A conservative two-phase flow model with a nonlinear degenerate diffusion

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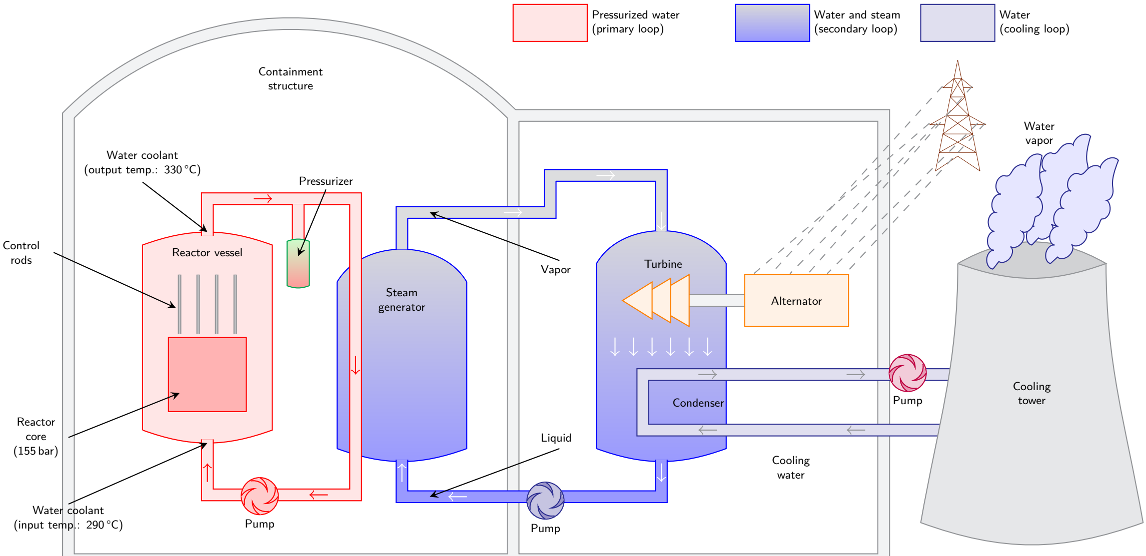
Outline of the presentation

Pressurized Water Reactor



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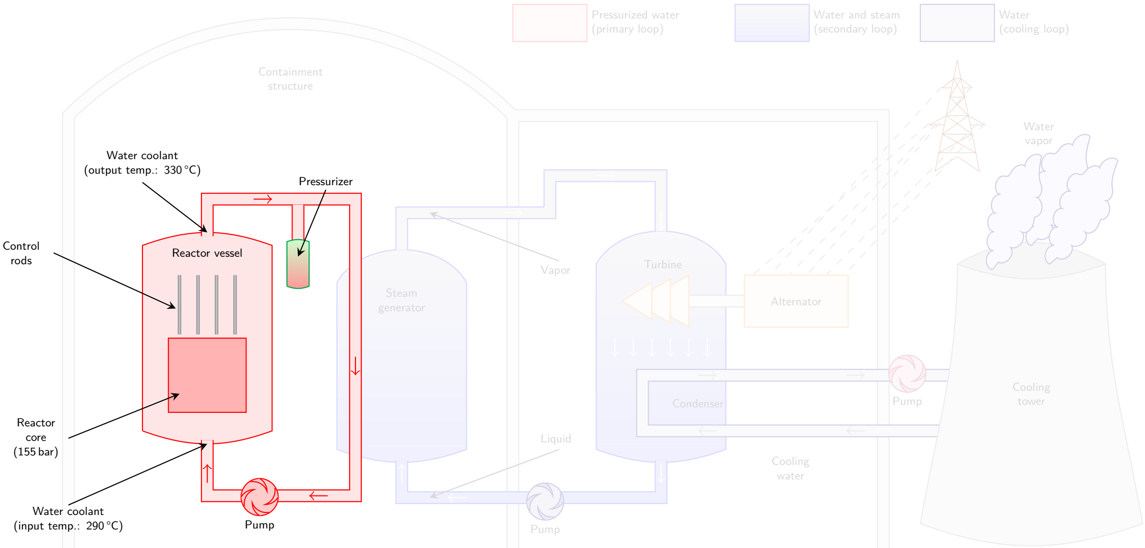
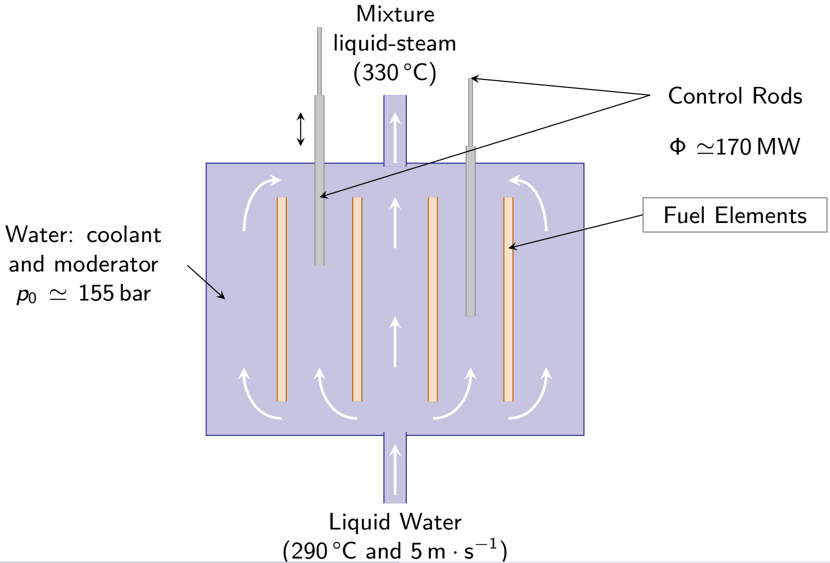


Core of a Pressurized Water Reactor



Core at Pressurized Water Reactor

Nominal regime[1]

- Inlet velocity: $|\mathbf{u}_e| \approx 5\,\mathrm{m}\cdot\mathrm{s}^{-1}$
- At $p_0 = 155\,\mathrm{bar}$ and $T = 300\,°\mathrm{C}$: speed of sound $c_\ell^* \simeq 1.0 \times 10^3\,\mathrm{m}\cdot\mathrm{s}^{-1}$
- Mach number (measure of compressibility) $\mathrm{M} = \dfrac{|\mathbf{u}_e|}{c_\ell^*} \simeq 5 \times 10^{-3} \ll 1$

Model with acoustics ($\mathrm{M} = \mathcal{O}(1)$) and heat transfers

$\rightsquigarrow$ Compressible Navier-Stokes/Euler system

- Acoustics negligible (no shock waves) $\mathrm{M} \ll 1$
- High heat transfers: $\nabla\cdot\mathbf{u} \neq 0$

$\rightsquigarrow$ An asymptotic low Mach number model

A model without acoustics $\mathrm{M} = 0$ and $\nabla\cdot\mathbf{u} = 0$

$\rightsquigarrow$ Incompressible model

[1] and some incidental/accidental regimes

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From Compressible Navier-Stokes-Fourier System to the LMNC model

Compressible Navier-Stokes-Fourier system ⇝ a Low Mach number model

$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \\ \partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p = \rho \boldsymbol{g} + \nabla \cdot \sigma(\mathbf{u}) \\ \partial_t (\rho h) + \nabla \cdot (\rho h \mathbf{u}) = \Phi + \nabla \cdot \left(\omega \nabla T\right) + \sigma(\mathbf{u}) : \nabla \mathbf{u} + \partial_t p \; + \mathbf{u} \cdot \nabla p \end{cases}$$

In Low Mach number regime $M \ll 1$ we have $p(t, \mathbf{x}) = p_* + \mathrm{M}^2 \bar{p}(t, \mathbf{x})$

Unknowns:

- $\mathbf{u}(t, \mathbf{x})$ velocity field
- $h(t, \mathbf{x})$ enthalpy
- $p(t, \mathbf{x})$ perturbational pressure

Given quantities:

- $\Phi(t, \mathbf{x}) \geq 0$ power density modelling the heating
- $\boldsymbol{g}$ gravity field, $\sigma(\mathbf{u})$ viscous effects
- $p_* > 0$ thermodynamic pressure (constant)

Equation of state

Density $\rho(h, p)$ and temperature $T(h, p)$

[S. Dellacherie, *On A Low Mach Nuclear Core Model*, ESAIM: Proc., 35 (2012)]

From Compressible Navier-Stokes-Fourier System to the LMNC model

Compressible Navier-Stokes-Fourier system $\rightsquigarrow$ a Low Mach number model

$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \\ \partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla \bar{p} = \rho \boldsymbol{g} + \nabla \cdot \sigma(\mathbf{u}) \\ \partial_t (\rho h) + \nabla \cdot (\rho h \mathbf{u}) = \Phi + \nabla \cdot \big(\omega \nabla T\big) + \sigma(\mathbf{u}) : \nabla \mathbf{u} \cancel{+ \partial_t p_* + \mathbf{u} \cdot \nabla p_*} \end{cases}$$

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Equation of state

Density $\rho(h, p_*)$ and temperature $T(h, p_*)$

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The model

When neglecting the viscous terms, the model becomes

$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \\ \partial_t(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla \bar{p} = \rho \boldsymbol{g} \\ \partial_t(\rho h) + \nabla \cdot (\rho h \mathbf{u}) = \Phi + \nabla \cdot (\omega \nabla T) \end{cases}$$

Unknowns:

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

Given quantities:

- $\Phi > 0$ constant power density
- $\boldsymbol{g}$ gravity field

Low Mach setting $\rightsquigarrow$ no hyperbolic structure! v can be interpreted as a Lagrange multiplier.

Closure: equation of state

- $\rho(h)$ specific density
- $T(h)$ temperature
- $\omega(h)$ heat conductivity

Without diffusion, many references (analytical solutions, numerical schemes, EoS, relaxation model...)

Diphasic equation of state with phase transition

Diffuse Interface Framework:
the (compressible) fluid can exist in liquid (ℓ) or vapor (g) phase or as a mixture of both

- Pure phase $\kappa \in \{\ell, g\}$ is described by a given (complete) EoS

$$(h, p) \mapsto T_\kappa(h, p)$$

- Mixture: at saturation (same pressure p, temperature T, chemical potential μ)

$$\mu_\ell(T, p) = \mu_g(T, p) \rightsquigarrow p \mapsto T^s(p)$$

temperature at saturation

Transition pure phase/mixture: $h^s_\kappa(p) \stackrel{\text{def}}{=} h_\kappa(T^s(p), p)$ the enthalpy of the phase κ at saturation

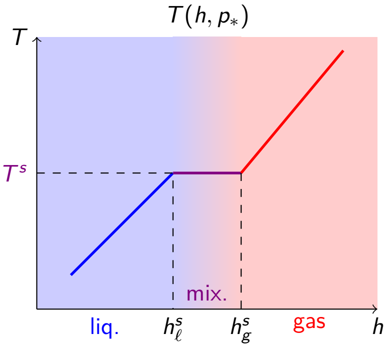
At pressure p, the fluid is

- in the liquid phase if $h \leq h^s_\ell(p)$
- a mixture at saturation if $h^s_\ell(p) < h < h^s_g(p)$
- in the vapor phase if $h \geq h^s_g(p)$

Thermal diffusion term

- In our EDP system, p_* is constant
- T is piecewise defined w.r.t. h_κ^s

$$T(h) = \begin{cases} T_\ell(h), & \text{if } h \le h_\ell^s \\ T^s, & \text{if } h_\ell^s < h < h_g^s \\ T_g(h), & \text{if } h \ge h_g^s \end{cases}$$



LMNC model $\partial_t(\rho h) + \nabla \cdot (\rho h \mathbf{u}) = \Phi(t, \mathbf{y}) + \nabla \cdot \Big(\omega(h, p_*)\nabla T(h, p_*)\Big)$

- ω constant in each phase & ∇T vanishes in the mixture $\rightsquigarrow$

$$\omega(h)\nabla T(h) = \begin{cases} \lambda_\ell \nabla h, & \text{if } h \le h_\ell^s, \\ 0, & \text{if } h_\ell^s < h < h_g^s, \\ \lambda_g \nabla h, & \text{if } h \ge h_g^s, \end{cases}$$

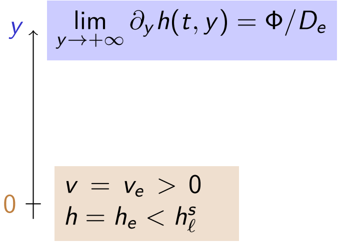
$$\lambda_\kappa \overset{\text{def}}{=} \frac{\omega_\kappa}{c_{p,\kappa}}$$

$$c_{p,\kappa} \overset{\text{def}}{=} \frac{\partial h}{\partial T}\Big|_p$$ isobar heat capacity

The 1D model

1. In 1D, v and h are solutions of the following system

$$\begin{cases} \partial_t \varrho + \partial_y(\varrho v) = 0 \\ \partial_t(\varrho h) + \partial_y(\varrho h v) = [\Phi + \partial_y\left(\lambda(h)\partial_y h\right)] \end{cases} \qquad \lambda(h) = \begin{cases} \lambda_\ell & \text{if } h \le h_\ell^s \\ 0 & \text{if } h_\ell^s < h < h_g^s \\ \lambda_g & \text{if } h \ge h_g^s \end{cases}$$



- $\rho(h)$ given by the EoS
- Constants: $\Phi > 0$, $D_e \stackrel{\text{def}}{=} v_e \varrho(h_e) > 0$
- Initial condition: $h(0, y) = h_e$ liquid phase

2. Additionally, $\bar{p}$ is a solution of

$$\partial_y \bar{p} = -\varrho g - \partial_t(\varrho v) - \partial_y(\varrho v^2)$$

Outline of the presentation

The 1D steady-state model

$$\begin{cases} \partial_y(\varrho v) = 0 \\ \partial_y(\varrho v h) = \left[\Phi + \partial_y\Big(\lambda(h)\partial_y h\Big)\right] & y \in [0; +\infty) \\ (\varrho v)(0) = \varrho(h_e)v_e \stackrel{\text{def}}{=} D_e > 0 \text{ constant} \\ \lim\limits_{y\to+\infty} \partial_y h(y) = \frac{\Phi}{D_e} \end{cases}$$

$$\Downarrow$$

$$\begin{cases} (\varrho v)(y) = D_e & \rightsquigarrow v(y) = \dfrac{D_e}{\varrho(h(y))} \\ D_e\partial_y h = \left[\Phi + \partial_y\Big(\lambda(h)\partial_y h\Big)\right] & \text{independent of } \varrho(h) \\ h(0) = h_e \\ \lim\limits_{y\to+\infty} \partial_y h(y) = \frac{\Phi}{D_e} \end{cases}$$

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The 1D steady-state model

Notation: $h' = \partial_y h$

EDO

$$D_e h'(y) - \Big(\lambda(h) h'(y)\Big)' = \Phi$$

Diffusion

$$\lambda(h) = \begin{cases} \lambda_\ell & \text{if } h \leq h_\ell^s \\ \lambda_m & \text{if } h_\ell^s < h < h_g^s \\ \lambda_g & \text{if } h \geq h_g^s \end{cases}$$

Different configurations:

- $\lambda_\ell = \lambda_m = \lambda_g = 0$: no diffusion $\rightsquigarrow$ $h(y) = h_e + \frac{\Phi}{D_e} y$
- $\lambda_\ell, \lambda_m, \lambda_g > 0$ $\rightsquigarrow$ continuous explicit h, defined piecewise
- $\lambda_m = 0$ and $\lambda_\ell, \lambda_g > 0$: model with a degenerate diffusion

If λ was degenerate in space but not on h, the solution would be continuous.

Remark

Due to the discontinuities in λ, the ODE should be interpreted as follows:

$$D_e h' - (L(h))'' = \Phi \qquad \text{with } L'(h) = \lambda(h)$$

Solution with $\lambda_m = 0$ and $\lambda_\ell, \lambda_g > 0$ (degenerate diffusion)

Proposition

When the mixture zone is present[a]*, the unique steady-state solution is discontinuous at y_g^s:*

$$h(y) = \begin{cases} h_\ell(y) \stackrel{\text{def}}{=} C_{\ell,1} + \dfrac{\Phi}{D_e} y + C_{\ell,2} \exp\left(\dfrac{y}{\lambda_\ell / D_e}\right) & \text{if } y \le y_\ell^s \\ h_m(y) \stackrel{\text{def}}{=} h_\ell^s + \dfrac{\Phi}{D_e}(y - y_\ell^s) & \text{if } y_\ell^s \le y < y_g^s \\ h_g(y) \stackrel{\text{def}}{=} h_g^s + \dfrac{\Phi}{D_e}(y - y_g^s) & \text{if } y \ge y_g^s \end{cases}$$

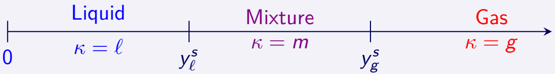
- *The constants $C_{\ell,1}$ and $C_{\ell,2}$ depend on y_ℓ^s, implicitly defined by $h_\ell(y_\ell^s) = h_\ell^s$ and $h_\ell'(y_\ell^s) = 0$.*
- *The position y_g^s is computed w.r.t. y_ℓ^s by $y_g^s = y_\ell^s + \frac{D_e}{\Phi}(h_g^s - h_\ell^s) - \frac{\lambda_g}{D_e}$.*

[a] This is the case when $\lambda_g \Phi / D_e^2 < h_g^s - h_\ell^s$

Liquid/mixture/gas

Proof – Solution on each region

- Given $\Phi > 0$, $D_e > 0$, we can prove that h increases. This leads to the division of space into three regions, ordered from low to high y values:

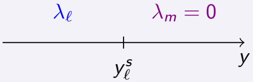


- In pure phase regions, we solve $D_e h_\kappa'(y) - \lambda_\kappa h_\kappa''(y) = \Phi$, yielding
$h_\kappa(y) = C_{\kappa,1} + \frac{\Phi}{D_e} y + C_{\kappa,2} \exp\left(\frac{y}{\lambda_\kappa / D_e}\right)$
- The boundary conditions give two relations:
  - Liquid region: $h_\ell(0) = h_e \rightsquigarrow C_{\ell,2} = h_e - C_{\ell,1}$
  - Vapor region: $\lim_{y \to \infty} h_g'(y) = \frac{\Phi}{D_e} \rightsquigarrow C_{g,2} = 0$
- In mixture region, we solve $D_e h_m'(y) = \Phi$, yielding $h_\kappa(y) = C_m + \frac{\Phi}{D_e} y$
- We need to compute $C_{\ell,1}$, C_m, $C_{g,1}$ and the transition points y_ℓ^s, y_g^s.

Liquid/mixture/gas

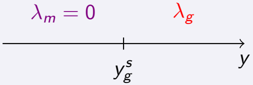
Proof – Jump relations $[\![D_e h]\!] - [\![\lambda(h)h']\!] = 0$.

- Liquid/Mixture transition: jump relation at y_ℓ^s:



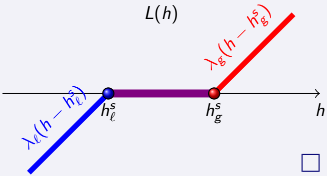
$$\underbrace{D_e[\![h(y_\ell^s)]\!]}_{\geq 0} - 0 \times h'(y_\ell^{s,+}) + \underbrace{\lambda_\ell h'(y_\ell^{s,-})}_{\geq 0} = 0 \quad \rightsquigarrow \quad \begin{cases} [\![h(y_\ell^s)]\!] = 0 \\ h'(y_\ell^{s,-}) = 0 \end{cases}$$

- Mixture/Gas transition: jump relation at y_g^s:



$$D_e[\![h(y_g^s)]\!] - \lambda_g h'(y_g^{s,+}) + 0 \times h'(y_g^{s,-}) = 0 \quad \rightsquigarrow \quad [\![h(y_g^s)]\!] = \frac{\lambda_g}{D_e}\frac{\Phi}{D_e}$$

- Jump in the mixture, since at a discontinuity point y_*:
  - $[\![L(h)]\!](y_*) = 0 \rightsquigarrow h_\ell^s \leq h(y_*^-) < h(y_*^+) \leq h_g^s$
  - $[\![(L(h))']\!](y_*) > 0 \rightsquigarrow h(y_*^+) = h_g^s$ or $h(y_*^-) = h_\ell^s$



□

Sharp interface models

What about if the condition $\dfrac{\lambda_g}{D_e}\dfrac{\Phi}{D_e} \leq h_g^s - h_\ell^s$ is not met?

A direct transition from liquid to gas must be considered.

It is a sharp interface model since no mixture region is present.

Link with the generalized stationary Stefan problem on temperature

Free boundary problem: find y^s such that

$$\begin{cases} c_{p,\ell} D_e T' - \omega_\ell T'' = \Phi \\ T(0) = T_e < T^s, \\ T(y^{s,-}) = T^s, \end{cases} \quad \text{in }]0, y^s[, \qquad \begin{cases} c_{p,g} D_e T' - \omega_g T'' = \Phi \\ T(y^{s,+}) = T^s, \\ \lim\limits_{y \to \infty} T'(y) = \frac{\Phi}{c_{p,g} D_e}, \end{cases} \quad \text{in }]y^s, +\infty[$$

& Interface condition: $\omega_g T'(y^{s,+}) - \omega_\ell T'(y^{s,-}) = D_e(h_g^s - h_\ell^s)$

Sharp interface models

Stefan problem

- Sharp interface framework (no mixture allowed).
- By assumption, jump equals to $h_g^s - h_\ell^s$.

Our model

- Diffuse interface framework allowing for mixture.
- Jump equals to $\min\left\{\frac{\lambda_g}{D_e}\frac{\Phi}{D_e}, h_g^s - h_\ell^s\right\}$

Same model when $\frac{\lambda_g}{D_e}\frac{\Phi}{D_e} \geq h_g^s - h_\ell^s$.

When our model involves a mixture, the Stefan problem yields non-physical solution

The last relation in the temperature formulation gives

$$\omega_g T'(y^{s,+}) - \omega_\ell T'(y^{s,-}) = D_e(h_g^s - h_\ell^s) \quad \rightsquigarrow \quad \omega_\ell T'(y^{s,-}) = \lambda_g \frac{\Phi}{D_e} - D_e(h_g^s - h_\ell^s).$$

If $\frac{\lambda_g}{D_e}\frac{\Phi}{D_e} < h_g^s - h_\ell^s$ (indicating the presence of the mixture in our model): $T'(y^{s,-}) < 0$ and thus the temperature must have exceeded T^s within the liquid phase.

Outline of the presentation

Time-dependent model

✓ Dynamical jump relations with or without the mixture zone

Travelling wave solutions

Let $c < 0$. We can construct the unique travelling wave solution with velocity c of the system with compatible initial conditions $h_0(y)$, $v_0(y)$ and boundary conditions $h_e(t) = h_0(-ct)$, $v_e(t) = c + D_e/\varrho(h_e(t))$ by

$$h(t,y) = h_0(y - ct), \qquad v(t,y) = c + D_e/\varrho(h(t,y)).$$

We can construct h_0 using the steady-state solution in both cases

- when the mixture zone is present
- when there is a liquid-gas transition

Challenges with the model

The steady solution exhibits...

a jump in $h \rightsquigarrow$ a jump in $\varrho(h) \rightsquigarrow$ a jump in v

We cannot work with the non-conservative form, keep the conservative one

$$\begin{cases} \partial_t \varrho + \partial_y(\varrho v) = 0 \\ \partial_t(\varrho h) + \partial_y(\varrho h v) - \partial_{yy} L(h) = \Phi \end{cases}$$

Numerical schemes

- Spatial discretization:

Gradient scheme: avoid writing the diffusion term as $\partial_y(\lambda_\kappa \partial_y h)$ [1]

- Time discretization:

Full explicit schemes are prohibited (no explicit time derivative of v, the system is not hyperbolic)

[1] [R. Eymard, P. Féron, T. Gallouët, R. Herbin, C. Guichard, *Gradient schemes for the Stefan problem*, Int. J. Finite Volumes, 2013]

Numerical schemes

$$\begin{cases} \partial_t \varrho + \partial_y(\varrho v) = 0 \\ \partial_t(\varrho h) + \partial_y(\varrho h v) - \partial_{yy} L(h) = \Phi \end{cases}$$

1. Explicit predictor-corrector approach
   - Observe that $h \mapsto \varrho(h)h$ can be non invertible (depending on the EoS)
   - Combine the two equations: $R = Q\varrho - \varrho h(\varrho)$, $Q > 0$ such that $\varrho \mapsto R$ invertible

     $$\partial_t R + \partial_y(Rv) - \partial_{yy} L(h) = -\Phi$$

   - Predictor step: compute R_i^{n+1} from

     $$\frac{R_i^{n+1} - R_i^n}{\Delta t} + \frac{(Rv)_i^n - (Rv)_{i-1}^n}{\Delta y} + \frac{L(h_{i+1}^n) - 2L(h_i^n) + L(h_{i-1}^n)}{\Delta y^2} = -\Phi$$

     Deduce ϱ_i^{n+1} by inversion of R, and h_i^{n+1} by the EoS
   - Corrector step: compute v_i^{n+1} from

     $$\frac{\varrho_i^{n+1} - \varrho_i^n}{\Delta t} + \frac{(\varrho v)_i^{n+1} - (\varrho v)_{i-1}^{n+1}}{\Delta y} = 0$$

2. Full implicit scheme

Validation of the schemes

Discrete jump relations

- Computed for both schemes, mimic the continuous ones
- At most one point in the jump

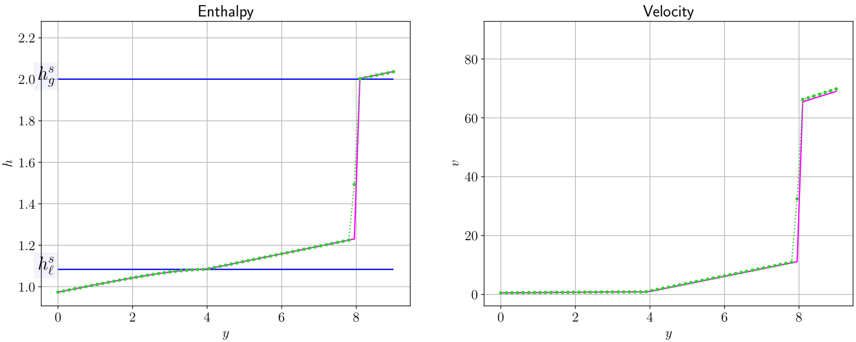
- EoS : Stiffened gas law in all phases

$$\varrho_\kappa(h) = \frac{\zeta_\kappa}{h - q_\kappa}$$

- Dimensionless setting
- Different configurations, depending on the presence of the different phases:
  $\rightsquigarrow$ adjust boundary conditions, power density, diffusion coefficients
- Constrained CFL for the explicit scheme (diffusion)
- Convergence of the Newton fixed point for the implicit scheme: $\rightsquigarrow$ adaptive time step
- Coarse grid (61 points)

Travelling wave solution with mixture phase

- Exact solution of velocity $c = -5$



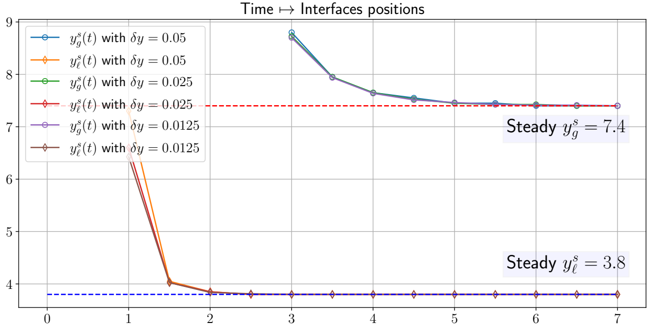
Play/Pause

- Comparison of the discrete displacement velocities of the interface: *e.g.* $-c_\varrho [\![w\varrho]\!]_i^{n+1} + [\![\varrho v]\!]_i^{n+1} = 0$
  Mean values $c_\varrho \simeq -4.97$, $c_{\varrho h} \simeq -4.97$
- Maximal error on the reconstructed position y_g^s of the jump < 0.07 (*cf.* $\Delta y = 0.15$)

Transient regime – Numerical results

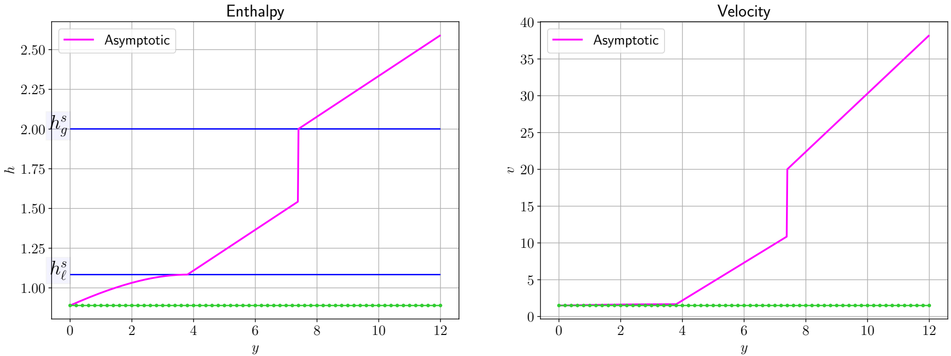
- $L = 12$, $\Delta y = 0.2$, $D_e = 20$
- Other parameters vary depending on the scenario

- Check grid convergence (error on h and v)
- Check precision of the transition points y_ℓ^s and y_g^s



Appearance of phases

Scenario 1: coexistence of all three phases [1]

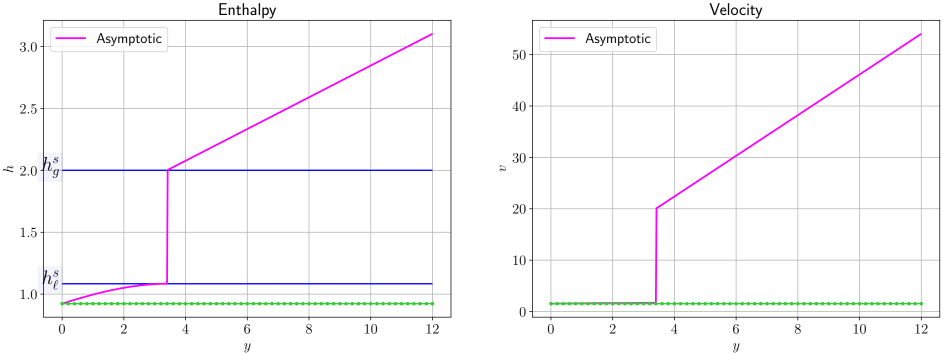


Play/Pause

[1]Parameters $h_e \simeq 0.89$, $\lambda_\ell \simeq 67.65$, $\lambda_g \simeq 71.05$, $\Phi \simeq 2.56$

Appearance of phases

Scenario 2: disappearance of the mixture phase, zero slope of the enthalpy at the liquid-gas transition point[2]

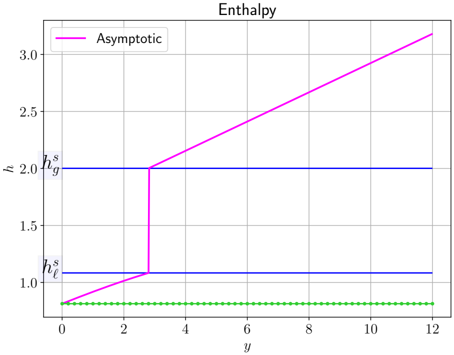


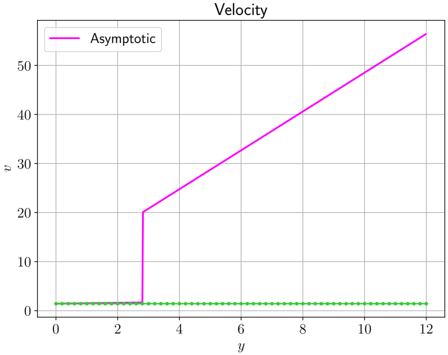
Play/Pause

[2]Parameters $h_e \simeq 0.92$, $\lambda_\ell \simeq 67.65$, $\lambda_g \simeq 143.05$, $\Phi \simeq 2.56$

Appearance of phases

Scenario 3: disappearance of the mixture phase, positive slope of the enthalpy at the liquid-gas transition point[3]





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[3]Parameters $h_e \simeq 0.81$, $\lambda_\ell \simeq 67.65$, $\lambda_g \simeq 185.97$, $\Phi \simeq 2.56$

Outline of the presentation

Conclusion and prospects

Conclusion

- 1D LMNC model with phase change and degenerate thermal diffusion
- Steady-state and travelling wave solutions with/without mixture zone
- Two numerical schemes which capture correctly the discontinuities at phase boundaries

Prospects

- Extension to 2D/3D
  - No post-processing for the equation on the pressure
  - Navier-Stokes-like equation but in conservative form
- Extension to the viscous case
  - Discontinuous solution in 1D
  - Low Mach number hypothesis not satisfied locally at phase change?
  - Relaxation from a more complex model describing non-instantaneous mass transfers between phases

Thank you for your attention!