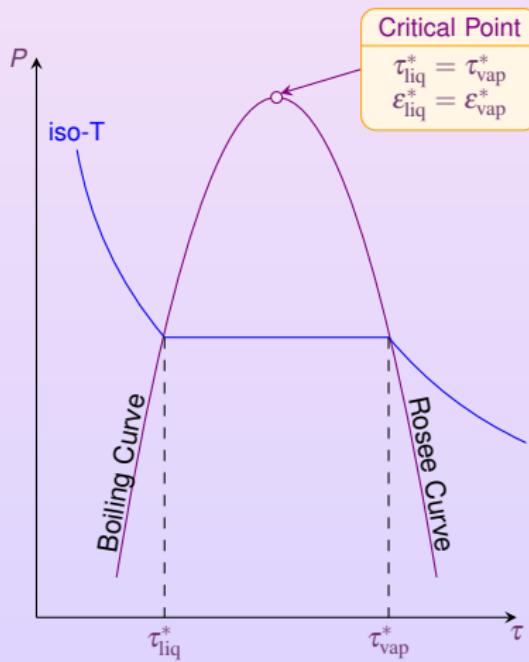
Metastability



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

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

Critical Point



PHYSIC

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

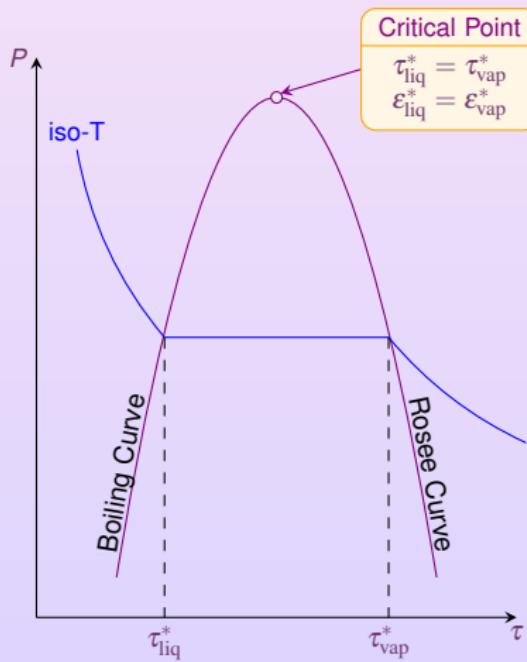
EOS

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

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

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

Critical Point



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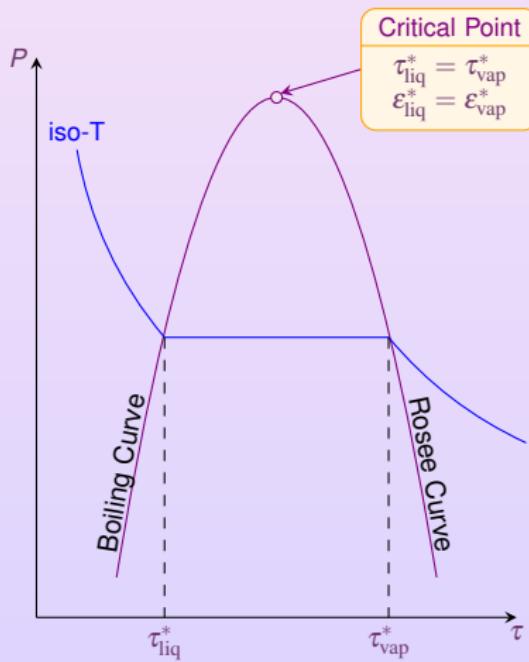
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Eq

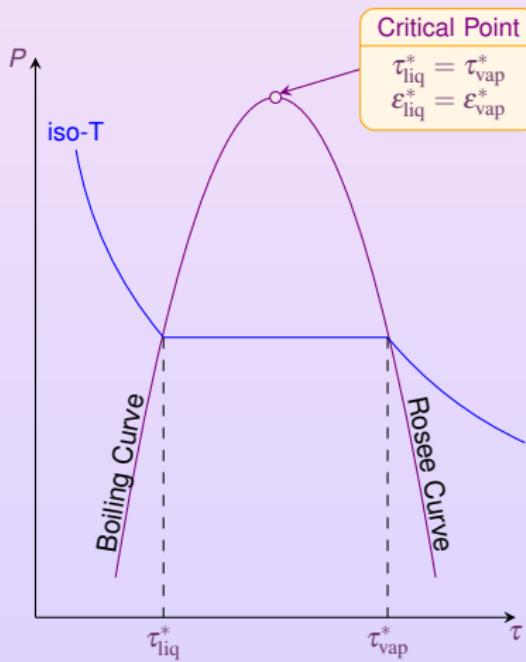
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