IGESA – Porquerolles, 31/5/2016

On a diphasic low Mach model for a heat exchanger

Theoretical and 1D/2D numerical results

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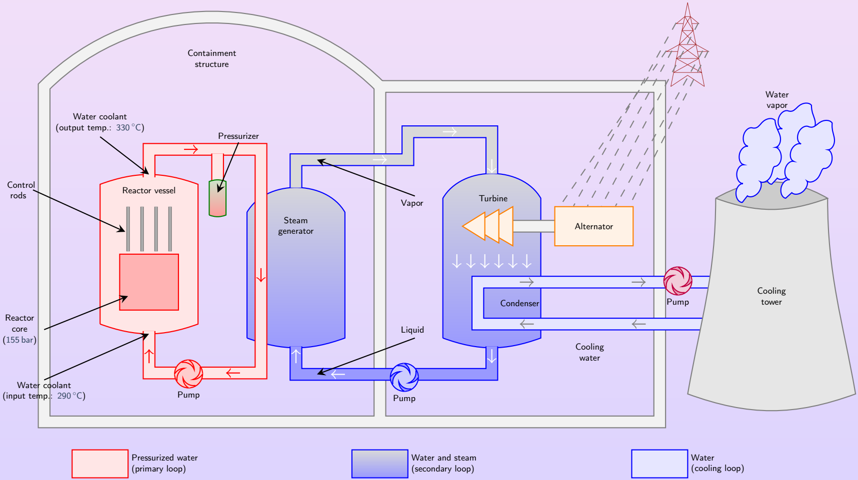
Outline

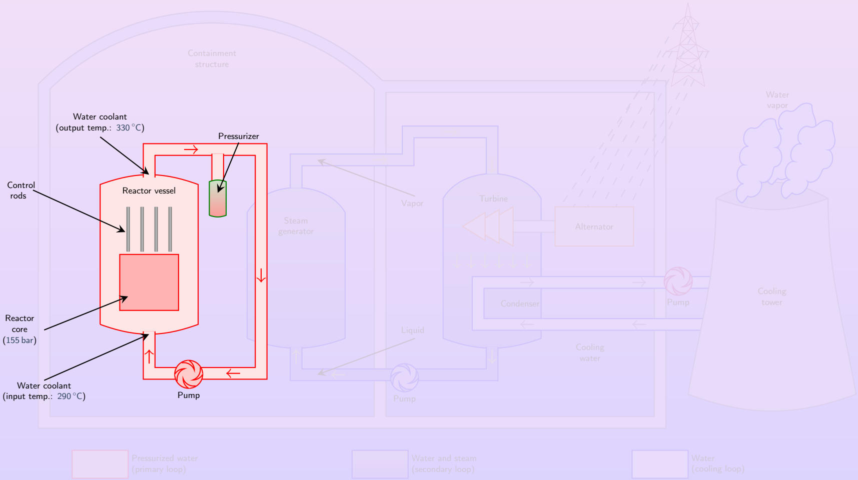
Section 1

Context

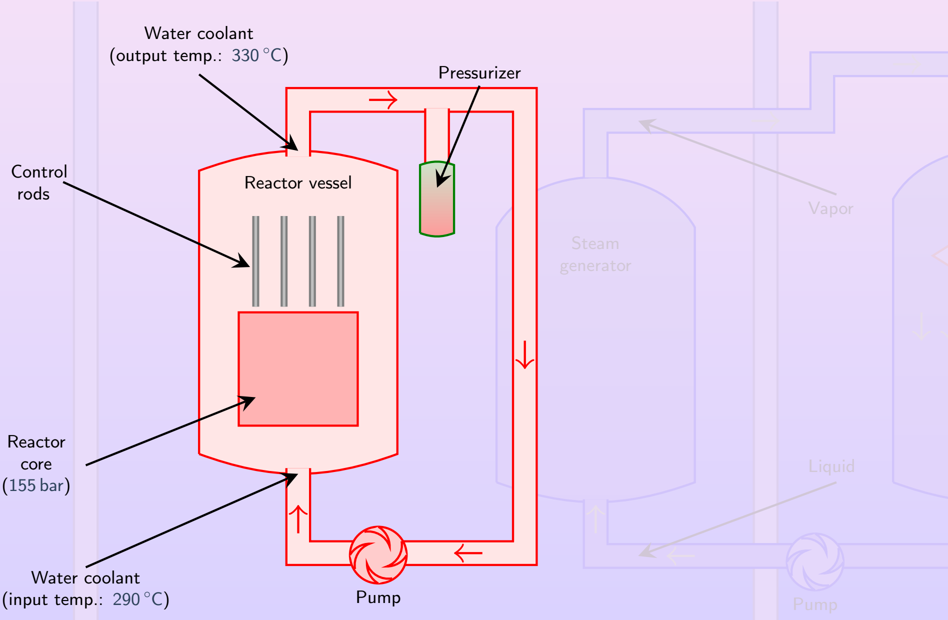
Pressurized Water Reactor



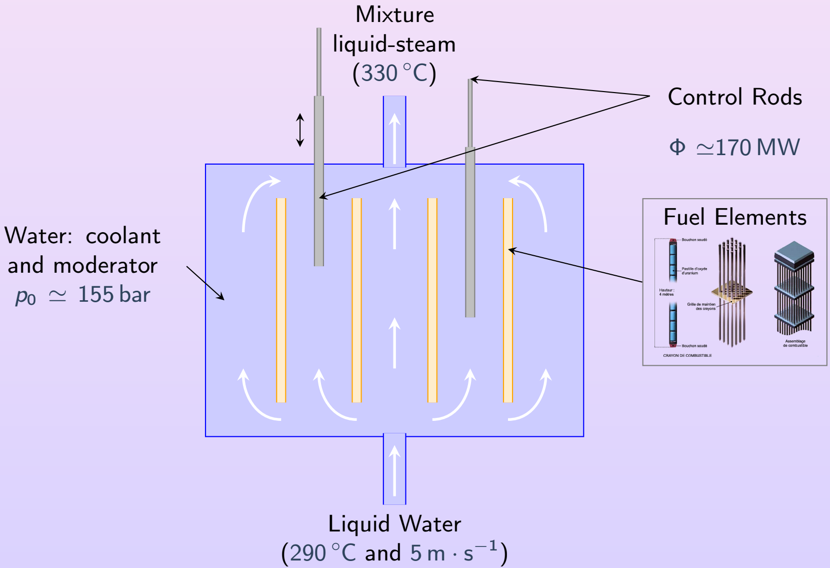
Pressurized Water Reactor



Pressurized Water Reactor



Core of a Pressurized Water Reactor



Section 2

The Low Mach Hypothesis

Core at Pressurized Water Reactor

Nominal regime

- Inlet velocity: $|\mathbf{u}| \simeq 5\,\mathrm{m\cdot s^{-1}}$
- Speed of sound at $p_0 = 155\,\mathrm{bar}$ and $T = 300\,^\circ\mathrm{C}$: $c_\ell^* \simeq 1.0\times 10^3\,\mathrm{m\cdot s^{-1}}$

$$\textbf{Mach number } \mathrm{M} = \frac{|\mathbf{u}|}{c_\ell^*} \simeq 5\times 10^{-3} \ll 1$$

This is also the case

- for incidental regime
- for some accidental scenarios such as a LOFA (Loss of Flow Accident)[1] induced by a coolant pump trip event *even if phase change occurs*

Acoustics negligible (no shock waves) BUT high heat transfers

[1] Except for a very fast depressurization such as a LOCA (Loss of Coolant Accident)

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Which model?

- Low Mach number: $\mathrm{M} \ll 1$
- High heat transfers: $\operatorname{div} \mathbf{u} \neq 0$

$$\Downarrow$$

1. Compressible Navier-Stokes system
   $\rightarrow$ model with acoustics and with heat transfers
2. Asymptotic low Mach model
   (obtained formally by filtering out the acoustics waves)
   $\rightarrow$ model without acoustics but with heat transfers

Section 3

A Low Mach model for a heat exchanger

- Governing equations
- Boundary Conditions
- Equation(s) of State

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A Low Mach model for a heat exchanger

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An Asymptotic Low Mach Model

$$p(t,\mathbf{x}) = p_0(t) + \bar{p}(t,\mathbf{x}) \text{ with } \frac{\bar{p}(t,\mathbf{x})}{p(t,\mathbf{x})} = \mathcal{O}(\mathrm{M}^2)$$

$$\begin{cases} \operatorname{div}(\mathbf{u}) = -\dfrac{p_0'(t)}{\varrho(h,p_0)(c^*(h,p_0))^2} + \dfrac{\beta(h,p_0)}{p_0(t)}[\Phi + \operatorname{div}(\lambda \cdot \nabla T(h,p_0))] \\ \varrho(h,p_0)\Big(\partial_t h + \mathbf{u}\cdot\nabla h\Big) = \Phi + p_0'(t) + \operatorname{div}(\lambda \cdot \nabla T(h,p_0)) \\ \varrho(h,p_0)\Big(\partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u}\Big) + \nabla\bar{p} = \operatorname{div}(\sigma(\mathbf{u})) + \varrho(h,p_0)\mathbf{g} \end{cases}$$

- **Unknowns**
- **Given quantities**
- **Equation Of State:**

An Asymptotic Low Mach Model

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Unknowns

- $(t,\mathbf{x}) \mapsto \mathbf{u}$ velocity
- $(t,\mathbf{x}) \mapsto h$ enthalpy
- $(t,\mathbf{x}) \mapsto \bar{p}$ dynamic pressure

Given quantities

Equation Of State:

An Asymptotic Low Mach Model

$$p(t,\mathbf{x}) = p_0(t) + \bar{p}(t,\mathbf{x}) \text{ with } \frac{\bar{p}(t,\mathbf{x})}{p(t,\mathbf{x})} = \mathcal{O}(\mathrm{M}^2)$$

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- **Unknowns**
- **Given quantities**
  - $(t,\mathbf{x}) \mapsto \Phi \geq 0$ power density
  - $\mathbf{g}$ gravity
  - $t \mapsto p_0$ thermodynamic pressure
- **Equation Of State:**

An Asymptotic Low Mach Model

$$p(t,\mathbf{x}) = p_0(t) + \bar{p}(t,\mathbf{x}) \text{ with } \frac{\bar{p}(t,\mathbf{x})}{p(t,\mathbf{x})} = \mathcal{O}(\mathrm{M}^2)$$

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- **Unknowns**
- **Given quantities**
- **Equation Of State:** $(h,p_0) \mapsto \varrho$ density

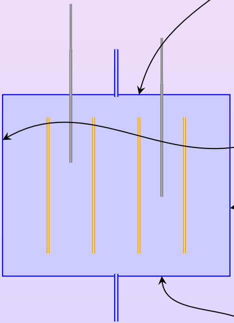
$$\Longrightarrow \begin{cases} (h,p_0) \mapsto \beta \stackrel{\text{def}}{=} -\dfrac{p_0}{\varrho^2(h,p_0)} \dfrac{\partial\varrho}{\partial h}\Big|_{p_0} & \text{compressibility coefficient} \\ (h,p_0) \mapsto T & \text{temperature} \\ (h,p_0) \mapsto c^* & \text{speed of sound} \end{cases}$$

Section 3

A Low Mach model for a heat exchanger

- Governing equations
- Boundary Conditions
- Equation(s) of State

Boundary conditions



Free outflow

$$\sigma(\mathbf{u})\mathbf{n} - \bar{p}\mathbf{n} = \mathbf{0}$$

Free-slip

$$\begin{cases} \mathbf{u} \cdot \mathbf{n} = 0 \\ (\sigma(\mathbf{u})\mathbf{n}) \cdot \boldsymbol{\tau} = 0 \end{cases}$$

Inflow

$$\begin{cases} h = h_e(t, x), \\ (\varrho\mathbf{u}) = (0, D_e(t, x)) \end{cases}$$

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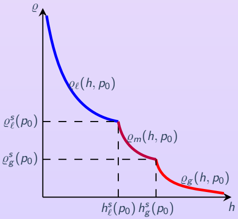
Diphasic EOS

- Liquid $\kappa = \ell$ and vapour $\kappa = g$ are characterized by their thermodynamic properties: $(h, p_0) \mapsto \varrho_\kappa$
- In the mixture, full equilibrium between liquid and vapour phases: $T = T^s(p_0)$ and we define values at saturation:

$$h^s_\kappa(p_0) \stackrel{\text{def}}{=} h_\kappa\big(p_0, T^s(p_0)\big), \qquad \varrho^s_\kappa(p_0) \stackrel{\text{def}}{=} \varrho_\kappa\big(p_0, T^s(p_0)\big) = \varrho_\kappa\big(h^s_\kappa, p_0\big).$$

$$\varrho(h, p_0) = \begin{cases} \varrho_\ell(h, p_0), & \text{if } h \le h^s_\ell(p_0), \\ \varrho_m(h, p_0) & \text{if } h^s_\ell(p_0) < h < h^s_g(p_0), \\ \varrho_g(h, p_0), & \text{if } h \ge h^s_g(p_0), \end{cases}$$



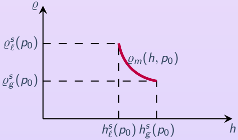
Mixture EoS

$$\begin{cases} \varrho = \alpha \varrho_g^s(p_0) + (1-\alpha)\varrho_\ell^s(p_0) \\ \varrho h = \alpha \varrho_g^s(p_0) h_g^s(p_0) + (1-\alpha)\varrho_\ell^s(p_0) h_\ell^s(p_0) \end{cases}$$

for $h \in [h_\ell^s(p_0); h_g^s(p_0)]$

$$\Downarrow$$

$$\boxed{\varrho_m(h,p_0) = \frac{p_0/\beta_m(p_0)}{h - q_m(p_0)}}$$



where

$$\beta_m(p_0) \stackrel{\text{def}}{=} p_0 \frac{\frac{1}{\varrho_g^s} - \frac{1}{\varrho_\ell^s}}{h_g^s - h_\ell^s} = -\frac{p_0}{\varrho_m(h,p_0)} \left.\frac{\partial \varrho_m}{\partial h}\right|_{p_0} \qquad q_m(p_0) \stackrel{\text{def}}{=} \frac{\varrho_g^s h_g^s - \varrho_\ell^s h_\ell^s}{\varrho_g^s - \varrho_\ell^s}$$

Pure phase EoS: Noble Able Stiffened Gas law

$$\frac{1}{\varrho_\kappa}(h, p_0) = \frac{\gamma_\kappa - 1}{\gamma_\kappa} \frac{h - q_\kappa}{p_0 + \pi_\kappa} + b_\kappa$$

- $\gamma_\kappa > 1$ adiabatic coefficient
- π_κ reference pressure
- q_κ binding energy
- b_κ covolume

$$\Downarrow$$

$$\beta_\kappa(p_0) = -\frac{p_0}{\varrho_\kappa^2(h, p_0)} \left.\frac{\partial \varrho}{\partial h}\right|_{p_0} = \frac{\gamma_\kappa - 1}{\gamma_\kappa} \frac{p_0}{p_0 + \pi_\kappa} \qquad \text{independent on } h$$

$$\Downarrow$$

$$\varrho_\kappa(h, p_0) = \frac{p_0/\beta_\kappa(p_0)}{h - \hat{q}_\kappa(p_0)}, \qquad \hat{q}_\kappa(p_0) \stackrel{\text{def}}{=} q_\kappa - \frac{p_0}{\beta_\kappa(p_0)} b_\kappa$$

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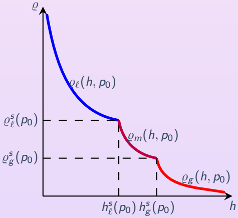
Diphasic Noble Able Stiffened Gas EOS

$$\varrho(h,p_0)=\frac{p_0/\beta(h,p_0)}{h-\hat{q}(h,p_0)}$$



where

$$\hat{q}_\kappa(p_0)\stackrel{\text{def}}{=}q_\kappa-\frac{p_0}{\beta_\kappa(p_0)}b_\kappa$$

$$[\beta,q,b](h,p_0)=\begin{cases}[\beta,q,b]_\ell, & \text{if } h\le h_\ell^s(p_0),\\ [\beta,q,0]_m & \text{if } h_\ell^s(p_0)<h<h_g^s(p_0),\\ [\beta,q,b]_g, & \text{if } h\ge h_g^s(p_0),\end{cases}$$

Section 4

Theoretical results: 1D-model

- Steady state solution
- Analytical solutions with NASG

The LMNC model

$$p_0(t) = 155\,\text{bar}\ \forall t$$

$$\lambda = 0\,\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$$

1D

$$\begin{cases} \partial_y v = \dfrac{\beta(h)}{p_0}\Phi \\ \partial_t h + v\partial_y h = \dfrac{\Phi}{\varrho(h)} \\ \partial_t(\varrho(h)v) + \partial_y(\varrho v^2 + \bar{p}) - \partial_y(\mu\partial_y v) = -g\,\varrho(h) \end{cases}$$

Section 4

Theoretical results: 1D-model

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Steady state solution

$$(h_e^\infty, D_e^\infty > 0, \Phi^\infty(y)) \stackrel{\text{def}}{=} \lim_{t\to+\infty} (h_e(t), D_e(t), \Phi(t,y))$$

1. **Enthalpy**
   Using $\partial_y(\varrho^\infty v^\infty) = 0$ we have $\partial_y h^\infty = \frac{\Phi^\infty}{D_e^\infty}$.

$$h^\infty(y) = h_e^\infty + \frac{\Psi(y)}{D_e^\infty}, \qquad \Psi(y) \stackrel{\text{def}}{=} \int_0^y \Phi^\infty(z)\, dz$$

2. **Velocity**

$$v^\infty(y) = \frac{D_e^\infty}{\varrho(h^\infty(y))}$$

3. **Dynamic pressure**
   Direct integration of $\partial_y \bar{p} = \partial_y(\mu\partial_y v) - \partial_y(\varrho v^2) - \varrho g$.

Section 4

Theoretical results: 1D-model

- Steady state solution
- Analytical solutions with NASG

Single phase

- **Velocity**
- **Enthalpy**

Single phase

- **Velocity**

  Direct integration of $\partial_y v = \frac{\bar{\beta}}{p_0}\Phi$.

$$v(t,y) = v_e(t) + \frac{\bar{\beta}}{p_0}\Psi(t,y), \qquad \Psi(t,y) \stackrel{\text{def}}{=} \int_0^y \Phi(t,z)\, \mathrm{d}z$$

- **Enthalpy**

Single phase

- ► **Velocity**
- ▼ **Enthalpy**

  Method of characteristics on $\partial_t h + v\partial_y h = \frac{\Phi}{\varrho(h)} = \Phi\left[\frac{\bar{\beta}}{p_0}(h - \hat{q})\right]$.

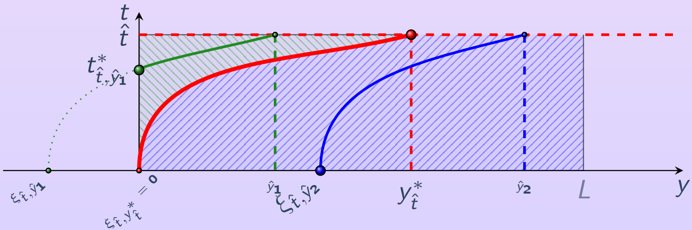
Single phase

- ▶ **Velocity**
- ▼ **Enthalpy**

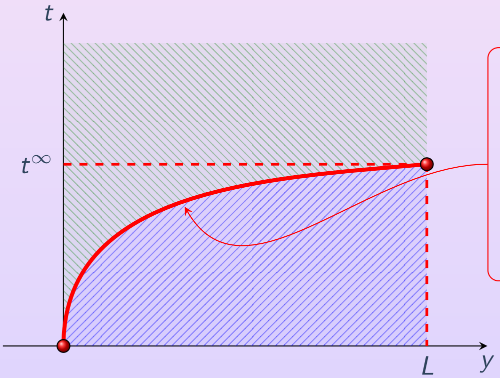
Method of characteristics on $\partial_t h + v\partial_y h = \frac{\Phi}{\varrho(h)} = \Phi\left[\frac{\bar{\beta}}{p_0}(h-\hat{q})\right]$.

Example: if Φ and v_e are constant, let $\hat{\Phi} \stackrel{\text{def}}{=} \frac{\bar{\beta}\Phi}{p_0}$ then

$$h(t,y) = \begin{cases} \hat{q} + \left(h_{\text{init}}(\xi_{t,y}) - \hat{q}\right) e^{\hat{\Phi} t} & \text{if } \xi_{t,y} \geq 0, \\ h_e(t^*_{t,y}) + \frac{\Phi}{D_e(t^*_{t,y})} y & \text{if } \xi_{t,y} < 0. \end{cases}$$



Single phase



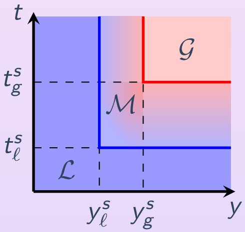
Characteristic $t = t(y)$:

$$y = \chi_{t^\infty,L}(t) = y_t^*$$

$$\Longrightarrow \begin{cases} \xi_{t^\infty,L} = 0 \\ t^*_{t^\infty,L} = 0 \\ y^*_{t^\infty} = L \\ y^*_0 = 0 \end{cases}$$

NASG two phases with phase transition

Φ, v_e, h_e, h_0: constant; IC and BC: liquid phase.

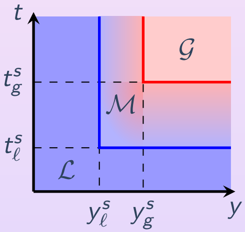


$$y_\ell^s = \frac{D_e}{\Phi}(h_\ell^s - h_e)$$
$$y_g^s = \frac{D_e}{\Phi}(h_g^s - h_e)$$
$$t_\ell^s = \frac{1}{\hat{\Phi}_\ell} \ln\left(\frac{h_\ell^s - \hat{q}_\ell}{h_0 - \hat{q}_\ell}\right)$$
$$t_g^s = t_\ell^s + \frac{1}{\hat{\Phi}_m} \ln\left(\frac{h_g^s - \hat{q}_m}{h_\ell^s - \hat{q}_m}\right)$$

- **Velocity**
- **Enthalpy**

NASG two phases with phase transition

Φ, v_e, h_e, h_0: constant; IC and BC: liquid phase.



$$
\begin{aligned}
y_\ell^s &= \frac{D_e}{\Phi}(h_\ell^s - h_e)\\
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t_\ell^s &= \frac{1}{\hat{\Phi}_\ell}\ln\left(\frac{h_\ell^s-\hat{q}_\ell}{h_0-\hat{q}_\ell}\right)\\
t_g^s &= t_\ell^s + \frac{1}{\hat{\Phi}_m}\ln\left(\frac{h_g^s-\hat{q}_m}{h_\ell^s-\hat{q}_m}\right)
\end{aligned}
$$

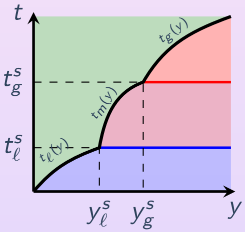
▼ **Velocity**: direct integration of $\partial_y v = \frac{\beta(h)}{p_0}\Phi$.

$$
v(t,y) = \begin{cases} v_e + y\hat{\Phi}_\ell & \text{if } (t,y)\in\mathcal{L},\\ v_e + y_\ell^s\hat{\Phi}_\ell + (y - y_\ell^s)\hat{\Phi}_m & \text{if } (t,y)\in\mathcal{M},\\ v_e + y_\ell^s\hat{\Phi}_\ell + (y_g^s - y_\ell^s)\hat{\Phi}_m + (y - y_g^s)\hat{\Phi}_g & \text{if } (t,y)\in\mathcal{G}, \end{cases}
$$

► **Enthalpy**

NASG two phases with phase transition

Φ, v_e, h_e, h_0: constant; IC and BC: liquid phase.



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$$t_g^s = t_\ell^s + \frac{1}{\hat{\Phi}_m} \ln\left(\frac{h_g^s - \hat{q}_m}{h_\ell^s - \hat{q}_m}\right)$$

- **Velocity**
- **Enthalpy**: method of characteristics on $\partial_t h + v\partial_y h = \frac{\beta(h)\Phi}{p_0}(h - \hat{q}(h))$.

$$h(t,y) = \begin{cases} q_\ell + (h_0 - \hat{q}_\ell)e^{\hat{\Phi}_\ell t} & \text{if } (t,y) \in \mathcal{L} \text{ and } t < t_\ell(y), \\ q_m + (h_\ell^s - \hat{q}_m)e^{\hat{\Phi}_m (t - t_\ell^s)} & \text{if } (t,y) \in \mathcal{M} \text{ and } t < t_m(y), \\ q_g + (h_g^s - \hat{q}_g)e^{\hat{\Phi}_g (t - t_g^s)} & \text{if } (t,y) \in \mathcal{G} \text{ and } t < t_g(y), \\ h_e + \frac{\Phi}{D_e} y & \text{otherwise.} \end{cases}$$

Section 5

Numerical schemes

- 1D Numerical schemes
- 2D Numerical scheme

Section 5

Numerical schemes

- 1D Numerical schemes
- 2D Numerical scheme

MOC-scheme

- **Enthalpy**
- **Velocity**

MOC-scheme

▼ **Enthalpy** - key idea:

$$\partial_t h(t^{n+1}, y_i) + v(t^{n+1}, y_i)\partial_y h(t^{n+1}, y_i) = \frac{\Phi(t^{n+1}, y_i)}{\varrho(h(t^{n+1}, y_i))}$$

$$\rightsquigarrow$$

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\tilde{h}_i^{n+1}(\tau) = \frac{\Phi\big(\tau, \chi(\tau; t^{n+1}, y_i)\big)}{\varrho(\tilde{h}_i^{n+1}(\tau))}$$

where $\bar{t} \in [t^n; t^{n+1}[$, $\tau \mapsto \tilde{h}_i^{n+1}(\tau) \stackrel{\text{def}}{=} h\big(\tau, \chi(\tau; t^{n+1}, y_i)\big)$ and χ is the characteristic flow defined as the solution of

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}\tau}\chi(\tau; t^{n+1}, y_i) = v\left(\tau, \chi(\tau; t^{n+1}, y_i)\right), & \tau \le t^{n+1}, \\ \chi(t^{n+1}; t^{n+1}, y_i) = y_i. \end{cases}$$

► **Velocity**

MOC-scheme

- **Enthalpy** - key idea:

$$\partial_t h(t^{n+1}, y_i) + v(t^{n+1}, y_i)\partial_y h(t^{n+1}, y_i) = \frac{\Phi(t^{n+1}, y_i)}{\varrho(h(t^{n+1}, y_i))}$$

$$\Downarrow$$

$$\int_{\bar{t}}^{t^{n+1}} \frac{\mathrm{d}}{\mathrm{d}\tau}\tilde{h}_i^{n+1}(\tau)\,\mathrm{d}\tau = \int_{\bar{t}}^{t^{n+1}} \frac{\Phi(\tau, \chi(\tau; t^{n+1}, y_i))}{\varrho(\tilde{h}_i^{n+1}(\tau))}\,\mathrm{d}\tau$$

where $\bar{t} \in [t^n; t^{n+1}[$, $\tau \mapsto \tilde{h}_i^{n+1}(\tau) \stackrel{\text{def}}{=} h(\tau, \chi(\tau; t^{n+1}, y_i))$ and χ is the characteristic flow defined as the solution of

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}\tau}\chi(\tau; t^{n+1}, y_i) = v\left(\tau, \chi(\tau; t^{n+1}, y_i)\right), & \tau \le t^{n+1}, \\ \chi(t^{n+1}; t^{n+1}, y_i) = y_i. \end{cases}$$

- **Velocity**

MOC-scheme

▼ **Enthalpy** - key idea:

$$\partial_t h(t^{n+1}, y_i) + v(t^{n+1}, y_i)\partial_y h(t^{n+1}, y_i) = \frac{\Phi(t^{n+1}, y_i)}{\varrho(h(t^{n+1}, y_i))}$$

$$\rightsquigarrow$$

$$h(t^{n+1}, y_i) - \tilde{h}_i^{n+1}(\bar{t}) = \int_{\bar{t}}^{t^{n+1}} \frac{\mathrm{d}}{\mathrm{d}\tau}\tilde{h}_i^{n+1}(\tau)\,\mathrm{d}\tau = \int_{\bar{t}}^{t^{n+1}} \frac{\Phi\left(\tau, \chi(\tau; t^{n+1}, y_i)\right)}{\varrho(\tilde{h}_i^{n+1}(\tau))}\,\mathrm{d}\tau$$

where $\bar{t} \in [t^n; t^{n+1}[$, $\tau \mapsto \tilde{h}_i^{n+1}(\tau) \stackrel{\text{def}}{=} h\left(\tau, \chi(\tau; t^{n+1}, y_i)\right)$ and χ is the characteristic flow defined as the solution of

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}\tau}\chi(\tau; t^{n+1}, y_i) = v\left(\tau, \chi(\tau; t^{n+1}, y_i)\right), & \tau \le t^{n+1}, \\ \chi(t^{n+1}; t^{n+1}, y_i) = y_i. \end{cases}$$

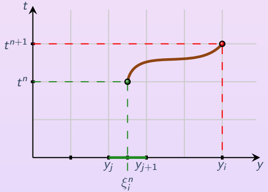
► **Velocity**

MOC-scheme

▼ **Enthalpy** - scheme: let $\xi_i^n \approx \chi(t^n; t^{n+1}, y_i)$.

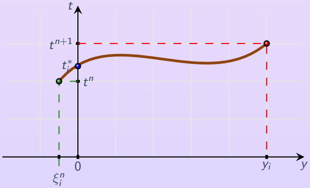
- If $\xi_i^n > 0$, let $\hat{h}_i^n \approx \tilde{h}_i^{n+1}(t^n)$ (at order 1 or higher) and then $\bar{t} = t^n$ and

$$h_i^{n+1} = \hat{h}_i^n + \Delta t \frac{\Phi(t^n, \xi_i^n)}{\varrho(\hat{h}_i^n)}$$



- If $\xi_i^n \le 0$, let $t_i^* = t^{n+1} - y_i/v_i^n \approx \tau$ such that $\chi(\tau; t^{n+1}, y_i) = 0$ and then $\bar{t} = t_i^*$ and

$$h_i^{n+1} = h_e(t_i^*) + (t^{n+1} - t_i^*) \frac{\Phi(t^*, 0)}{\varrho(h_e(t_i^*))}$$



► **Velocity**

MOC-scheme

- **Enthalpy**
- **Velocity** : $\partial_y v = \frac{\beta(h)\Phi}{p_0}$

$$
\begin{aligned}
v_i^{n+1} &= v_{i-1}^{n+1} + \frac{1}{p_0}\int_{y_{i-1}}^{y_i} \beta(h(t^{n+1},z))\Phi(t^{n+1},z)\,\mathrm{d}z \\
&\approx v_{i-1}^{n+1} + \frac{\Delta y}{p_0}\beta(h_{i-1}^{n+1})\Phi(t^{n+1},y_{i-1}).
\end{aligned}
$$

β is discontinuous at phase change points, so that if $h_\kappa^s \in (h_{i-1}^{n+1}, h_i^{n+1})$, let $y^* = y_{i-1} + \Delta y \frac{h_\kappa^s - h_{i-1}^{n+1}}{h_i^{n+1} - h_{i-1}^{n+1}}$ and then

$$
\begin{aligned}
&\int_{y_{i-1}}^{y_i} \beta(h(t^{n+1},z))\Phi(t^{n+1},z)\,\mathrm{d}z \\
&\approx (y^* - y_{i-1})\beta(h_{i-1}^{n+1})\Phi(t^{n+1},y_{i-1})\,\mathrm{d}y + (y_i - y^*)\beta(h_i^{n+1})\Phi(t^{n+1},y_i)\,\mathrm{d}y
\end{aligned}
$$

INTMOC-scheme (NASG)

- **Enthalpy** - key idea:

$$\frac{\frac{\mathrm{d}}{\mathrm{d}\tau}\tilde{h}_i^{n+1}(\tau)}{\beta(\tilde{h}_i^{n+1}(\tau))\left(\tilde{h}_i^{n+1}(\tau)-\hat{q}(\tilde{h}_i^{n+1}(\tau))\right)}=\frac{\Phi\big(\tau,\chi(\tau;t^{n+1},y_i)\big)}{p_0}$$

$$\Downarrow$$

$$\int_{\tilde{h}_i^{n+1}(\bar{t})}^{\tilde{h}_i^{n+1}(t^{n+1})}\frac{1}{\beta(h)(h-\hat{q}(h))}\,\mathrm{d}h=\frac{1}{p_0}\int_{\bar{t}}^{t^{n+1}}\Phi\big(\tau,\chi(\tau;t^{n+1},y_i)\big)\,\mathrm{d}\tau$$

so that

$$\tilde{h}_i^{n+1}(t^{n+1})=R^{-1}\left(R(\tilde{h}_i^{n+1}(\bar{t}))+\frac{1}{p_0}\int_{\bar{t}}^{t^{n+1}}\Phi\big(\tau,\chi(\tau;t^{n+1},y_i)\big)\,d\tau\right)$$

where

$$R(h)\stackrel{\mathrm{def}}{=}\int_0^{\tilde{h}}\frac{1}{\beta(h)(h-\hat{q}(h))}\,\mathrm{d}h$$

INTMOC-scheme (NASG)

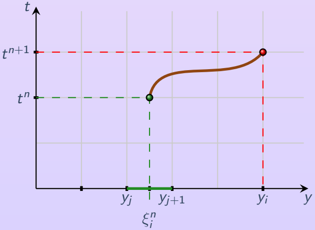
▼ **Enthalpy** - scheme: let $\xi_i^n \approx \chi(t^n; t^{n+1}, y_i)$.

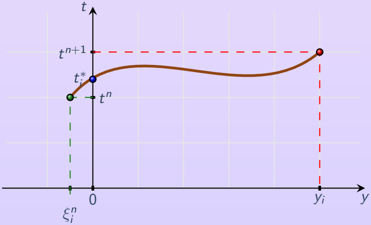
- If $\xi_i^n > 0$, let $\hat{h}_i^n \approx \tilde{h}_i^{n+1}(t^n)$ (at order 1 or 2) and then $\bar{t} = t^n$ and

$$h_i^{n+1} = R^{-1}\left(R(\hat{h}_i^n) + \frac{\Delta t}{p_0}\frac{\Phi(t^n, \xi_i^n) + \Phi(t^{n+1}, y_j)}{2}\right)$$

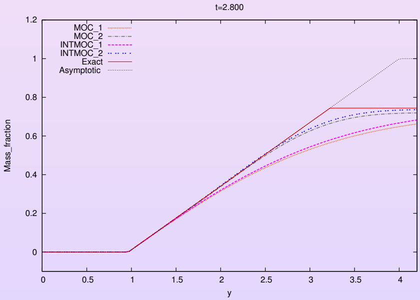
- If $\xi_i^n \leq 0$, let $t_i^* = t^{n+1} - y_i/v_i^n \approx \tau$ such that $\chi(\tau; t^{n+1}, y_i) = 0$ and then $\bar{t} = t_i^*$ and

$$h_i^{n+1} = R^{-1}\left(R(h_e(t_i^*)) + \frac{t^{n+1} - t_i^*}{p_0}\frac{\Phi(t_i^*, 0) + \Phi(t^{n+1}, y_i)}{2}\right)$$



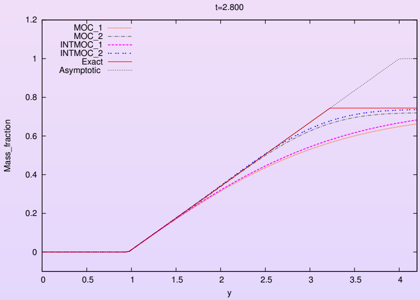


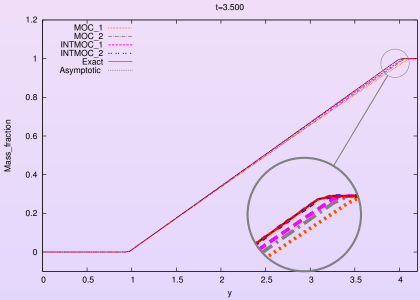
SG: MOC (order 1 or 2) vs INTMOC (order 1 or 2)



- Initially the domain is filled with liquid phase
- At $t = 1.769\,\text{s}$ mixture appears for $y > y_\ell^s \simeq 0.964\,\text{m}$
- At $t = 2.929\,\text{s}$ pure vapor phase appears for $y > y_g^s \simeq 4.002\,\text{m}$
- The asymptotic state is reached at $t = 2.957\,\text{s}$

SG: MOC (order 1 or 2) vs INTMOC (order 1 or 2)





- Initially the domain is filled with liquid phase
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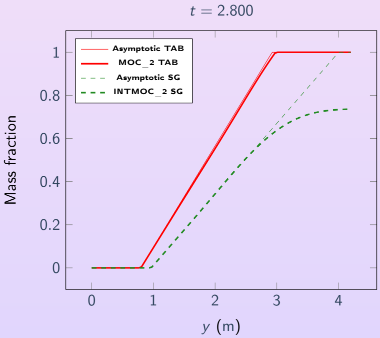
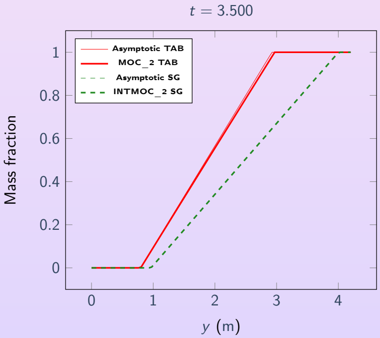
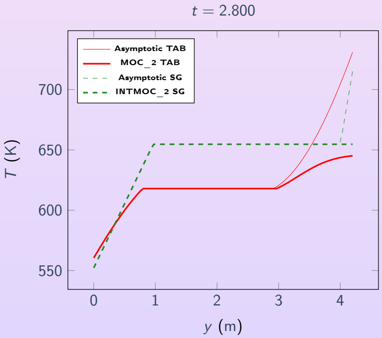
- The asymptotic state is reached at $t = 2.957\,\text{s}$

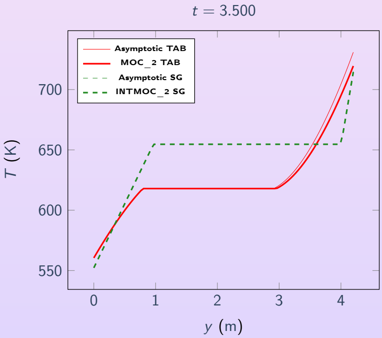
SG (INTMOC 2) vs TAB (MOC 2)



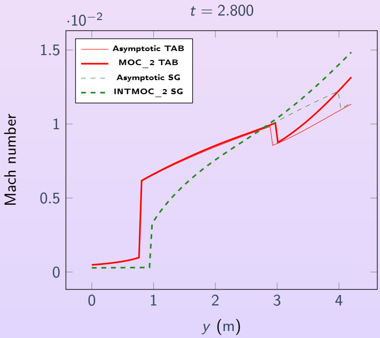


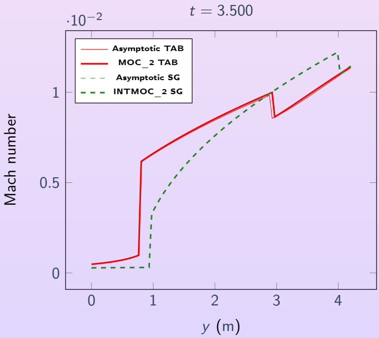
SG (INTMOC 2) vs TAB (MOC 2)





SG (INTMOC 2) vs TAB (MOC 2)

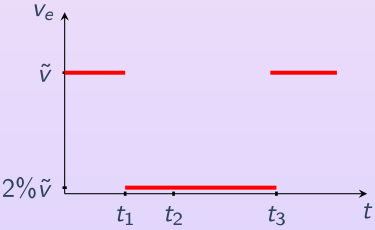


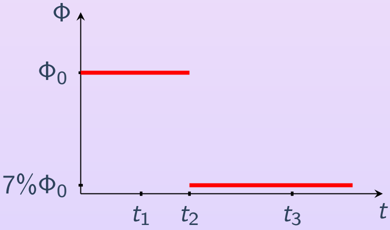


Loss of Flow Accident

$$v_e(t) = \begin{cases} \tilde{v} & \text{if } 0 \leq t < t_1, \\ 2\%\tilde{v} & \text{if } t_1 \leq t < t_3, \\ \tilde{v} & \text{if } t \geq t_3, \end{cases}$$

$$\Phi(t) = \begin{cases} \Phi_0 & \text{if } 0 \leq t < t_2, \\ 7\%\Phi_0 & \text{if } t \geq t_2. \end{cases}$$





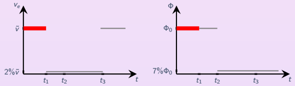
Coolant pump trip event

- pumps are stopped when $t = t_1$
- and re-started when $t = t_3$

Emergency stop

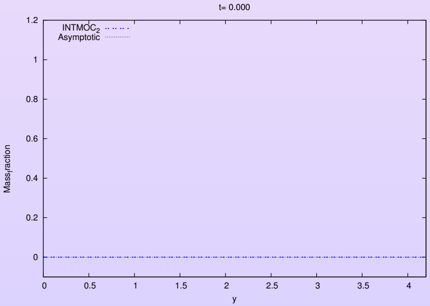
Control rods drop into the core when $t = t_2$

Loss of Flow Accident

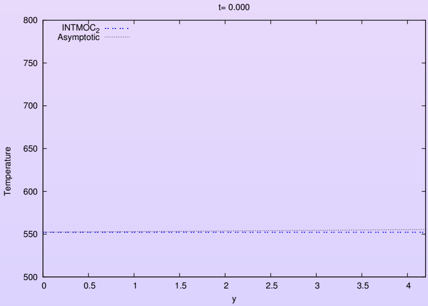


Initial data: $v_e(t) = \tilde{v}$ and $\Phi(t, y) = \Phi_0$.

Mass fraction

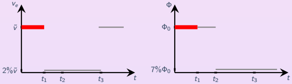


Temperature



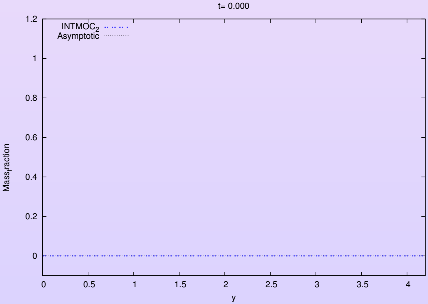
Description [$t_0 - t_1$] [$t_1 - t_2$] [$t_2 - t_3$] $t > t_3$ Fin

Loss of Flow Accident

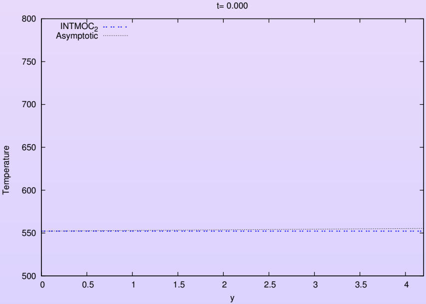


Initial data: $v_e(t) = \tilde{v}$ and $\Phi(t, y) = \Phi_0$.

Mass fraction

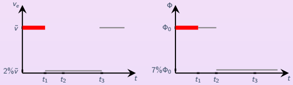


Temperature



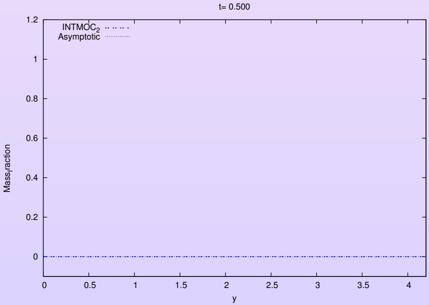
Description | $[t_0 - t_1]$ | $[t_1 - t_2]$ | $[t_2 - t_3]$ | $t > t_3$ | Fin

Loss of Flow Accident

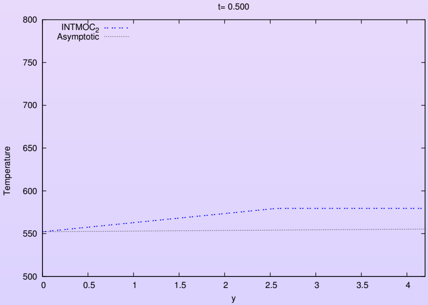


Initial data: $v_e(t) = \tilde{v}$ and $\Phi(t, y) = \Phi_0$.

Mass fraction

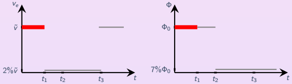


Temperature



◂ Description ▸ $[t_0 - t_1]$ ▸ $[t_1 - t_2]$ ▸▸ $[t_2 - t_3]$ ▸▸ $t > t_3$ ▸▸ Fin

Loss of Flow Accident



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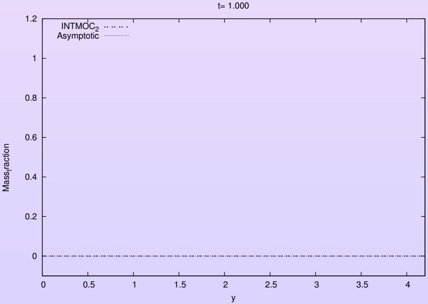
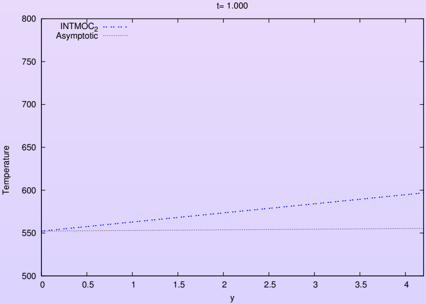
Mass fraction

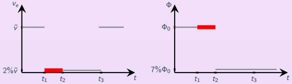


Temperature



Description | $[t_0 - t_1]$ | $[t_1 - t_2]$ | $[t_2 - t_3]$ | $t > t_3$ | Fin

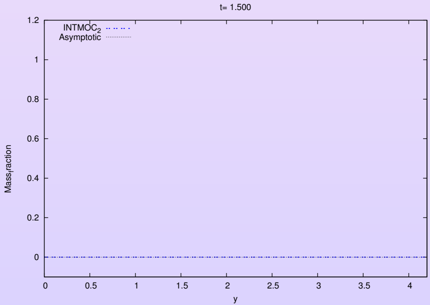
Loss of Flow Accident

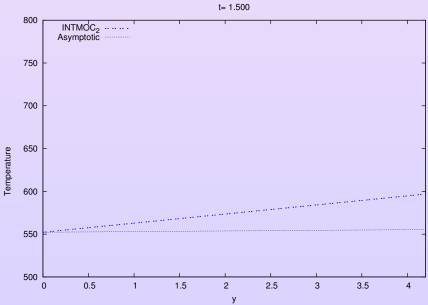


At t_1 most of the pumps stop $\implies v_e(t) \searrow$.

Mass fraction

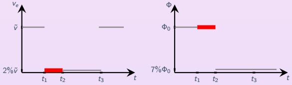
Temperature





◀ Description ▶ $[t_0 - t_1]$ ▶ $[t_1 - t_2]$ ▶▶ $[t_2 - t_3]$ ▶▶ $t > t_3$ ▶▶ Fin

Loss of Flow Accident



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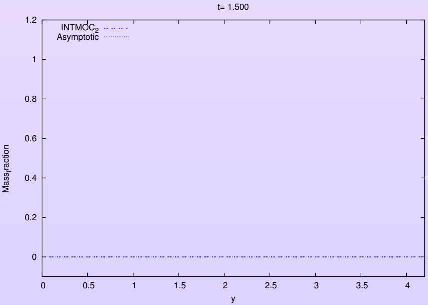
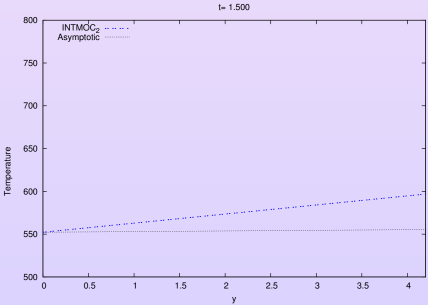
Mass fraction

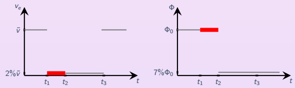


Temperature



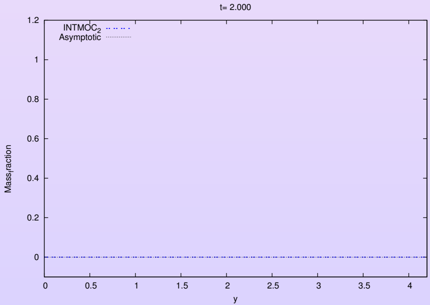
Description | $[t_0 - t_1]$ | $[t_1 - t_2]$ | $[t_2 - t_3]$ | $t > t_3$ | Fin

Loss of Flow Accident

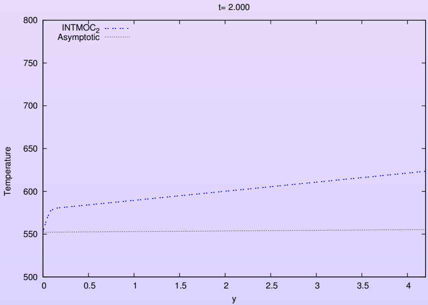


At t_1 most of the pumps stop $\Longrightarrow$ $v_e(t) \searrow$.

Mass fraction

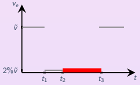


Temperature



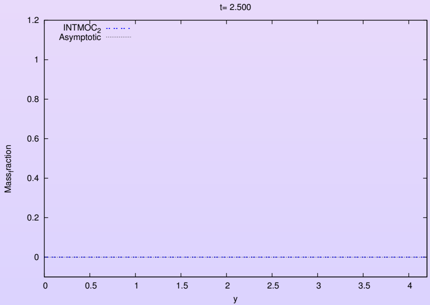
Description | $[t_0 - t_1]$ | $[t_1 - t_2]$ | $[t_2 - t_3]$ | $t > t_3$ | Fin

Loss of Flow Accident

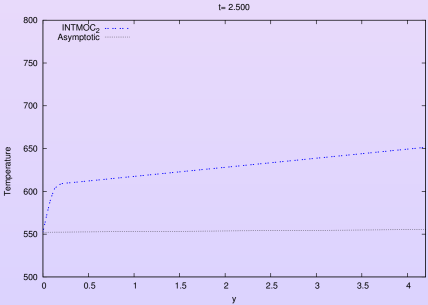


At t_2 the security system drops control rods into the core $\implies \Phi(t) \searrow 7\%\Phi_0$.

Mass fraction

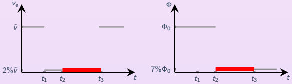


Temperature



◂ Description ▸ $[t_0 - t_1]$ ▸ $[t_1 - t_2]$ ▸▸ $[t_2 - t_3]$ ▸▸ $t > t_3$ ▸▸ Fin

Loss of Flow Accident



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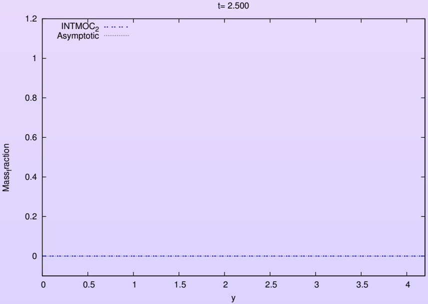
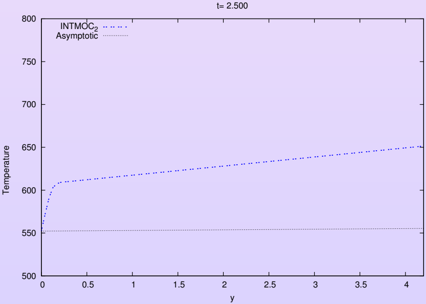
Mass fraction

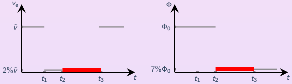


Temperature



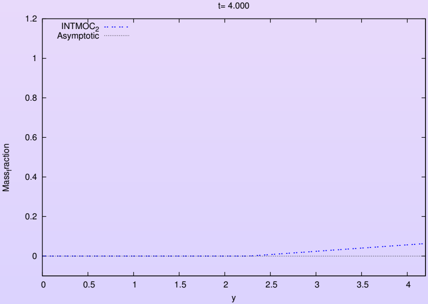
Description | $[t_0 - t_1]$ | $[t_1 - t_2]$ | $[t_2 - t_3]$ | $t > t_3$ | Fin

Loss of Flow Accident

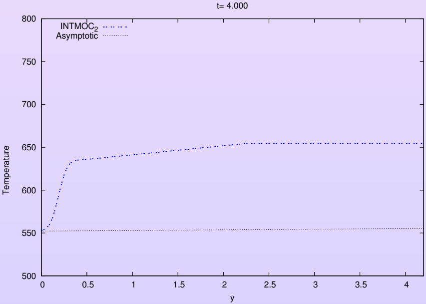


At t_2 the security system drops control rods into the core $\Longrightarrow \Phi(t) \searrow 7\%\Phi_0$.

Mass fraction

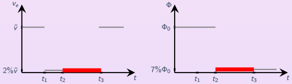


Temperature



◂ Description ▸ $[t_0 - t_1]$ ▸ $[t_1 - t_2]$ ▸▸ $[t_2 - t_3]$ ▸▸ $t > t_3$ ▸▸ Fin

Loss of Flow Accident



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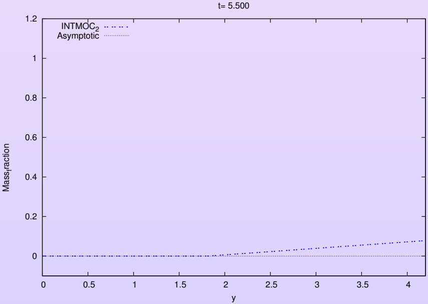
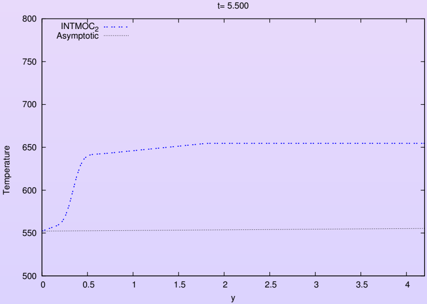


Temperature



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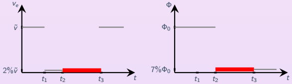

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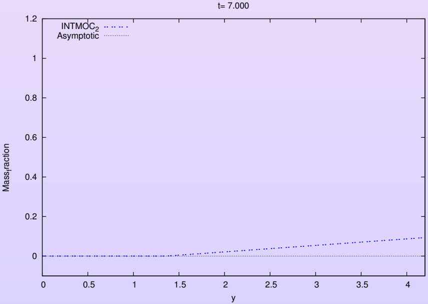
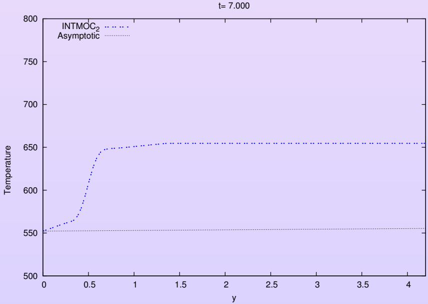


Temperature



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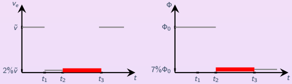

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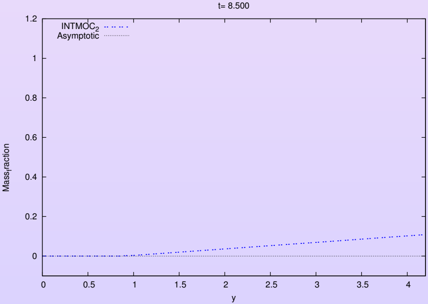
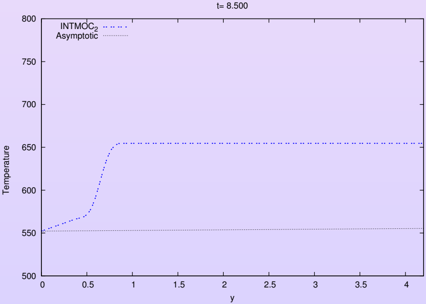
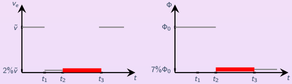


Temperature



◂ Description ▸ $[t_0 - t_1]$ ▸ $[t_1 - t_2]$ ▸▸ $[t_2 - t_3]$ ▸▸ $t > t_3$ ▸▸ Fin

Loss of Flow Accident



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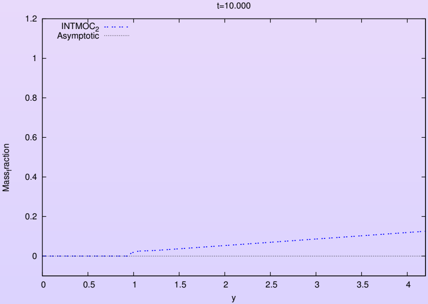
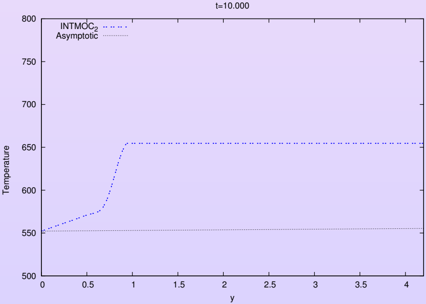


Temperature



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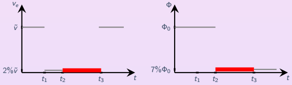

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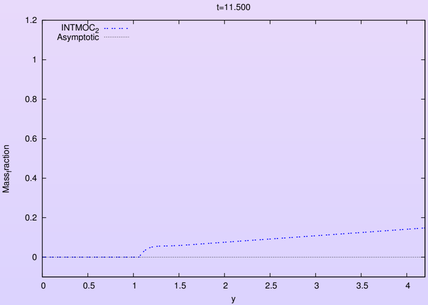
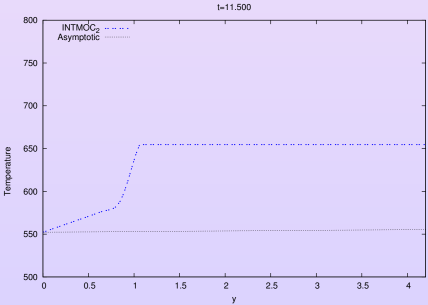


Temperature



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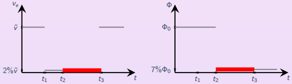

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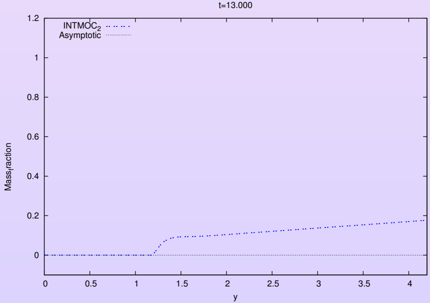
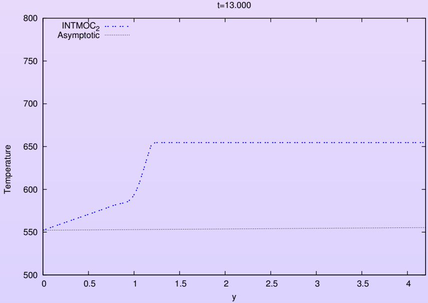


Temperature



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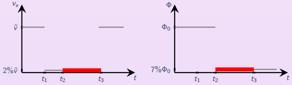

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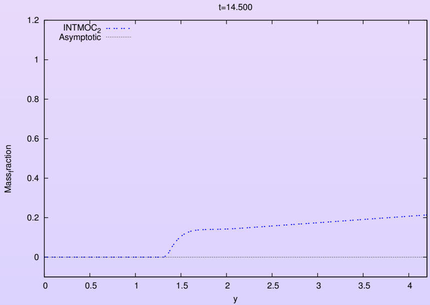
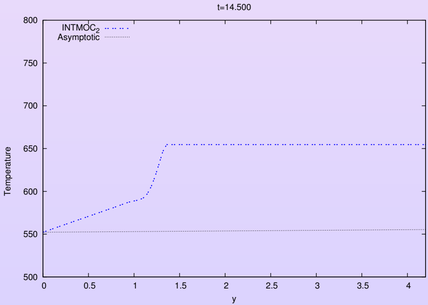


Temperature



◂ Description ▸ $[t_0 - t_1]$ ▸ $[t_1 - t_2]$ ▸▸ $[t_2 - t_3]$ ▸▸ $t > t_3$ ▸▸ Fin

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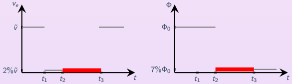

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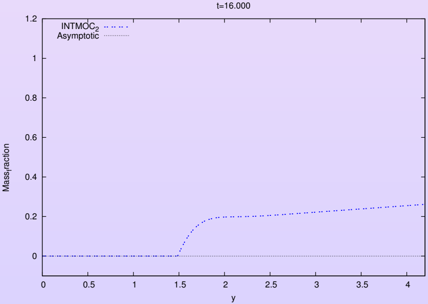
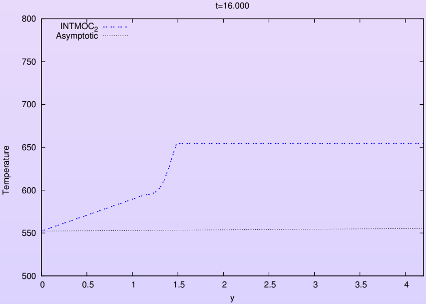


Temperature



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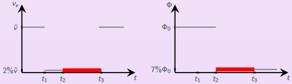

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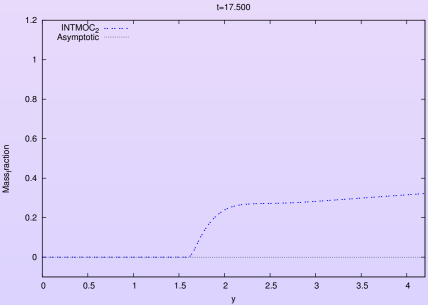
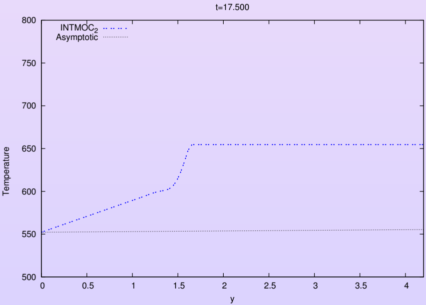


Temperature



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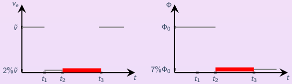

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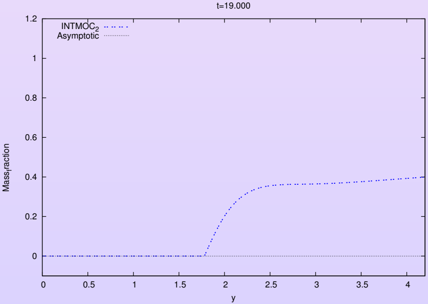

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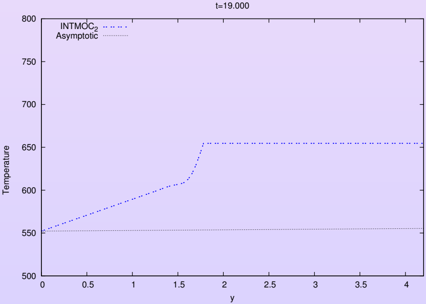

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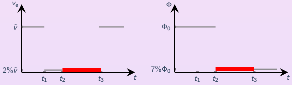

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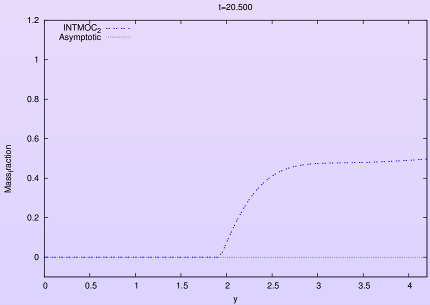

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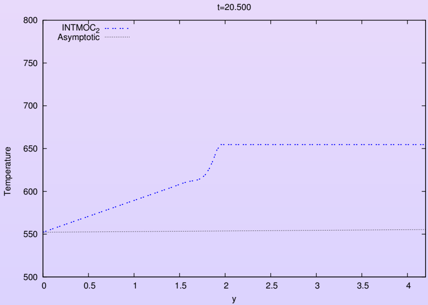

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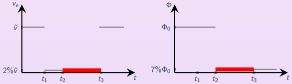

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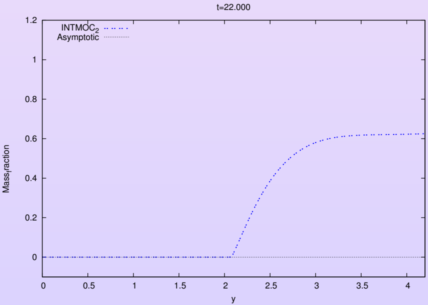

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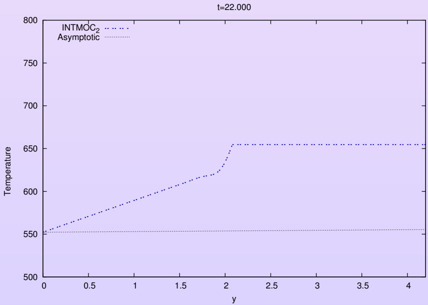

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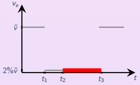

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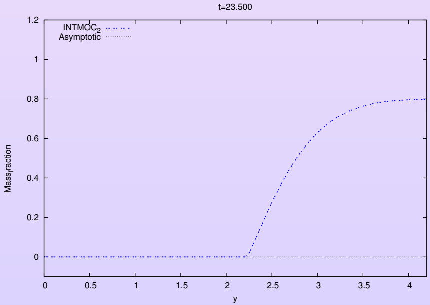

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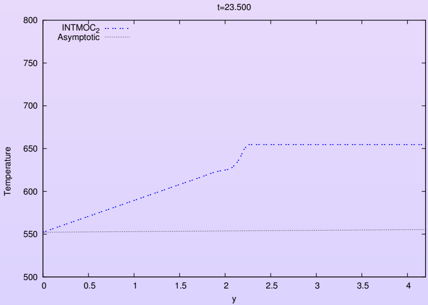

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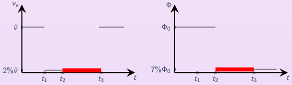

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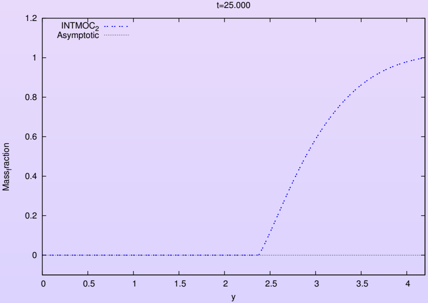

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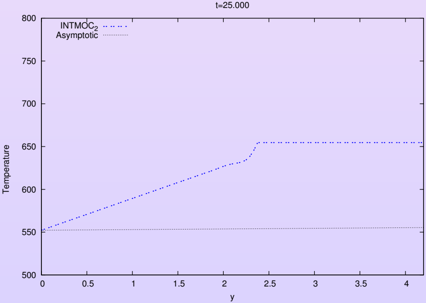

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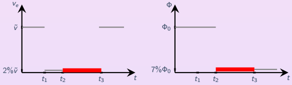

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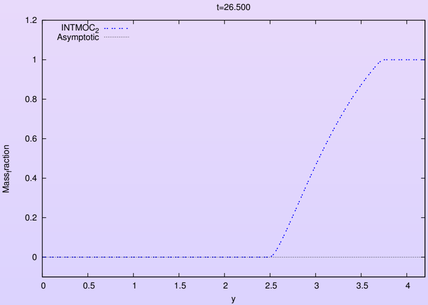

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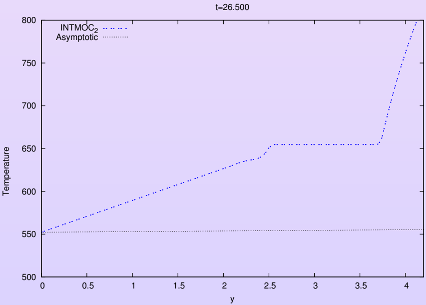

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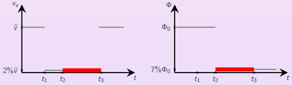

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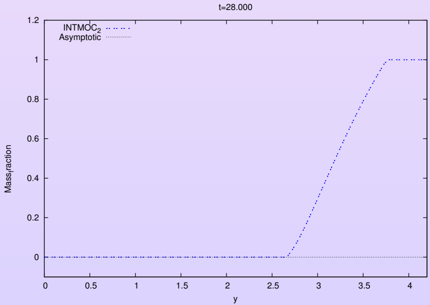

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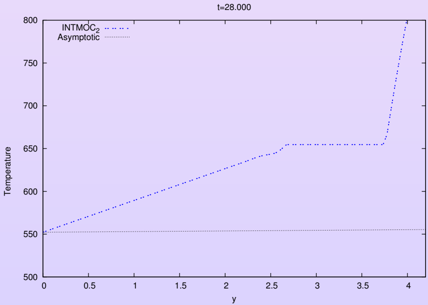

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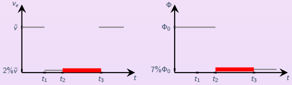

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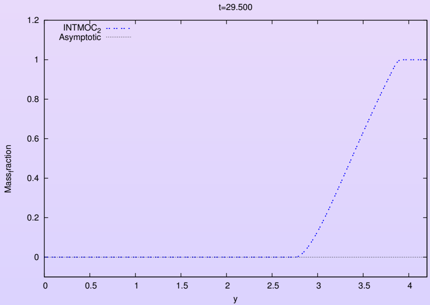

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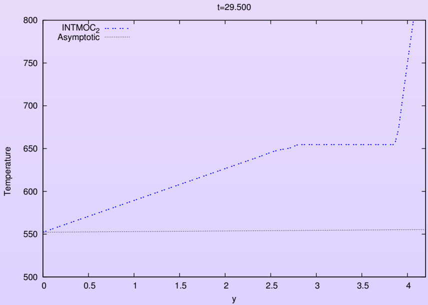

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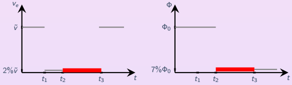

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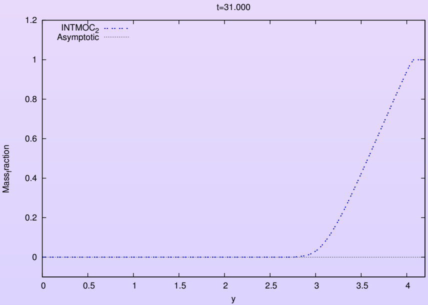

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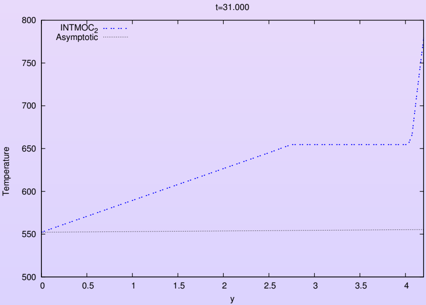

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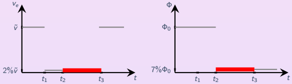

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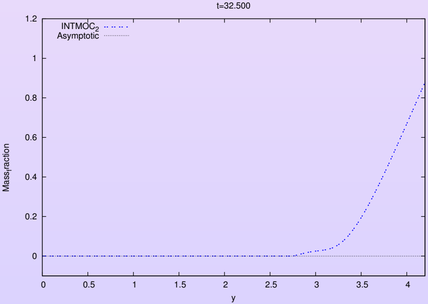
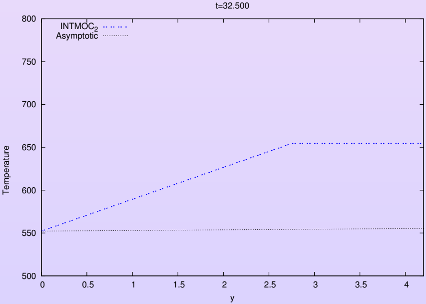
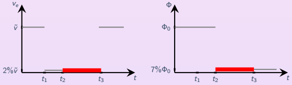


Temperature



Description | $[t_0 - t_1]$ | $[t_1 - t_2]$ | $[t_2 - t_3]$ | $t > t_3$ | Fin

Loss of Flow Accident



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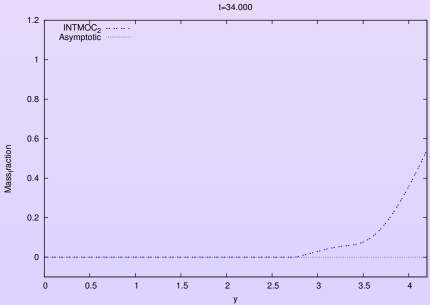

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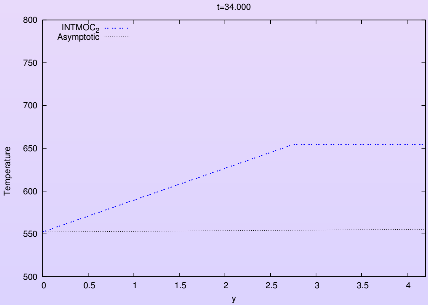

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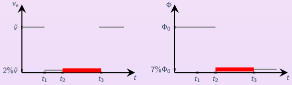

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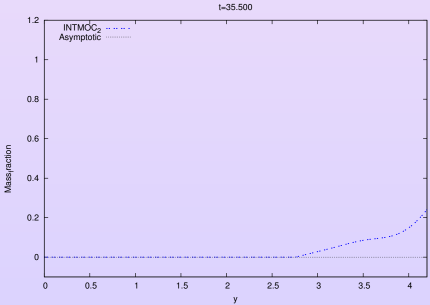

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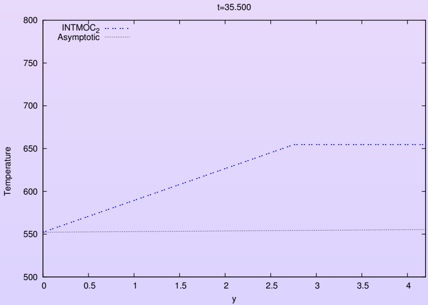

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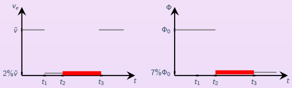

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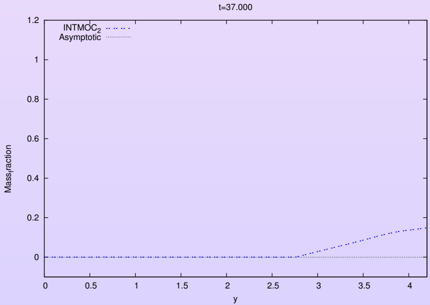

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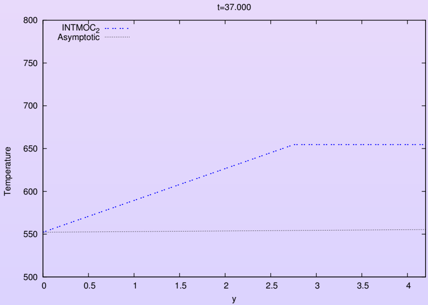

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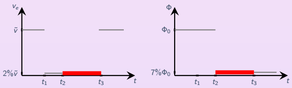

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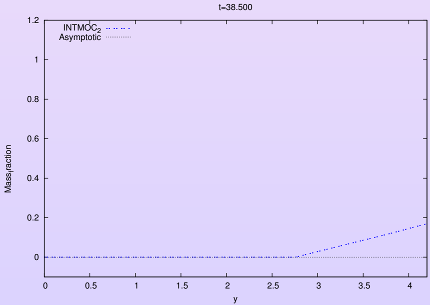

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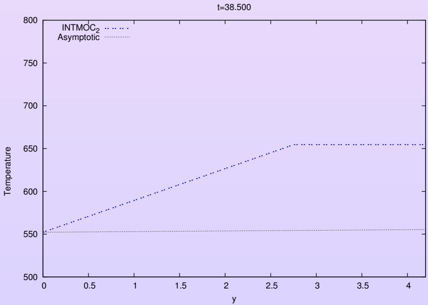

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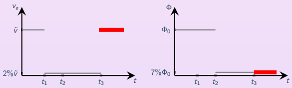

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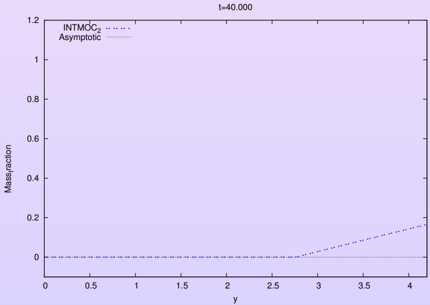

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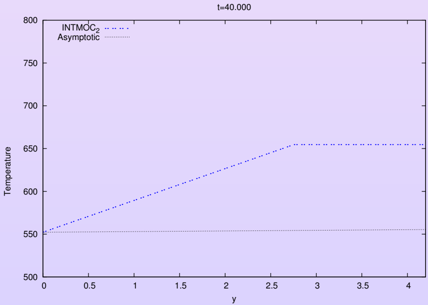

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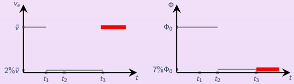

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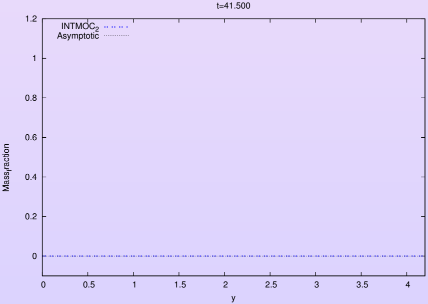

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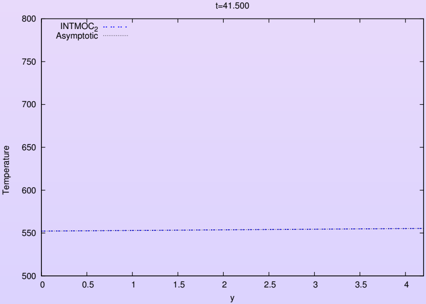

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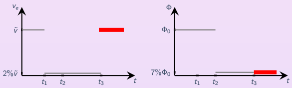

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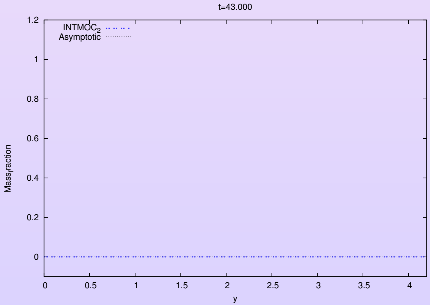
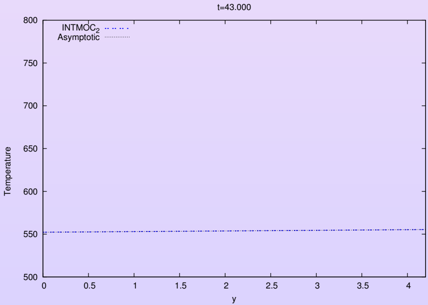


Temperature



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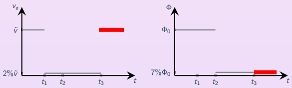

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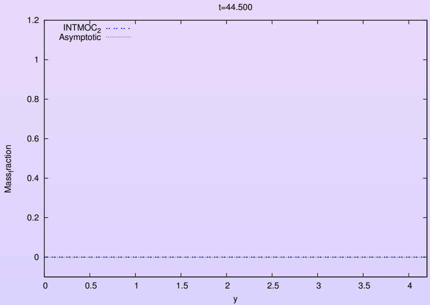

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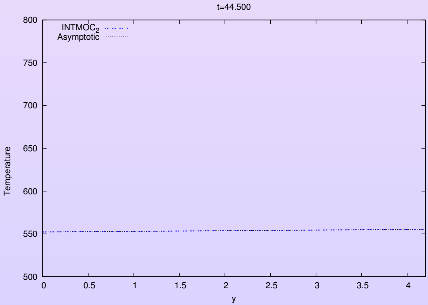

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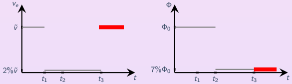

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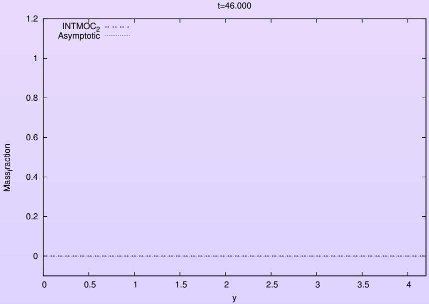

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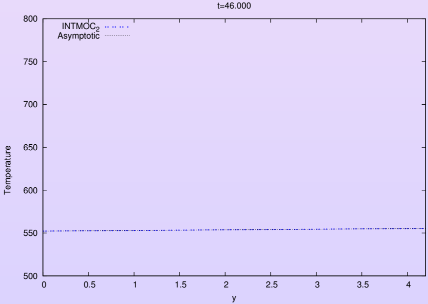

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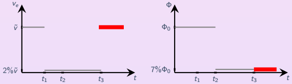

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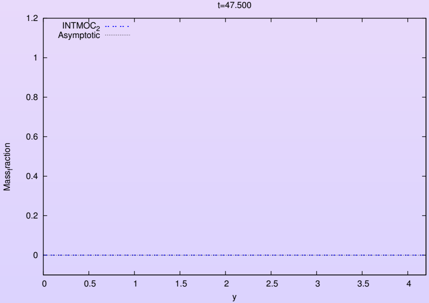

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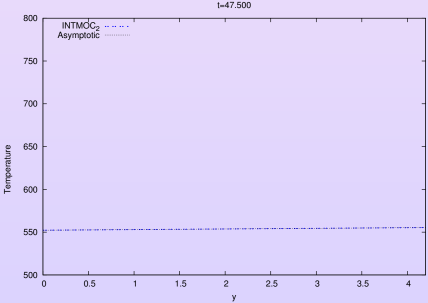

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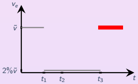

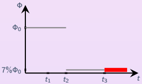

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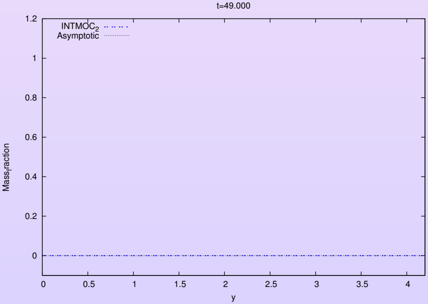

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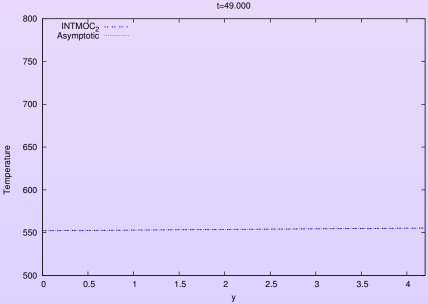

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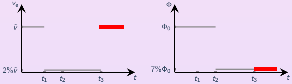

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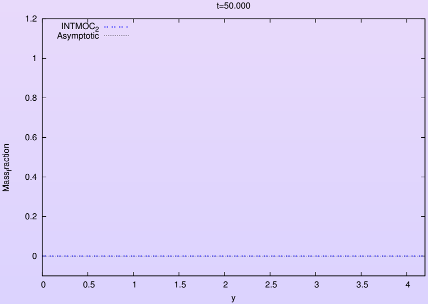

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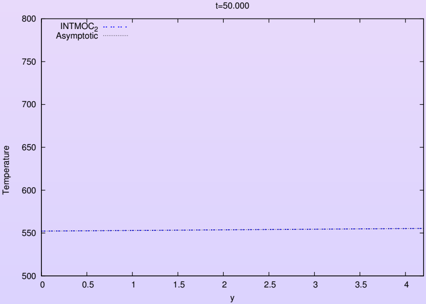

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Section 5

Numerical schemes

- 1D Numerical schemes
- 2D Numerical scheme

FreeFem++ (1)

- Let ξ^n the foot at time t^n of the characteristic issuing from $\mathbf{x}$ at time t^{n+1}, then the convective part of the system can be approximated by

$$[\partial_t \star + (\mathbf{u} \cdot \nabla)\star](t^{n+1}, \mathbf{x}) \approx \frac{\star(t^{n+1}, \mathbf{x}) - \star(t^n, \xi^n)}{\Delta t}, \qquad \star = \mathbf{u} \text{ or } h$$

- Weak formulation of a semi-implicit temporal discretization: at time t^{n+1} find $(\mathbf{u}^{n+1}, \bar{p}^{n+1}, h^{n+1}) \in (\mathbf{u}_e + \mathcal{U}) \times \mathcal{P} \times (h_e + \mathcal{H})$ defined by
  - $\mathcal{U} = \left\{ \mathbf{v} \in (H^1(\Omega))^2 | \mathbf{v}(x, 0) = \mathbf{0}, \mathbf{v} \cdot \mathbf{n}(0, y) = \mathbf{v} \cdot \mathbf{n}(L_x, y) = 0 \right\}$
  - $\mathcal{P} = L^2_0(\Omega) = \left\{ q \in L^2(\Omega) | \int_\Omega q(\mathbf{x}) \, d\mathbf{x} = 0 \right\}$
  - $\mathcal{H} = \left\{ k \in H^1(\Omega) | k(x, 0) = 0 \right\}$

  such that ...

FreeFem++ (2)

- $\forall \mathbf{u}_{\text{test}} \in \mathcal{U}$

$$\begin{aligned}
&\frac{1}{\Delta t}\int_\Omega \varrho(h^n)(\mathbf{u}^{n+1} - \mathbf{u}^n(\xi^n)) \cdot \mathbf{u}_{\text{test}} \, \mathrm{d}\mathbf{x} \\
&\quad + \int_\Omega \mu(h^n)((\nabla \mathbf{u}^{n+1} + (\nabla \mathbf{u}^{n+1})^T) : \nabla(\mathbf{u}_{\text{test}})) \, \mathrm{d}\mathbf{x} \\
&\quad + \int_\Omega \eta(h^n) \operatorname{div}(\mathbf{u}^{n+1}) \operatorname{div}(\mathbf{u}_{\text{test}}) \, \mathrm{d}\mathbf{x} - \int_\Omega \bar{p}^{n+1} \operatorname{div}(\mathbf{u}_{\text{test}}) \, \mathrm{d}\mathbf{x} \\
&= \int_\Omega \varrho(h^n)\mathbf{g} \cdot \mathbf{u}_{\text{test}} \, \mathrm{d}\mathbf{x}
\end{aligned}$$

- $\forall p_{\text{test}} \in \mathcal{P}$

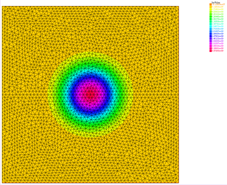
$$\int_\Omega \operatorname{div}(\mathbf{u}^{n+1}) p_{\text{test}} \, \mathrm{d}\mathbf{x} = \frac{1}{p_0}\int_\Omega \beta(h^n)\Phi(t^{n+1}) p_{\text{test}} \, \mathrm{d}\mathbf{x}$$

- $\forall h_{\text{test}} \in \mathcal{H}$

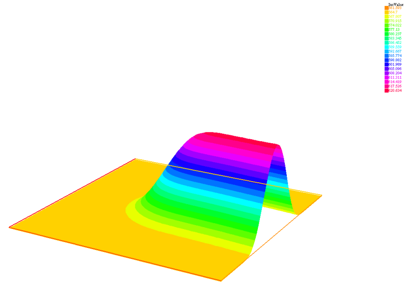
$$\frac{1}{\Delta t}\int_\Omega (h^{n+1} - h^n(\xi^n)) h_{\text{test}} \, \mathrm{d}\mathbf{x} = \int_\Omega \frac{\Phi(t^{n+1})}{\varrho(h^n)} h_{\text{test}} \, \mathrm{d}\mathbf{x}$$

A 2D test

- Power density localized in the center of the core
- Gravity along $(1, -1)$



Power density and mesh



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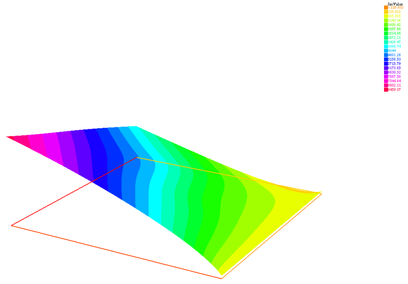

Pressure $(\bar{p} - \min_{\Omega} \bar{p})$

Section 6

Conclusion & Perspectives

Summary & Perspectives

- Model
  - ✓ mono/diphasic low Mach model with phase transition (Noble Able Stiffened Gas & Tabulated EoS),
  - ✓ $t \mapsto p_0(t)$,
  - ✓ Heat diffusion,
- Theoretical study (1D)
  - ✓ unsteady exact solutions on some cases (NASG with phase transition), steady exact solutions (also with tabulated EOS),
- Numerical Method
  - ✓ preliminary results: 1D (MOC, unconditionally positive)& 2D (MOC+FE)

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  - ✗ Coupling with a neutronics model
  - ✗ EoS for MSFR

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- Numerical Method
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  - ✗ 3D (FV with projection, C. Galusinski, J.-M. Maurizi).

Appendix

- References
- Compressible Navier-Stokes system
- Computing saturation values from two pure phase laws
- $p \to T^s$
- NIST vs SG
- Tabulated laws
- MOC

References

- S. Dellacherie.
  On a low Mach nuclear core model.
  ESAIM Proc., 35:79–106, 2012.

- M. Bernard, S. Dellacherie, G. Faccanoni, B. Grec, O. Lafitte, T.-T. Nguyen and Y. Penel.
  Study of low Mach nuclear core model for single-phase flow.
  ESAIM Proc., 38:118–134, 2012.

- M. Bernard, S. Dellacherie, G. Faccanoni, B. Grec and Y. Penel.
  Study of low Mach nuclear core model for two-phase flows with phase transition I: stiffened gas law.
  Submitted.

- S. Dellacherie, G. Faccanoni, B. Grec, E. Nayir and Y. Penel.
  2D numerical simulation of a low Mach nuclear core model with stiffened gas using FreeFem++
  Submitted

- S. Dellacherie, G. Faccanoni, B. Grec and Y. Penel.
  Study of a low Mach model for two-phase flows with phase transition II: tabulated laws.
  In preparation.

Compressible Navier-Stokes system

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0 \\ \partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \operatorname{div}(\sigma(\mathbf{u})) + \varrho \mathbf{g} \\ \partial_t(\varrho h) + \operatorname{div}(\varrho h \mathbf{u}) = \partial_t p + \mathbf{u} \cdot \nabla p + \sigma(\mathbf{u}) \colon \nabla \mathbf{u} + \Phi \end{cases}$$

where

$$\sigma(\mathbf{u}) \stackrel{\text{def}}{=} \nu\left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T\right) + \eta \nabla \mathbf{u}$$

- **Unknowns**
- **Given quantities**
- **Equation Of State**

Compressible Navier-Stokes system

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0 \\ \partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \operatorname{div}(\sigma(\mathbf{u})) + \varrho \mathbf{g} \\ \partial_t(\varrho h) + \operatorname{div}(\varrho h \mathbf{u}) = \partial_t p + \mathbf{u} \cdot \nabla p + \sigma(\mathbf{u}) : \nabla \mathbf{u} + \Phi \end{cases}$$

where

$$\sigma(\mathbf{u}) \stackrel{\text{def}}{=} \nu\left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T\right) + \eta \nabla \mathbf{u}$$

- **Unknowns**
  - $(t, \mathbf{x}) \mapsto \mathbf{u}$ velocity,
  - $(t, \mathbf{x}) \mapsto h$ enthalpy,
  - $(t, \mathbf{x}) \mapsto p$ pressure;
- **Given quantities**
- **Equation Of State**

Compressible Navier-Stokes system

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0 \\ \partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \operatorname{div}(\sigma(\mathbf{u})) + \varrho \mathbf{g} \\ \partial_t(\varrho h) + \operatorname{div}(\varrho h \mathbf{u}) = \partial_t p + \mathbf{u} \cdot \nabla p + \sigma(\mathbf{u}) : \nabla \mathbf{u} + \Phi \end{cases}$$

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- **Unknowns**
- **Given quantities**
  - $(t, \mathbf{x}) \mapsto \Phi \geq 0$ power density,
  - $\mathbf{g}$ gravity;
- **Equation Of State**

Compressible Navier-Stokes system

$$\begin{cases} \partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0 \\ \partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \operatorname{div}(\sigma(\mathbf{u})) + \varrho \mathbf{g} \\ \partial_t(\varrho h) + \operatorname{div}(\varrho h \mathbf{u}) = \partial_t p + \mathbf{u} \cdot \nabla p + \sigma(\mathbf{u}) \colon \nabla \mathbf{u} + \Phi \end{cases}$$

where

$$\sigma(\mathbf{u}) \stackrel{\text{def}}{=} \nu\left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T\right) + \eta \nabla \mathbf{u}$$

- **Unknowns**
- **Given quantities**
- **Equation Of State**
  - $(h, p) \mapsto \nu, \eta$ such that $2\mu + 3\eta > 0$,
  - $(h, p) \mapsto \varrho$ density.

Saturation values

- Liquid $\kappa = \ell$ and vapor $\kappa = g$ are characterized by their EoS

$$(h, p) \mapsto \varrho_\kappa = \frac{\gamma_\kappa}{\gamma_\kappa - 1} \frac{p + \pi_\kappa}{h - q_\kappa}$$

(see Le Metayer and Saurel for parameters of liquid water and steam)

- Second principle of thermodynamics: when phases coexist, they have the same pressures, the same temperatures and their chemical potentials are equal:

$$g_\ell(p, T) = g_g(p, T) \qquad \Longrightarrow \qquad T = T^s(p).$$

- We define saturation values at $p = p_0$:

$$h^s_\kappa \overset{\text{def}}{=} h_\kappa\big(p_0, T^s(p_0)\big), \qquad \varrho^s_\kappa \overset{\text{def}}{=} \varrho_\kappa\big(h^s_\kappa, p_0\big).$$

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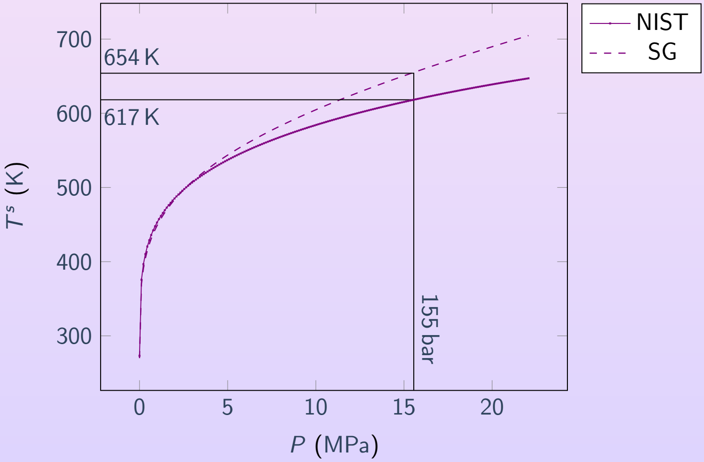
$p \mapsto T^s$

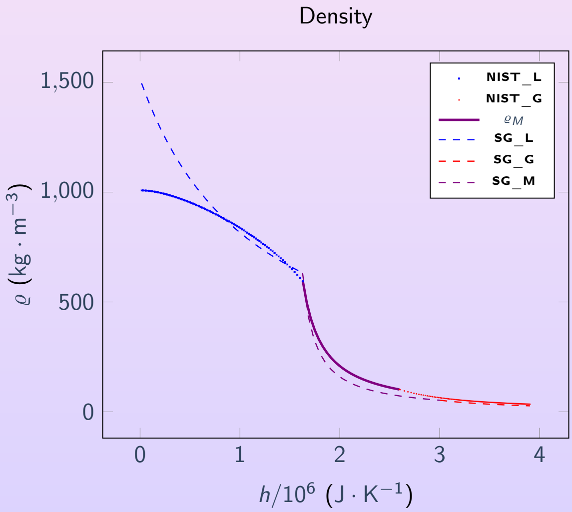


700
600
500
400
300
654 K
617 K
155 bar
Tˢ (K)
0
5
10
15
20
P (MPa)
NIST
SG

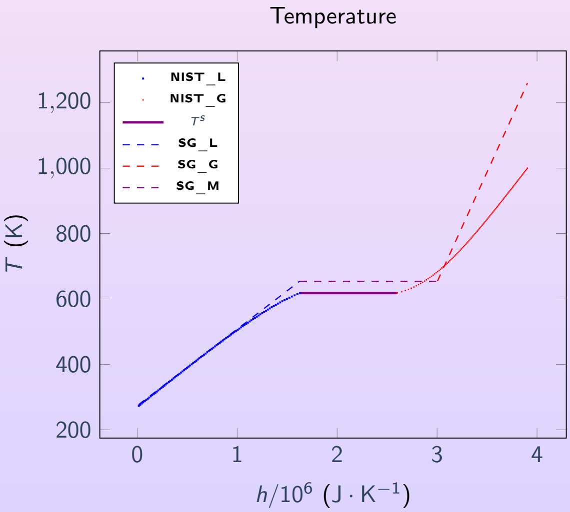
NIST vs SG

	NIST	SG
T^s	$617\,\mathrm{K}$	$654\,\mathrm{K}$
h_ℓ^s	$1.629 \times 10^6\ \mathrm{J} \cdot \mathrm{K}^{-1}$	$1.627 \times 10^6\ \mathrm{J} \cdot \mathrm{K}^{-1}$
h_g^s	$2.596 \times 10^6\ \mathrm{J} \cdot \mathrm{K}^{-1}$	$3.004 \times 10^6\ \mathrm{J} \cdot \mathrm{K}^{-1}$
ϱ_ℓ^s	$594.38\,\mathrm{kg} \cdot \mathrm{m}^{-3}$	$632.663\,\mathrm{kg} \cdot \mathrm{m}^{-3}$
ϱ_g^s	$101.93\,\mathrm{kg} \cdot \mathrm{m}^{-3}$	$52.937\,\mathrm{kg} \cdot \mathrm{m}^{-3}$

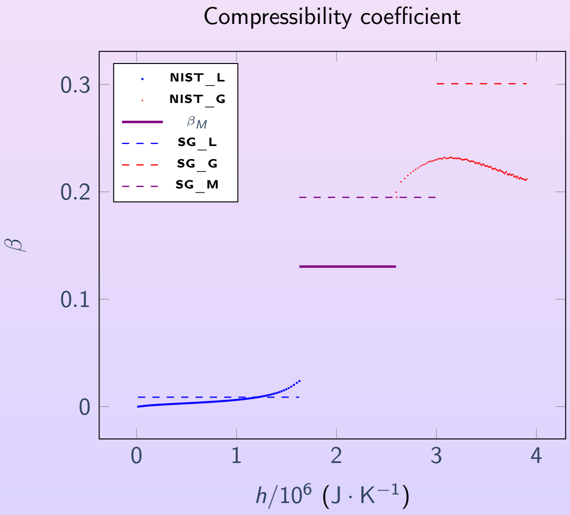
NIST vs SG: $h \mapsto \varrho$



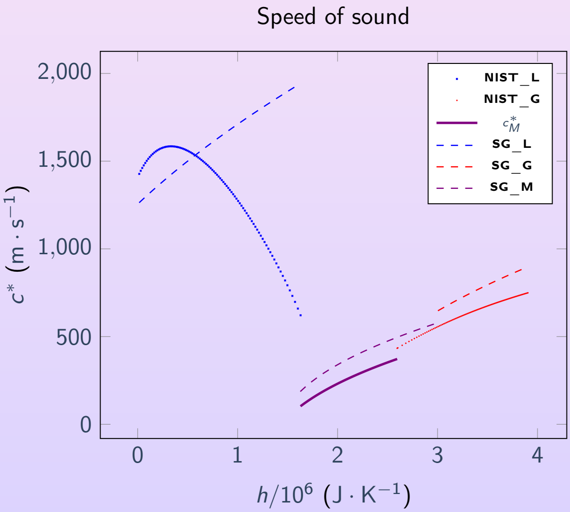
NIST vs SG: $h \mapsto T$



NIST vs SG: $h \mapsto \beta$



NIST vs SG: $h \mapsto c^*$



Pure phase EoS: Tabulated laws at $p = p_0$

κ	h [kJ/kg]	ϱ_κ [kg/m^3]	T_κ [K]	c^*_κ [m · s^{-1}]	β_κ
ℓ	15.608	1007.5	273.16	1427.4	✗
ℓ	30.678	1007.5	276.79	1445.0	✗
⋮	⋮	⋮	⋮	⋮	⋮
ℓ	1602.8	609.10	614.77	659.56	✗
ℓ	h^s_ℓ	594.38	T^s	621.43	✗
g	h^s_g	101.93	T^s	433.40	✗
g	2602.6	101.06	618.41	435.61	✗
⋮	⋮	⋮	⋮	⋮	⋮
g	2.5299	35.139	996.37	747.83	✗
g	2.5290	34.985	1000.0	749.37	✗

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

Pure phase EoS: Tabulated laws at $p = p_0$

Liquid phase

- Discretization of the enthalpy interval $[1.56 \times 10^4; h_\ell^s]$:

$$h_i \simeq (1.56 + 1.68i) \times 10^4, \qquad i \in \mathfrak{I} = \{1, \dots, 96\}$$

- Approximation of $\beta_\ell(h_i) = -\frac{p_0}{\varrho_\ell^2(h_i)} \varrho_\ell'(h_i)$ by finite differences
- Least squares polynomial approximation over the set of discrete values $((\varrho_\ell, \beta_\ell, T_\ell, c_\ell^*)(h_i))_{i \in \mathfrak{I}}$:

$$(\varrho_\ell, \beta_\ell, T_\ell, c_\ell^*)\left(\frac{h}{10^6}\right) = \sum_{j=0}^{N} \left(\frac{h}{10^6}\right)^i a_j, \qquad N \leq 6$$

Pure phase EoS: Tabulated laws at $p = p_0$

Vapor phase

- Discretization of the enthalpy interval $[h_g^s; 25.29 \times 10^6]$:

$$h_i \simeq (2.596 + 0.0122i) \times 10^6, \qquad i \in \mathfrak{I} = \{1, \dots, 107\}$$

- Approximation of $\beta_g(h_i) = -\frac{p_0}{\varrho_g^2(h_i)} \varrho_g'(h_i)$ by finite differences
- Least squares polynomial approximation over the set of discrete values $((\varrho_g, \beta_g, T_g, c_g^*)(h_i))_{i \in \mathfrak{I}}$:

$$(\varrho_g, \beta_g, T_g, c_g^*) \left(\frac{h}{10^6} \right) = \sum_{j=0}^{N} \left(\frac{h}{10^6} \right)^j a_j, \qquad N \leq 6$$

MOC scheme details

1. Foot of the characteristic $\xi_i^n \approx \chi(t^n; t^{n+1}, y_i)$.
2. $\hat{h}_i^n \approx h(t^n, \xi_i^n) \approx \tilde{h}_i^{n+1}(t^n)$.

MOC scheme details

1. Foot of the characteristic $\xi_i^n \approx \chi(t^n; t^{n+1}, y_i)$.
   This approximation is computed either at order one or two:
   1. at order one in time we have $\xi(t^n, y_i) \approx y_i - \Delta t \cdot v(t^n, y_i)$ so that we set
   $$\xi_i^n = y_i - \Delta t \cdot v_i^n,$$
   2. at order two in time we have
   $$\xi(t^n, y_i) \approx y_i - \Delta t \cdot v(t^n, y_i) - \frac{1}{2}\Delta t^2 \left(\partial_t v(t^n, y_i) - \frac{\beta(h(t^n, y_i))}{p_0} v(t^n, y_i)\Phi(t^n, y_i)\right)$$
   so that we set
   $$\xi_i^n = y_i - \Delta t \left(\frac{3}{2}v_i^n - \frac{1}{2}v_i^{n-1}\right) + \frac{\Delta t^2}{2}\frac{\beta(h_i^n)}{p_0} v_i^n \Phi(t^n, y_i).$$
2. $\hat{h}_i^n \approx h(t^n, \xi_i^n) \approx \tilde{h}_i^{n+1}(t^n)$.

MOC scheme details

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MOC scheme details

1. Foot of the characteristic $\xi_i^n \approx \chi(t^n; t^{n+1}, y_i)$.
2. $\hat{h}_i^n \approx h(t^n, \xi_i^n) \approx \tilde{h}_i^{n+1}(t^n)$.
   If $\xi_i^n > 0$, let j be the index such that $\xi_i^n \in [y_j, y_{j+1})$ and $\theta_{ij}^n \stackrel{\text{def}}{=} \frac{y_{j+1} - \xi_i^n}{\Delta x}$.
   1. At order one $\hat{h}_i^n = \theta_{ij}^n h_j^n + (1 - \theta_{ij}^n) h_{j+1}^n$.
   2. At order two $\hat{h}_i^n = \lambda_i^n h_j^- + (1 - \lambda_i^n) h_j^+$ where

$$\lambda_i^n \stackrel{\text{def}}{=} \begin{cases} \frac{1+\theta_{ij}^n}{3}, & \text{if } \mathcal{P}_j^+(\theta_{ij}^n) \geq 0 \text{ and } \mathcal{P}_j^-(\theta_{ij}^n) \geq 0, \\ 0, & \text{if } \mathcal{P}_j^+(\theta_{ij}^n) \geq 0 \text{ and } \mathcal{P}_j^-(\theta_{ij}^n) < 0, \\ 1, & \text{if } \mathcal{P}_j^+(\theta_{ij}^n) < 0 \text{ and } \mathcal{P}_j^-(\theta_{ij}^n) \geq 0, \\ \theta_{ij}^n, & \text{otherwise,} \end{cases}$$

$$h_j^- \stackrel{\text{def}}{=} \begin{cases} h_j^n, \text{ if } \mathcal{P}_j^+(\theta_{ij}^n) < 0 \text{ and } \mathcal{P}_j^-(\theta_{ij}^n) < 0, \\ \dfrac{(\theta_{ij}^n)^2}{2}\left(h_{j-1}^n - 2h_j^n + h_{j+1}^n\right) - \dfrac{\theta_{ij}^n}{2}\left(h_{j-1}^n - 4h_j^n + 3h_{j+1}^n\right) + h_{j+1}^n, \text{ otherwise,} \end{cases}$$

$$h_j^+ \stackrel{\text{def}}{=} \begin{cases} h_{j+1}^n, \text{ if } \mathcal{P}_j^+(\theta_{ij}^n) < 0 \text{ and } \mathcal{P}_j^-(\theta_{ij}^n) < 0, \\ \dfrac{(\theta_{ij}^n)^2}{2}\left(h_{j+2}^n - 2h_{j+1}^n + h_j^n\right) - \dfrac{\theta_{ij}^n}{2}\left(h_{j+2}^n - h_j^n\right) + h_{j+1}^n, \text{ otherwise,} \end{cases}$$

   and $\mathcal{P}_j^{\pm}(\theta) \stackrel{\text{def}}{=} (\theta - \delta_j^{\pm})(\theta - \delta_{j+1}^{\pm})$ where

$$\delta_j^- \stackrel{\text{def}}{=} \frac{2(h_{j+1}^n - h_j^n)}{h_{j-1}^n - 2h_j^n + h_{j+1}^n}, \qquad \delta_j^+ \stackrel{\text{def}}{=} \frac{2(h_{j+1}^n - h_j^n)}{h_j^n - 2h_{j+1}^n + h_{j+2}^n},$$

$$\delta_{j+1}^- \stackrel{\text{def}}{=} \frac{h_{j-1}^n - 4h_j^n + 3h_{j+1}^n}{h_{j-1}^n - 2h_j^n + h_{j+1}^n}, \qquad \delta_{j+1}^+ \stackrel{\text{def}}{=} \frac{h_{j+2}^n - h_j^n}{h_j^n - 2h_{j+1}^n + h_{j+2}^n}.$$