Low Mach number models: some advantages for numerical simulations of weakly compressible flows with high heat transfers

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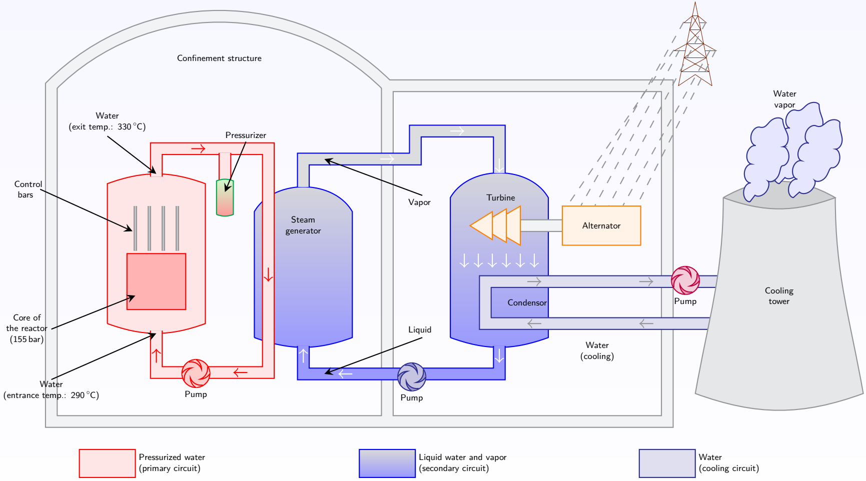
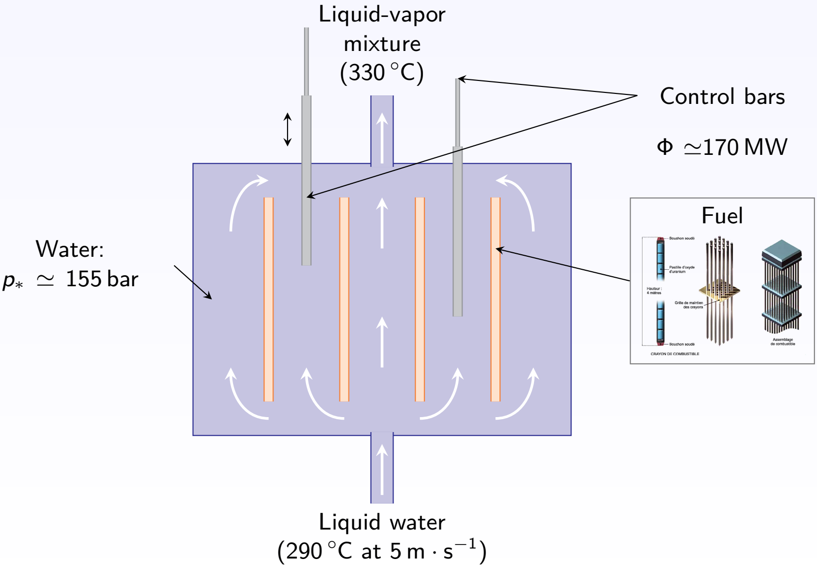
Outline of the talk

Pressurized Water Reactor (PWR)



Core of a Pressurized Water Reactor (PWR)



Low Mach number: which model for which regime?

Nominal regime

- Entrance velocity: $|\boldsymbol{u}| \simeq 5\,\mathrm{m}\cdot\mathrm{s}^{-1}$
- Sound speed at $p_0 = 155\,\mathrm{bar}$ and $T = 300\,°\mathrm{C}$: $c_\ell^* \simeq 1.0 \times 10^3\,\mathrm{m}\cdot\mathrm{s}^{-1}$
- Mach number (measures the compressibility of the flow):

$$\mathrm{Ma} = \frac{|\boldsymbol{u}|}{c_\ell^*} \simeq 5 \times 10^{-3} \ll 1$$

Choice of the model:

- Compressible Navier-Stokes/Euler?
- Incompressible?
- Adapted model for the low Mach regime?

Negligible acoustic phenomena (no shock waves)
BUT high heat transfers: $\operatorname{div} \boldsymbol{u} \neq 0$
$\Rightarrow$ Asymptotic model at low Mach number

From compressible Navier-Stokes to LMNC model

Compressible Navier-Stokes system

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho \boldsymbol{u}) = 0, \\ \partial_t(\rho h) + \operatorname{div}(\rho h \boldsymbol{u}) = \Phi + \operatorname{div}\big(\lambda \nabla T\big) + \partial_t p + \boldsymbol{u} \cdot \nabla p + \sigma(\boldsymbol{u}) :: \sigma(\boldsymbol{u}), \\ \partial_t(\rho \boldsymbol{u}) + \operatorname{div}(\rho \boldsymbol{u} \otimes \boldsymbol{u}) - \operatorname{div} \sigma(\boldsymbol{u}) + \nabla p = \rho \boldsymbol{g}. \end{cases}$$

- Unknowns
  - $(t, \boldsymbol{x}) \mapsto \boldsymbol{u}$: velocity
  - $(t, \boldsymbol{x}) \mapsto h$: enthalpy
  - $(t, \boldsymbol{x}) \mapsto p$: pressure
  - ρ, T: density and temperature linked to h and p through the equation of state
- Data
  - $(t, \boldsymbol{x}) \mapsto \Phi \geq 0$: power density
  - $\boldsymbol{g}$: gravity
  - λ: thermal conductivity
  - $\sigma(\boldsymbol{u})$ stress tensor (viscosity)

From compressible Navier-Stokes to LMNC model

Compressible Navier-Stokes system

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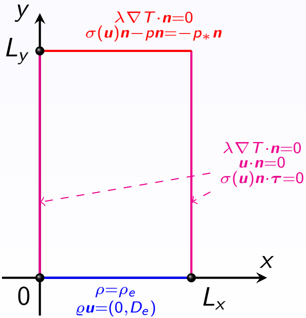
- Boundary conditions



From compressible Navier-Stokes to LMNC model

Compressible Navier-Stokes system

$$\begin{cases} \partial_t \rho + \mathrm{div}(\rho \boldsymbol{u}) = 0, \\ \partial_t(\rho h) + \mathrm{div}(\rho h \boldsymbol{u}) = \Phi + \mathrm{div}\big(\lambda \nabla T\big) + \partial_t p + \boldsymbol{u} \cdot \nabla p + \mathcal{O}(\varepsilon^2), \\ \partial_t(\rho \boldsymbol{u}) + \mathrm{div}(\rho \boldsymbol{u} \otimes \boldsymbol{u}) - \mathrm{div}\,\sigma(\boldsymbol{u}) + \frac{1}{\varepsilon^2} \nabla p = \rho \boldsymbol{g}. \end{cases}$$

- Dimensionless system: $\mathrm{Ma} = \varepsilon$ and asymptotic expansion

$$p = p^{(0)} + \varepsilon p^{(1)} + \varepsilon^2 p^{(2)} + \mathcal{O}(\varepsilon^3)$$

- $\nabla p^{(0)} = \nabla p^{(1)} = 0$ with outlet boundary condition independent of t

$$\Longrightarrow p(t, \boldsymbol{x}) = p_* + \varepsilon^2 \bar{p}(t, \boldsymbol{x}).$$

Pressure is decomposed into a thermodynamical constant part p_* and a dynamical part of order ε^2 $\bar{p}$.

Low Mach number model

LMNC Model

$$
\begin{cases}
\operatorname{div} \boldsymbol{u} = \dfrac{\beta(h, p_*)}{p_*}\left[\Phi + \operatorname{div}\left(\Lambda(h, p_*)\nabla h\right)\right], \\
\rho(h, p_*)\left(\partial_t h + \boldsymbol{u}\cdot\nabla h\right) = \Phi + \operatorname{div}\left(\Lambda(h, p_*)\nabla h\right), \\
\rho(h, p_*)\left(\partial_t \boldsymbol{u} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u}\right) + \nabla\bar{p} = \operatorname{div}(\sigma(\boldsymbol{u})) + \rho(h, p_*)\boldsymbol{g}.
\end{cases}
$$

- Compressibility coefficient $\beta(h, p_*) = -\dfrac{p_*}{\rho^2}\dfrac{\partial\rho}{\partial h}(h, p_*)$
- Equation of state: analytical or tabulated
  $\rightsquigarrow$ for example, stiffened gas (SG) : $\rho(h, p_*) = \dfrac{\gamma}{\gamma-1}\dfrac{p_*+\pi}{h-q}$
- Rewriting the thermal diffusion term

$$
\lambda(h, p_*)\nabla T = \frac{\lambda(h, p_*)}{c_p(h, p_*)}\nabla h = \Lambda(h, p_*)\nabla h
$$

- Stress tensor $\sigma(\boldsymbol{u}) = \mu(h, p_*)\left(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T\right) + \eta(h, p_*)(\operatorname{div}\boldsymbol{u})\,\mathbf{Id}$

Low Mach number model

LMNC Model

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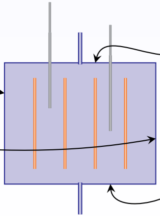
Initial and boundary conditions

Free outflow + adiabatic

$$\begin{cases} \sigma(\boldsymbol{u})\boldsymbol{n} - \bar{p}\boldsymbol{n} = \boldsymbol{0} \\ \Lambda\nabla h\cdot\boldsymbol{n} = 0 \end{cases}$$

Slip + adiabatic

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



Entrance

$$\begin{cases} \rho = \rho_e(t,x), \\ \rho\boldsymbol{u} = (0, D_e(t,x)) \end{cases}$$

Analysis of low Mach number models

- Applications in combustion: Majda, Klein, ...
- Applications in astrophysics Colella, Almgren, ...
- Applications in nuclear industry: Bell, Paillère, Dellacherie, ...

Theoretical studies

- Klainerman & Majda ('81, '82): barotropic models (some domains)
- Schochet ('94): convergence for barotropic Euler with any IC
- Desjardins, Grenier, Lions & Masmoudi ('99): bounded domains
- Danchin ('01, '05): extension to Besov spaces
- Alazard ('05): extension to general equations of state

Numerical aspects

- Klein ('95): operator splitting
- Guillard *et al.* ('99, '04, '08): asymptotic expansion in Ma in the schemes
- Dellacherie *et al.* ('10, '13): analysis of schemes thanks to Schochet decomposition, stability of the discrete kernels

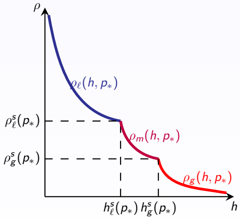
Outline of the talk

Diphasic equation of state

- Liquid $\kappa = \ell$ and vapor $\kappa = g$ are characterized by their thermodynamical properties: $(h, p_*) \mapsto \rho_\kappa$
- In the mixture, equilibrium between liquid and vapor phases: $T = T^s(p_*)$. Saturation values can be defined

$$h^s_\kappa(p_*) \stackrel{\text{def}}{=} h_\kappa\big(p_*, T^s(p_*)\big), \qquad \rho^s_\kappa(p_*) \stackrel{\text{def}}{=} \rho_\kappa\big(h^s_\kappa, p_*\big).$$

$$\rho(h, p_*) = \begin{cases} \rho_\ell(h, p_*), & \text{if } h \le h^s_\ell(p_*), \\ \rho_m(h, p_*) & \text{if } h^s_\ell(p_*) < h < h^s_g(p_*), \\ \rho_g(h, p_*), & \text{if } h \ge h^s_g(p_*). \end{cases}$$



Equation of state in the mixture and analytical laws

Defining α the volume fraction of vapor phase, equilibrium gives

$$\begin{cases} \rho = \alpha \rho_g^s(p_*) + (1-\alpha)\rho_\ell^s(p_*) \\ \rho h = \alpha \rho_g^s(p_*) h_g^s(p_*) + (1-\alpha)\rho_\ell^s(p_*) h_\ell^s(p_*) \end{cases} \quad \text{for } h \in [h_\ell^s(p_*); h_g^s(p_*)]$$

Density in the mixture

$$\rho_m(h, p_*) = \frac{p_*/\beta_m(p_*)}{h - q_m(p_*)},$$ where β_m and q_m depend only on the saturation values.

Noble Able Stiffened Gas (NASG)

$$\frac{1}{\rho_\kappa}(h, p_*) = \frac{\gamma_\kappa - 1}{\gamma_\kappa} \frac{h - q_\kappa}{p_* + \pi_\kappa} + b_\kappa$$

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

We compute $\beta_\kappa(p_*)$ independent of h

New expression of ρ

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

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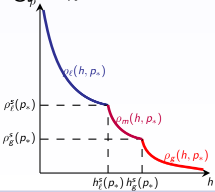

Equation of state for pure phases: tabulated data

κ	h_κ [$\mathrm{kJ \cdot kg^{-1}}$]	ϱ_κ [$\mathrm{kg \cdot m^{-3}}$]	T_κ [K]	$\cdots$	β_κ
ℓ	978.702	842.783	500.000	$\cdots$	✗
ℓ	980.223	842.359	500.336	$\cdots$	✗
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
ℓ	1627.450	595.733	617.667	$\cdots$	✗
ℓ	h^s_ℓ=1629.880	594.379	T^s=617.939	$\cdots$	✗
g	h^s_g=2596.119	101.930	T^s=617.939	$\cdots$	✗
g	2596.965	101.816	618.00	$\cdots$	✗
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
g	3066.962	60.540	699.667	$\cdots$	✗
g	3068.184	60.473	700.000	$\cdots$	✗

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

Quantities c^*_κ, c_{p_κ}, c_{v_κ}, λ_κ, μ_κ are also tabulated.

Equation of state for pure phases: tabulated data at p_*

New expression of the compressibility coefficient:

$$\beta = \frac{p}{\rho c^* \sqrt{T}} \sqrt{\frac{1}{c_v} - \frac{1}{c_p}}$$

$\Longrightarrow$ fitting of β for tabulated data for T, c_v, c_p, c^*, ρ

$$\beta_\kappa(h, p_*) \approx \tilde{\beta}_\kappa(h) := \sum_{j=0}^{d_{\beta,\kappa}} b_{\kappa,j} \left(\frac{h}{10^6}\right)^j .$$

Reconstruction of ρ

$$\frac{1}{\rho}(h, p_*) \approx \frac{1}{\tilde{\rho}(h)} := \begin{cases} \frac{1}{\tilde{\rho}_\ell}(h) := \frac{1}{\rho_\ell^s(p_*)} + \int_{h_\ell^s}^{h} \frac{\tilde{\beta}_\ell(h)}{p_*} dh, & \text{if } h \le h_\ell^s, \\ \frac{1}{\rho_m}(h), & \text{if } h_\ell^s < h < h_g^s, \\ \frac{1}{\tilde{\rho}_g}(h) := \frac{1}{\rho_g^s(p_*)} + \int_{h_g^s}^{h} \frac{\tilde{\beta}_g(h)}{p_*} dh, & \text{if } h \ge h_g^s. \end{cases}$$

Equation of state for pure phases: tabulated data at p_*

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$$\beta_\kappa(h, p_*) \approx \tilde{\beta}_\kappa(h) := \sum_{j=0}^{d_{\beta,\kappa}} b_{\kappa,j} \left(\frac{h}{10^6}\right)^j .$$

Proposition

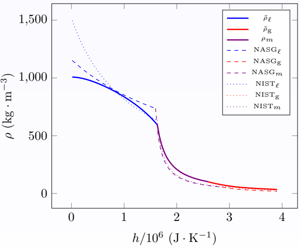
1. *The relation* $\tilde{\beta} = -\frac{p_*}{\tilde{\rho}^2} \frac{\partial \tilde{\rho}}{\partial h}$ *is satisfied exactly;*
2. $h \mapsto \tilde{\rho}(h)$ *is continuous, positive and decreasing on* (h_{min}, h_{max}).

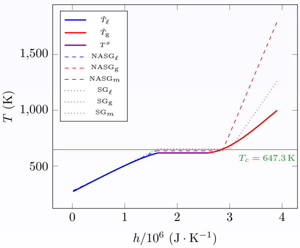
Choice of the degree $d_{\beta,\kappa}$ according to desired precision

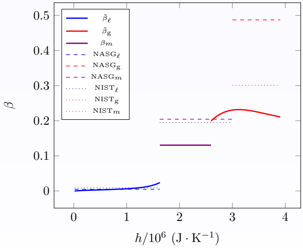
$\rightsquigarrow$ Even with $d_{\beta,\kappa} = 0$, better results than with analytical EOS such as (NA)SG

Comparison of the equations of state

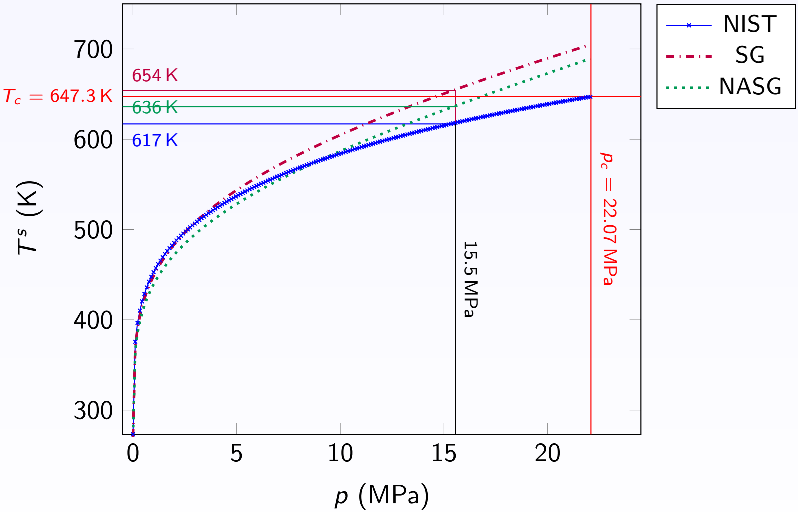
	SG	NASG	NIST
h_ℓ^s	$1.627 \times 10^6\,\mathrm{J \cdot kg^{-1}}$	$1.596 \times 10^6\,\mathrm{J \cdot kg^{-1}}$	$1.629 \times 10^6\,\mathrm{J \cdot kg^{-1}}$
h_g^s	$3.004 \times 10^6\,\mathrm{J \cdot kg^{-1}}$	$2.861 \times 10^6\,\mathrm{J \cdot kg^{-1}}$	$2.596 \times 10^6\,\mathrm{J \cdot kg^{-1}}$
ρ_ℓ^s	$632.663\,\mathrm{kg \cdot m^{-3}}$	$737.539\,\mathrm{kg \cdot m^{-3}}$	$594.38\,\mathrm{kg \cdot m^{-3}}$
ρ_g^s	$52.937\,\mathrm{kg \cdot m^{-3}}$	$55.486\,\mathrm{kg \cdot m^{-3}}$	$101.93\,\mathrm{kg \cdot m^{-3}}$
T^s	$654.65\,\mathrm{K}$	$636.47\,\mathrm{K}$	$617.939\,\mathrm{K}$







Comparison of the equations of state



Incomplete equation of state adapted to the low Mach approach where $p = p_*$!

Tabulated data when taking into account thermal diffusion

We can use (independently) the same approach to define $T(h, p_*)$ and $c_p(h, p_*)$.

Fitting $1/c_p$ from tabulated data

$$\frac{1}{{c_p}_\kappa(h, p_*)} \approx \frac{1}{{\tilde{c}_p}_\kappa(h)} := \sum_{j=0}^{d_{c_p,\kappa}} c_{\kappa,j} \left(\frac{h}{10^6}\right)^j.$$

Reconstruction of T

$$T(h, p_*) \approx \tilde{T}(h) := \begin{cases} \tilde{T}_\ell(h) := T^s + \displaystyle\int_{h_\ell^s}^{h} \frac{1}{{\tilde{c}_p}_\ell(h)} dh, & \text{if } h \leq h_\ell^s, \\ T^s, & \text{if } h_\ell^s < h < h_g^s, \\ \tilde{T}_g(h) := T^s + \displaystyle\int_{h_g^s}^{h} \frac{1}{{\tilde{c}_p}_g(h)} dh, & \text{if } h \geq h_g^s. \end{cases}$$

For the quantities with low variations on the considered range for h (μ, λ, ...), we can use the same approach with $d = 0$.

Outline of the talk

Analysis of the 1D model without thermal diffusion

Influence of heating and choice of the model: steady solutions (monophasic ideal gas, no viscosity nor gravity, Φ, h_e, v_e constant)

- Compressible Euler without Φ

$$h^\infty = h_e, \qquad v^\infty = v_e$$

- Compressible Euler with Φ [1]

$$\begin{cases} h^\infty = h_e \dfrac{2\gamma\tilde{p}_e + \gamma - 1 + \tilde{\Phi}y}{\gamma(\tilde{p}_e+1) + \sqrt{(\gamma\tilde{p}_e+1)^2 - (\gamma^2-1)\tilde{\Phi}y}}, \\ v^\infty = \dfrac{v_e}{\gamma+1}\left(\gamma(\tilde{p}_e+1) - \sqrt{(\gamma\tilde{p}_e-1)^2 - (\gamma^2-1)\tilde{\Phi}y}\right) \end{cases}$$

- Low Mach model with Φ

$$h^\infty = h_e + \frac{\Phi}{\rho_e v_e}y, \qquad v^\infty = v_e + \frac{\beta\Phi}{p_0}y$$

- Incompressible with Φ (Boussinesq approximation)

$$h^\infty = h_e + \frac{\Phi}{\rho_e v_e}y, \qquad v^\infty = v_e$$

[1] $\tilde{\Phi} = 2\Phi/\rho_e v_e^3$, $\tilde{p}_0 = p_0/\rho_e v_e^2$, $\tilde{p}_e = \left(1 - \tilde{p}_0 + \sqrt{(\gamma\tilde{p}_0 - 1)^2 + \tilde{\Phi}L}\right)/(\gamma-1)$.

Analysis of the 1D model without thermal diffusion

$$\begin{cases} \partial_y v = \frac{\beta(h,p_*)}{p_*}\Phi = -\frac{\rho'(h)}{\rho(h)^2}\Phi, \\ \rho(h)(\partial_t h + v\partial_y h) = \Phi, \\ \rho(h)(\partial_t v + v\partial_y v) + \partial_y \bar{p} = \partial_y(\mu\partial_x v) - \rho(h)g. \end{cases}$$

Steady solution for any equation of state

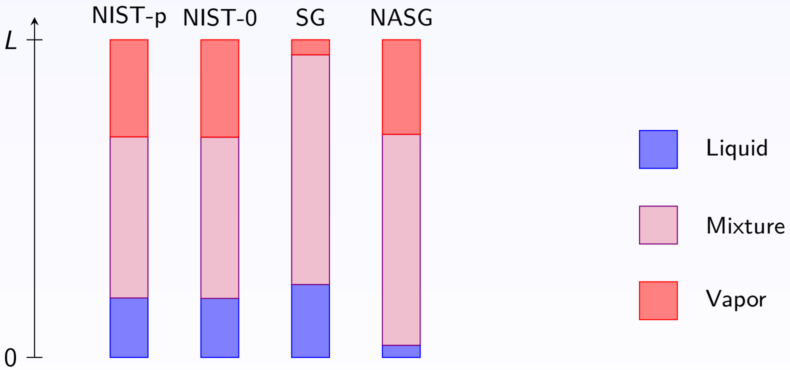
1. Observe that $\rho(h)v$ is constant (equal to D_e), thus $\boxed{v^\infty(y) = \dfrac{D_e}{\rho(h^\infty(y))}}$
2. Deduce enthalpy:

$$\boxed{h^\infty(y) = h_e + \frac{\Psi(y)}{D_e}, \qquad \text{where } \Psi(y) := \int_0^y \Phi^\infty(z)\,\mathrm{d}z}$$

3. Dynamical pressure $\bar{p}$: integrate the third equation

Analysis of the 1D model without thermal diffusion

Comparison of different EOS (analytical and tabulated): steady solutions

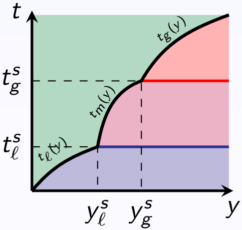


Importance of approximating precisely the saturation values!

Analysis of the 1D model without thermal diffusion

Exact solution with phase transition (NASG)

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



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

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

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

Outline of the talk

Higher dimensions: Weak formulation

- Equivalent formulation when taking into account thermal diffusion

$$\begin{cases} \operatorname{div} \boldsymbol{u} = \dfrac{\beta(h)}{p_0}[\Phi + \operatorname{div}(\Lambda(h)\nabla h)] = \dfrac{\beta(h)\rho(h)}{p_0}[\partial_t h + \boldsymbol{u} \cdot \nabla h] \\ \rho(h)\Big(\partial_t h + \boldsymbol{u} \cdot \nabla h\Big) = \Phi + \operatorname{div}(\Lambda(h)\nabla h) \\ \rho(h)\Big(\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u}\Big) + \nabla \bar{p} = \operatorname{div}(\sigma(\boldsymbol{u})) + \rho(h)\boldsymbol{g} \end{cases}$$

- Allows to avoid boundary terms (after integration by parts) on $\{\boldsymbol{x} \in \Omega \ : \ h(t, \boldsymbol{x}) = h^s_\kappa\}$, thus avoid
  - to improve the regularity of the function space of p_{test}
  - to approximate $\dfrac{\partial \beta}{\partial h}$

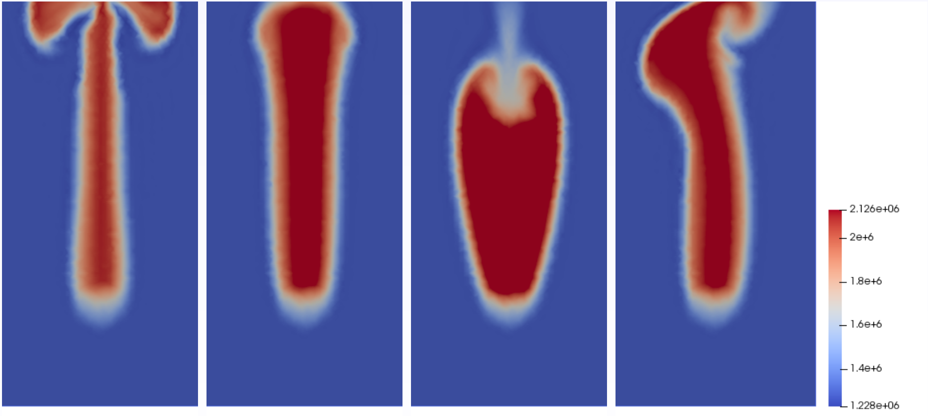
  and numerically, at each time step,
  - to define the curves $h(t^n, \cdot) = h^s_\kappa$,
  - to remesh to capture these zones.

Test case with localized heating and phase change

$$D_e = 375\,\mathrm{kg}\cdot\mathrm{m}^{-2}\cdot\mathrm{s}^{-1},\ \rho_e = 750\,\mathrm{kg}\cdot\mathrm{m}^{-3},\ \Phi = 170\times 10^6\,\mathrm{W}\cdot\mathrm{m}^{-3}\mathbb{1}_D$$

Influence of gravity

Enthalpy at time 0.55 s for several orientations of $\boldsymbol{g}$ (with phase change)



(a) $\boldsymbol{g} = (0, -g)$ (b) $\boldsymbol{g} = (0, 0)$ (c) $\boldsymbol{g} = (0, g)$ (d) $\boldsymbol{g} = (g, 0)$

Rayleigh-Taylor instability / Gravity in competition with convection

Outline of the talk

Conclusion and prospects

Conclusions

- Low Mach number model, fine treatment of the thermodynamics of phase change
- Easier for mathematical analysis (steady and exact solutions)
- Easier for numerical simulations

Work in progress and prospects

- Analysis of the mode without thermal diffusion (boundary conditions)
- Analysis of the model with thermal diffusion (discontinuity of Λ)
- Deriving a hierarchy of models (relaxation of the different equilibria, cf. n-equations models in the compressible setting)

  $\rightarrow$ convergences between the different models
- Coupling with simplified neutronics equations to determine Φ

Thank you for your attention!