Journées scientifiques du GdR MaNu — Croisic, 23-27/10/2023

# An advection-diffusion equation within a nonlinear degenerate diffusion in a diffuse interface framework

## A liquid-vapour flows with phase transition in an heat exchanger

Gloria Faccanoni

joint work with C. Galusinski, B. Grec and Y. Penel

# Outline

# 1. Introduction

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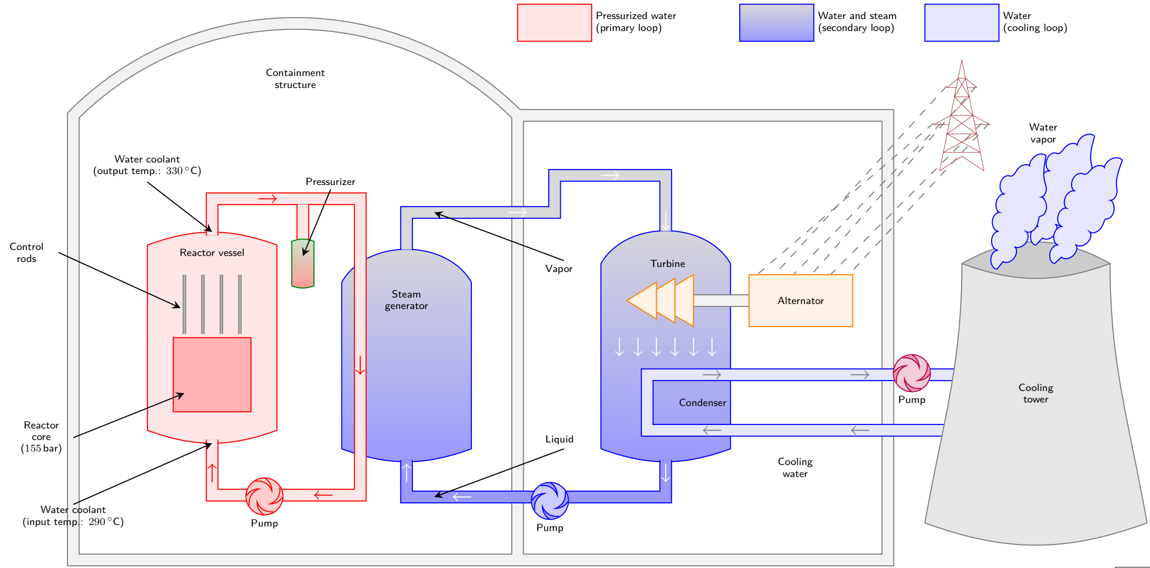
# Pressurized Water Reactor



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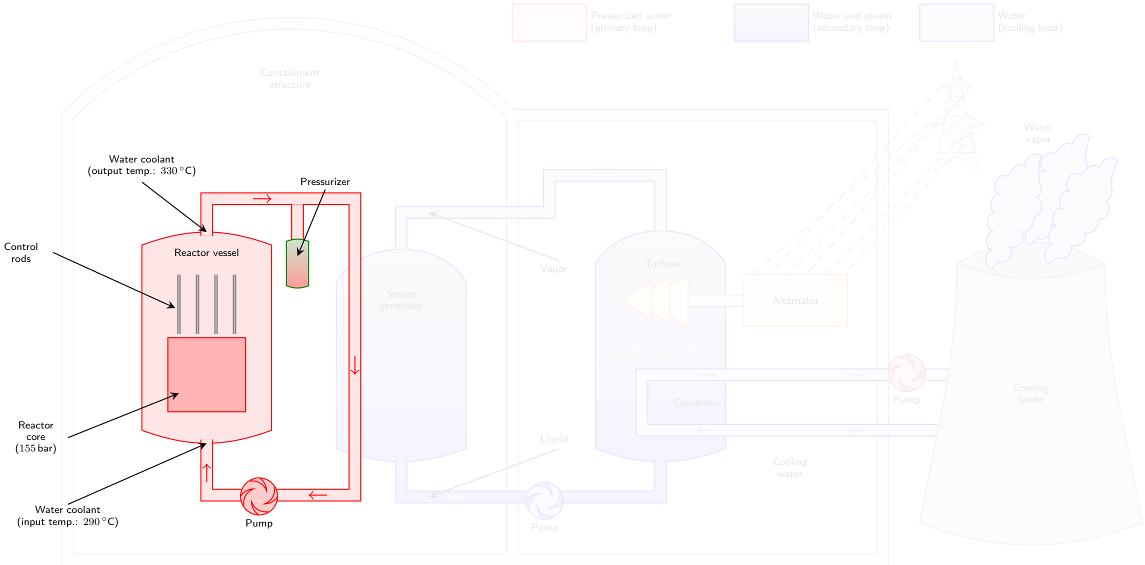
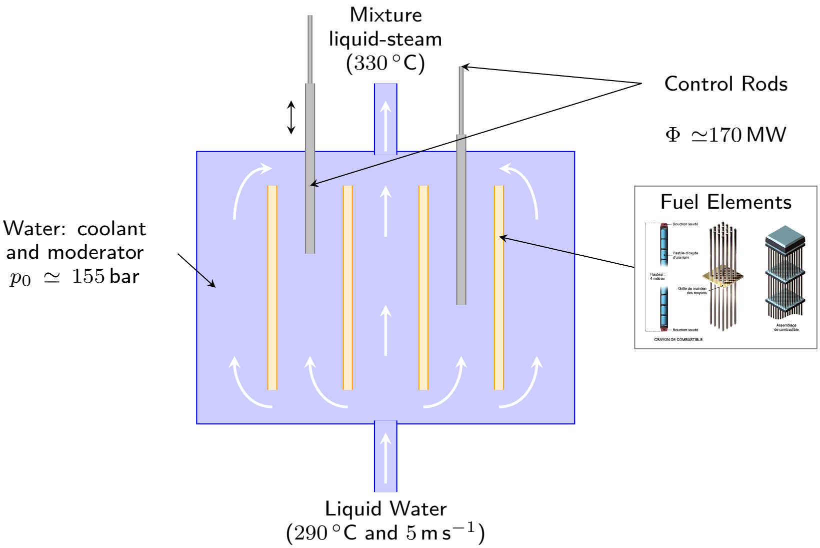
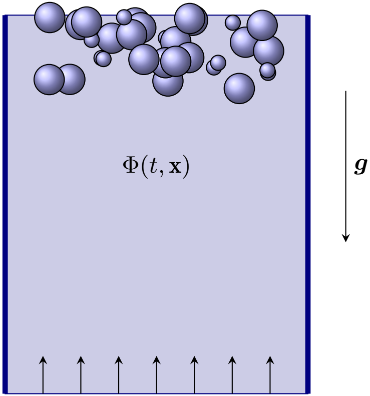


# Core of a Pressurized Water Reactor



# A heat exchanger



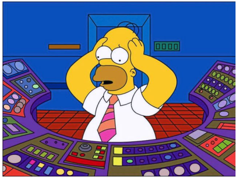

$v_e(t, \mathbf{x})$ and $T_e(t, \mathbf{x})$

# 1. Introduction

# Core at Pressurized Water Reactor

### Nominal regime

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



This hypothesis also applies to:

- Incidental Regime
- Certain accidental scenarios, such as a LOFA (Loss of Flow Accident)[1] *even if phase change occurs*

[1] Except for very rapid depressurization scenarios like a LOCA (Loss of Coolant Accident) induced by a coolant pump trip event

# Which model?

A model with acoustics $\mathrm{M} \geq 1$ 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 $\nabla \cdot \mathbf{u} = 0$

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# 1. Introduction

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

## Compressible Navier-Stokes-Fourier system $\rightsquigarrow$ a Low Mach Number Model

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

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

### Unknowns

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

### Given

- $(t,\mathbf{x}) \mapsto \Phi \geq 0$ power density modelling the heating
- $\omega$ heat conductivity
- $\boldsymbol{g}$ gravity field, $\sigma(\mathbf{u})$ viscous effects
- $p_* > 0$ thermodynamic pressure (constant)
- EoS: $(h, p) \mapsto \rho$ (density) and $(h, p) \mapsto T$ (temperature)

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

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

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# The model

By neglecting the viscous terms and the dependency on the constant pressure $p_*$, the model becomes

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

### Unknowns

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

### Given

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

### Closure

Diphasic equation of state: $h \mapsto T(h)$ (temperature) and $h \mapsto \rho(h)$ (specific density)

# 1. Introduction

# The LMNC model without Thermal Diffusion

## Summary

- Analytical Solutions (1D)
  - Steady-state for every choice of EoS for pure phases
  - Transitory solutions for Noble-Abel Stiffened-Gas (NASG) for pure phases
- Numerical Schemes
  - 1D non-cons. formulation: MOC, INTMOC (exponential), WB schemes
  - 3D non-cons. formulation: prediction-projection method
- EoS with Phase Transition at Saturation
  - SG, NASG for pure phases
  - IAPWS ⇝ incomplete SG exact on the boundaries of the saturation
  - Cubic (Van der Waals, Berthelot, Clausius...) with Maxwell construction

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- A Relaxation Model (4-LMNC model)
  - EDP + BGK term
  - EoS (Chemical Potential Disequilibrium)
  - Formal Convergence
  - WB and AP Schemes

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- G.F., B. Grec, ESAIM: Proc. 2023


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G.F., B. Grec, Y. Penel, ESAIM: M2AN 2021

# The LMNC model without Thermal Diffusion

## The conservative model ⇝ a non-conservative formulation

### Conservative formulation

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

$$\rightsquigarrow \tau \stackrel{\text{def}}{=} 1/\varrho$$

### Non-conservative formulation

$$\begin{cases} \partial_t h + \mathbf{u} \cdot \nabla h = \Phi(t, \mathbf{y}) \tau(h) \\ \nabla \cdot \mathbf{u} = \Phi(t, \mathbf{y}) \tau'(h) \\ \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} + \tau(h) \nabla \bar{p} = \mathbf{g} \end{cases}$$

### 1D Conservative formulation

$$\begin{cases} \partial_t \rho + \partial_y (\rho v) = 0 \\ \partial_t (\rho h) + \partial_y (\rho h v) = \Phi \end{cases}$$

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

$$\rightsquigarrow$$

### 1D Non-conservative formulation

$$\begin{cases} \partial_t h + v \partial_y h = \Phi \tau(h) \\ \partial_y v = \Phi \tau'(h) \end{cases}$$

and $\tau(h) \partial_y \bar{p} = -g - \partial_t v - v \partial_y v$

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# The LMNC model without Thermal Diffusion

## Schemes

We employ a standard projection method based on a non-conservative formulation on a staggered grid ($\simeq$ for Navier-Stokes):

1. First, we solve the transport equation for enthalpy.

$$\partial_t h + \mathbf{u} \cdot \nabla h = \Phi(t, \mathbf{y})\tau(h)$$

2. Next, the other equations are solved using a pressure-correction method.

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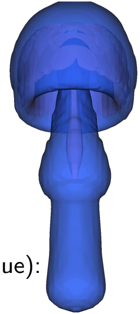
This involves two substeps per time step (repeated until the divergence reaches the desired value):

- Velocity prediction considering the pressure explicit in the first substep.
- Pressure correction in the second substep by projecting the predicted velocity onto the space of a "divergence-fixed" field.



**Next Step:** What happens with thermal diffusion?

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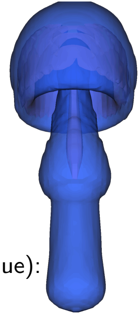

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# 1. Introduction

# Diphasic equation of state with phase transition

- **Diffuse Interface Framework**:
  the (compressible) fluid can exist in liquid ($\ell$) or vapor ($_g$) phase or as a mixture of both

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

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

- **Mixture**: at saturation (same pressure $p$, temperature $T$, chemical potential $\mu$)

$$\mu_\ell(T, p) = \mu_g(T, p) \rightsquigarrow p \mapsto T^{sat}(p)$$

*temperature at saturation*

- **Transition** pure phase/mixture: $h_\kappa^{sat}(p) \stackrel{\text{def}}{=} h_\kappa(T^{sat}(p), p)$ the enthalpy of the phase $\kappa$ at saturation

At pressure $p$, the fluid is

- in the liquid phase if $h \leq h_\ell^{sat}(p)$
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# Diphasic equation of state with phase transition

## Temperature with Phase Transition at Constant Pressure

- $T$ is piecewise defined w.r.t. $h_\kappa^{sat}(p)$

$$(h,p) \mapsto T(h,p) = \begin{cases} T_\ell(h,p), & \text{if } h \leq h_\ell^{sat}(p) \\ T^{sat}(p), & \text{if } h_\ell^{sat}(p) < h < h_g^{sat}(p) \\ T_g(h,p), & \text{if } h \geq h_g^{sat}(p) \end{cases}$$

- In our EDP system, the **thermodynamic** pressure $p_*$ is constant

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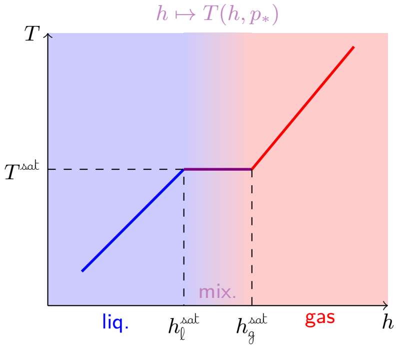


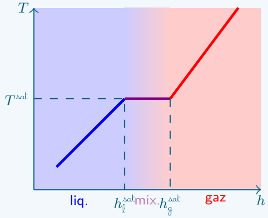
# Diffusion term

## Temperature in the LMNC model

- LMNC model

$$\partial_t(\rho h) + \nabla \cdot (\rho h \mathbf{u}) = \left[\Phi(t,\mathbf{y}) + \nabla \cdot \left(\omega(h,p_*)\nabla T(h,p_*)\right)\right]$$

- Mixture at saturation and thermodynamic pressure $p_*$ constant:




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

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

$c_{p,\kappa} \stackrel{\text{def}}{=} \left.\frac{\partial h}{\partial T}\right|_p$ isobar heat capacity

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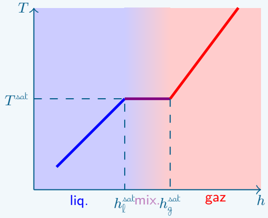


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$c_{p,\kappa} \overset{\text{def}}{=} \left.\dfrac{\partial h}{\partial T}\right|_p$ isobar heat capacity

# 1. Introduction

# The 1D model

1. $v$ and $h$ are solutions of

$$\begin{cases} \partial_t \varrho + \partial_y(\varrho v) = 0 \\ \partial_t(\varrho h) + \partial_y(\varrho h v) = [\Phi + \partial_y(\lambda(h)\partial_y h)] \end{cases}$$

$$h \mapsto \lambda(h) = \begin{cases} \lambda_\ell & \text{if } h \le h_\ell^{sat} \\ 0 & \text{if } h_\ell^{sat} < h < h_g^{sat} \\ \lambda_g & \text{if } h \ge h_g^{sat} \end{cases}$$

$$h \mapsto \varrho(h)$$

- Domain: $y \in \mathbb{R}^+$
- Boundary conditions:
  - $y = 0$: Dirichlet (injection) $v(t,0) = v_e > 0$ and $h(t,0) = h_e < h_\ell^{sat}$ constant,
  - $y \to +\infty$: asymptotic behavior $\lim_{y\to+\infty} \partial_y h(t,y) = \Phi/D_e$
- Constants: $\Phi > 0$, $D_e \stackrel{\text{def}}{=} v_e \varrho(h_e) > 0$
- Initial conditions: $h(0,y) = h_e$ liquid phase

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

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

## 2. Steady-state model

# 2. Steady-state model

# The 1D steady-state model

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

$$\Downarrow$$

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

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# The 1D steady-state model

**EDO**

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

- Constants: $\Phi > 0$, $D_e > 0$
- Domain: $[0, +\infty)$
- Boundary conditions:
  - Dirichlet (inlet) $h(0) = h_e < h_\ell^{sat}$
  - Asymptotic behavior $\lim_{y\to\infty} h'(y) = \frac{\Phi}{D_e}$

**Diffusion**

$$\lambda(h) = \begin{cases} \lambda_\ell & \text{if } h \le h_\ell^{sat} \\ \lambda_m & \text{if } h_\ell^{sat} < h < h_g^{sat} \\ \lambda_g & \text{if } h \ge h_g^{sat} \end{cases}$$

We will consider three cases:

- $\lambda_\ell = \lambda_m = \lambda_g = 0$: model without diffusion
- $\lambda_\ell, \lambda_m, \lambda_g > 0$: model with strictly positive diffusion
- $\lambda_m = 0$ and $\lambda_\ell, \lambda_g > 0$: model with a degenerate diffusion

**Remark**

Due to the discontinuities in $\lambda$, the ODE should be interpreted as follows:

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

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## 2. Steady-state model

# Solution with $\lambda_\ell = \lambda_m = \lambda_g = 0$ (without diffusion)

## Proposition 1

*If $\lambda(h) \equiv 0$ the steady enthalpy solution is*

$$h(y) = h_e + \frac{\Phi}{D_e} y$$

**Proof.**

$$\begin{cases} D_e h'(y) = \Phi \\ h(0) = h_e \\ \lim_{y \to +\infty} h'(y) = \frac{\Phi}{D_e} \end{cases} \implies h(y) = h_e + \frac{\Phi}{D_e} y$$

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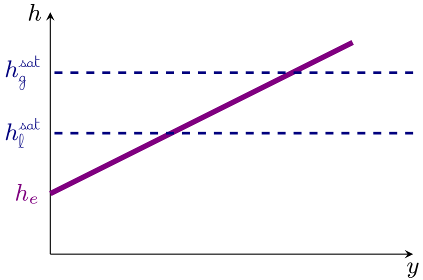

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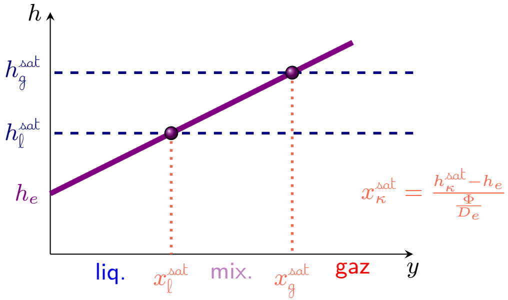


# 2. Steady-state model

## Solution with $\lambda_\ell, \lambda_m, \lambda_g > 0$ (strictly positive diffusion)

### Proposition 2

*Without degeneracy of diffusion, the unique solution is continuous and can be written as*

$$h(y) = \begin{cases} h_\ell(y) \overset{\text{def}}{=} C_{\ell,1} + \dfrac{\Phi}{D_e} y + C_{\ell,2} \exp\left(\dfrac{y}{\lambda_\ell / D_e}\right) & \textit{if } y \leq y_\ell^{sat} \\ h_m(y) \overset{\text{def}}{=} C_{m,1} + \dfrac{\Phi}{D_e} y + C_{m,2} \exp\left(\dfrac{y}{\lambda_m / D_e}\right) & \textit{if } y_\ell^{sat} \leq y < y_g^{sat} \\ h_g(y) \overset{\text{def}}{=} h_g^{sat} + \dfrac{\Phi}{D_e}(y - y_g^{sat}) & \textit{if } y \geq y_g^{sat} \end{cases}$$

*where the 4 constants $C_{\kappa,1}$ and $C_{\kappa,2}$ depend on $y_\ell^{sat}$ and $y_g^{sat}$.*

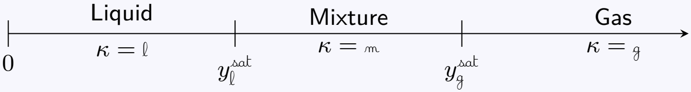
*The boundaries $y_\ell^{sat}$ and $y_g^{sat}$ satisfies the continuity flux*

$$\lambda_\ell h_\ell'(y_\ell^{sat}) = \lambda_m h_m'(y_\ell^{sat}) \quad \textit{and} \quad \lambda_m h_m'(y_g^{sat}) = \lambda_g h_g'(y_g^{sat}).$$

# Solution with $\lambda_\ell, \lambda_m, \lambda_g > 0$ (strictly positive diffusion)

**Proof – Solution in Each Region.**

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




- In each region, we solve $D_e h'_\kappa(y) - \lambda_\kappa h''_\kappa(y) = \Phi$, yielding $h_\kappa(y) = C_{\kappa,1} + \frac{\Phi}{D_e} y + C_{\kappa,2} \exp\left(\frac{y}{\lambda_\ell / D_e}\right)$.
- The boundary conditions give two relations:
  - Liquid region: $h_\ell(0) = h_e \rightsquigarrow C_{\ell,2} = h_e - C_{\ell,1}$
  - Vapor region: $\lim_{y\to\infty} h'_g(y) = \frac{\Phi}{D_e} \rightsquigarrow C_{g,2} = 0$
- We need to compute $C_{\ell,1}$, $C_{m,1}$, $C_{m,2}$, $C_{g,1}$ and the transition points $y_\ell^{sat}$, $y_g^{sat}$.

□

# Solution with $\lambda_\ell, \lambda_m, \lambda_g > 0$ (strictly positive diffusion)

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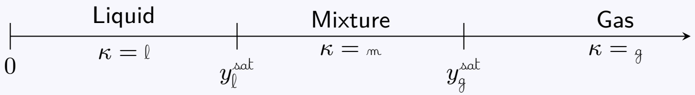


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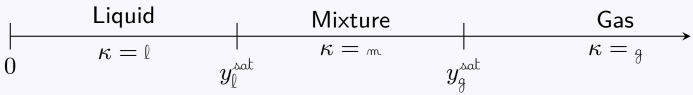


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$\square$

## Solution with $\lambda_\ell, \lambda_m, \lambda_g > 0$ (strictly positive diffusion)

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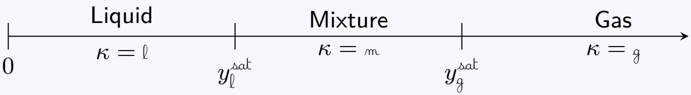


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# Solution with $\lambda_\ell, \lambda_m, \lambda_g > 0$ (strictly positive diffusion)

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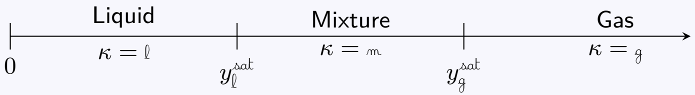


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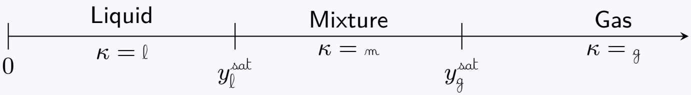


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□

# Solution with $\lambda_\ell, \lambda_m, \lambda_g > 0$ (strictly positive diffusion)

**Proof – Transition Points.**

- Continuity at $y_\ell^{sat}$ and $y_g^{sat}$:
  - Liquid region: $h_\ell(y_\ell^{sat}) = h_\ell^{sat} \rightsquigarrow C_{\ell,1}$ function of $y_\ell^{sat}$;
  - Mixture region: $h_m(y_\ell^{sat}) = h_\ell^{sat}$, $h_m(y_g^{sat}) = h_g^{sat} \rightsquigarrow C_{m,1}, C_{m,2}$ functions of $y_\ell^{sat}$ and $y_g^{sat}$;
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- The positions of the transition points, $y_\ell^{sat}$ and $y_g^{sat}$, are **implicitly** determined by the continuity conditions of flux:

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Let's take a look at the graphs to observe the limit as $\lambda_m \to 0$.

$\rightsquigarrow$ **Jupyter Notebook**

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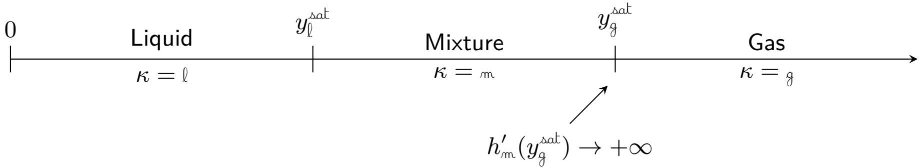

# 2. Steady-state model

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

Before delving into the analytical solution, let's take a look at the graphs $\rightsquigarrow$ **Jupyter Notebook**

If $\lambda_m = 0$, we have two distinct cases:

1. Liquid/mixture/gas
2. Liquid/gas (the mixture is not permitted)

**Remark**

Due to the jump in $h$, the ODE $D_e h'(y) - (\lambda(h)h'(y))' = \Phi$ should be interpreted as follows:

$$D_e h' - (L \circ h)'' = \Phi \qquad L(h) \stackrel{\text{def}}{=} \begin{cases} \lambda_\ell(h - h_\ell^{\text{sat}}) & \text{if } h \le h_\ell^{\text{sat}} \\ 0 & \text{if } h_\ell^{\text{sat}} < h < h_g^{\text{sat}} \\ \lambda_g(h - h_g^{\text{sat}}) & \text{if } h \ge h_g^{\text{sat}} \end{cases} \qquad (\text{thus, } L'(h) = \lambda(h))$$

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# Solution with $\lambda_m = 0$ and $\lambda_\ell, \lambda_g > 0$ (degenerate diffusion)- I: Liquid/mixture/gas

$$\boxed{\text{Case } \frac{\lambda_g}{D_e}\frac{\Phi}{D_e} < h_g^{sat} - h_\ell^{sat}}$$

Summary of the observations:

- Mixture presence
- Position $y_\ell^{sat}$ implicitly defined by $h_\ell(y_\ell^{sat}) = h_\ell^{sat}$ and we have $(h_\ell)'(y_\ell^{sat}) = 0$
- Position $y_g^{sat}$ computed w.r.t. $y_\ell^{sat}$ by $y_g^{sat} = y_\ell^{sat} + \frac{D_e}{\Phi}(h_g^{sat} - h_\ell^{sat}) - \frac{\lambda_g}{D_e}$
- Gas diffusion reduces mixture region for steady solution $(y_g^{sat} - y_\ell^{sat}) = (x_g^{sat} - x_\ell^{sat}) - \frac{\lambda_g}{D_e}$
- Jump occurs within the mixture region and

$$[\![h]\!](y_g^{sat}) = h_g^{sat} - h_m(y_g^{sat}) = \frac{\lambda_g}{D_e}\frac{\Phi}{D_e} \quad \left[< h_g^{sat} - h_\ell^{sat}\right]$$

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## Proposition 3

*The mixture zone is present and the unique solution is discontinuous at $y_g^{sat}$ and can be written as*

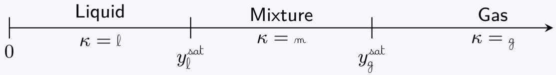
$$h(y) = \begin{cases} h_\ell(y) \stackrel{\text{def}}{=} C_{\ell,1} + \dfrac{\Phi}{D_e} y + C_{\ell,2} \exp\left(\dfrac{y}{\lambda_\ell / D_e}\right) & \text{if } y \le y_\ell^{sat} \\ h_m(y) \stackrel{\text{def}}{=} h_\ell^{sat} + \dfrac{\Phi}{D_e}(y - y_\ell^{sat}) & \text{if } y_\ell^{sat} \le y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

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

# Solution with $\lambda_m = 0$ and $\lambda_\ell, \lambda_g > 0$ (degenerate diffusion)- I: Liquid/mixture/gas

**Proof – Solution on each region.**

- Given $\Phi > 0$, $D_e > 0$, we observe 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: $h_\ell(0) = h_e \rightsquigarrow C_{\ell,2} = h_e - C_{\ell,1}$
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- 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 $y_\ell^{sat}$, $y_g^{sat}$.

$\square$

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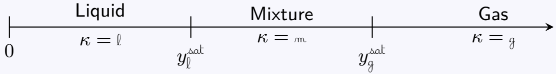


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□

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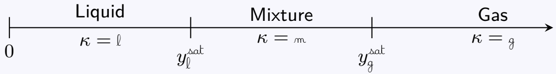


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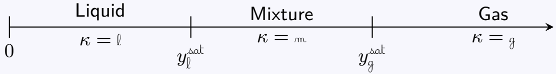


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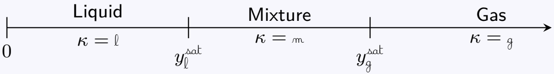


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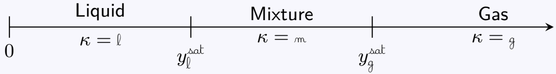


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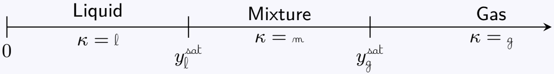


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# Solution with $\lambda_m = 0$ and $\lambda_\ell, \lambda_g > 0$ (degenerate diffusion)- I: Liquid/mixture/gas

**Proof – Liquid/Mixture transition.**

- Jump relation at $y_\ell^{sat}$:

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

- Continuity:
  - $h_\ell(y_\ell^{sat}) = h_\ell^{sat} \rightsquigarrow C_{\ell,1}$ is a function of $y_\ell^{sat}$
  - $h_m(y_\ell^{sat}) = h_\ell^{sat} \rightsquigarrow C_m$ is a function of $y_\ell^{sat}$
- Slope in the liquid region:
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□

# Solution with $\lambda_m = 0$ and $\lambda_\ell, \lambda_g > 0$ (degenerate diffusion)- I: Liquid/mixture/gas

**Proof – Liquid/Mixture transition.**

- Jump relation at $y_\ell^{sat}$:

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

- Continuity:
  - $h_\ell(y_\ell^{sat}) = h_\ell^{sat} \rightsquigarrow C_{\ell,1}$ is a function of $y_\ell^{sat}$
  - $h_m(y_\ell^{sat}) = h_\ell^{sat} \rightsquigarrow C_m$ is a function of $y_\ell^{sat}$
- Slope in the liquid region:
  - The position $y_\ell^{sat}$ is implicitly defined by $h'(y_\ell^{sat,-}) = 0$

□

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- Jump relation at $y_\ell^{sat}$:

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$\square$

# Solution with $\lambda_m = 0$ and $\lambda_\ell, \lambda_g > 0$ (degenerate diffusion)- I: Liquid/mixture/gas

**Proof – Mixture/Gas transition.**

- Jump relation at $y_g^{sat}$:

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

- An infinite number of solutions

$$h_g(y_g^{sat}) \in \left[ h_g^{sat}, h_g^{sat} + \frac{\lambda_g}{D_e}\frac{\Phi}{D_e} \right[ \quad \rightsquigarrow \quad h_m(y_g^{sat}) = h_g(y_g^{sat}) - [\![h(y_g^{sat})]\!]$$

- The viscosity solution corresponds to the smallest mixture region: $h_g(y_g^{sat}) = h_g^{sat}$
- This fixes $y_g^{sat}$ and thus $C_{g,1}$.

$\square$

# Solution with $\lambda_m = 0$ and $\lambda_\ell, \lambda_g > 0$ (degenerate diffusion)- I: Liquid/mixture/gas

Proof – Mixture/Gas transition.

- Jump relation at $y_g^{sat}$:

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

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

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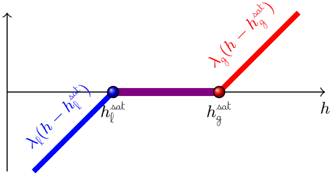
□

# Solution in the sense of distribution

**No need viscosity solution when $\lambda_m = 0$ and uniqueness of the continuous solution when $\lambda_m > 0$**

$D_e h' - (L \circ h)'' = \Phi$ with $h \mapsto L(h)$ which has the graph




Suppose that $[\![h]\!](y_*) > 0$ at a point $y_*$. What about $(L \circ h)(y_*)$ and $y_*$?

- We prove that $[\![L \circ h]\!](y_*) = 0$:

$$\begin{cases} [\![h]\!](y_*) > 0 \\ [\![L \circ h]\!](y_*) > 0 \end{cases} \Longrightarrow \begin{cases} h' \text{ contains a } \delta_{y_*} \\ (L \circ h)' \text{ contains a } \delta_{y_*} \end{cases} \Longrightarrow \begin{cases} h' \text{ order } 0 \\ (L \circ h)'' \text{ order } 1 \end{cases} \lightning$$

Since $L(h(y_*^+)) = L(h(y_*^-))$, this implies $h_\ell^{sat} \le h(y_*^-) < h(y_*^+) \le h_g^{sat}$

Note that, if $\lambda_m > 0$, we have $[\![L \circ h]\!](y_*) = 0$ iff $[\![h]\!](y_*) = 0$: jumps are not allowed.

- What about $[\![(L \circ h)']\!](y_*)$?

$$\begin{cases} [\![h]\!](y_*) > 0 \\ D_e h - (L \circ h)' \text{ continuous} \end{cases} \Longrightarrow [\![(L \circ h)']\!](y_*) > 0 \Longrightarrow h(y_*^+) = h_g^{sat} \text{ or } h(y_*^-) = h_\ell^{sat}$$

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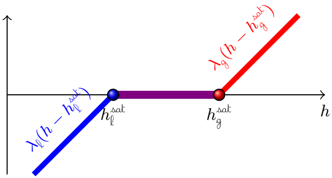


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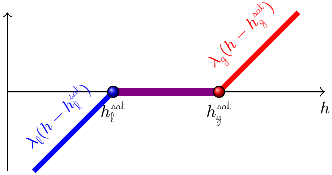


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# Solution with $\lambda_m = 0$ and $\lambda_\ell, \lambda_g > 0$ (degenerate diffusion)

What about if the condition $\frac{\lambda_g}{D_e}\frac{\Phi}{D_e} \leq h_g^{sat} - h_\ell^{sat}$ 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.

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# Solution with $\lambda_m = 0$ and $\lambda_\ell, \lambda_g > 0$ (degenerate diffusion)- II: Liquid/gas (no mixture)

$$\boxed{\text{Case } \frac{\lambda_g}{D_e}\frac{\Phi}{D_e} \geq h_g^{sat} - h_\ell^{sat}}$$

Summary of observations:

- Mixture does not exist
- If $\lambda_\ell > 0$, the jump is constant $[\![h]\!](y^{sat}) = h_g(y^{sat}) - h_\ell(y^{sat}) = h_g^{sat} - h_\ell^{sat}$
- Position $y^{sat} = y_\ell^{sat} = y_g^{sat}$ is implicitly defined by $h_\ell(y^{sat}) = h_\ell^{sat}$ with

$$(h_\ell)'(y^{sat}) = \frac{\frac{\lambda_g}{D_e}\frac{\Phi}{D_e} - (h_g^{sat} - h_\ell^{sat})}{\frac{\lambda_\ell}{D_e}} \qquad \left[\geq 0 \text{ and } \xrightarrow[\lambda_\ell \to 0]{} +\infty\right]$$

- If $\lambda_\ell = 0$, the jump occurs within the liquid region and $h_\ell(y^{sat}) < h_\ell^{sat}$:

$$[\![h]\!](y^{sat}) = h_g^{sat} - h_\ell(y^{sat}) = \frac{\lambda_g}{D_e}\frac{\Phi}{D_e} \geq h_g^{sat} - h_\ell^{sat}$$

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$$\boxed{\text{Case } \frac{\lambda_g}{D_e}\frac{\Phi}{D_e} \geq h_g^{sat} - h_\ell^{sat}}$$

## Proposition 4

*The mixture zone is not present and the unique solution is discontinuous and can be written as*

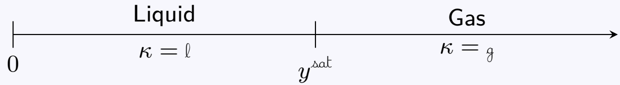
$$h(y) = \begin{cases} h_\ell(y) \stackrel{\text{def}}{=} C_{\ell,1} + \dfrac{\Phi}{D_e} y + C_{\ell,2} \exp\left(\dfrac{y}{\lambda_\ell / D_e}\right) & \text{if } y \leq y^{sat} \\ h_g(y) \stackrel{\text{def}}{=} h_g^{sat} + \dfrac{\Phi}{D_e}(y - y^{sat}) & \text{if } y \geq y^{sat} \end{cases}$$

- *The constants $C_{\ell,1}$ and $C_{\ell,2}$ depend on $y^{sat}$.*
- *The position $y^{sat}$ is implicitly defined by $D_e\left(h_g^{sat} - h_\ell^{sat}\right) = \lambda_g h'(y^{sat,+}) - \lambda_\ell h'(y^{sat,-})$*

# Solution with $\lambda_m = 0$ and $\lambda_\ell, \lambda_g > 0$ (degenerate diffusion)- II: Liquid/gas (no mixture)

**Proof – Solution on each region.**

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




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

$\square$

# Solution with $\lambda_m = 0$ and $\lambda_\ell, \lambda_g > 0$ (degenerate diffusion)- II: Liquid/gas (no mixture)

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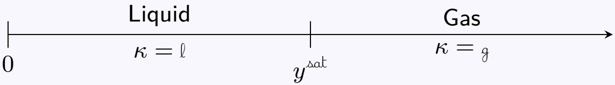


- In each region, we solve $D_e h'_\kappa(y) - \lambda_\kappa h''_\kappa(y) = \Phi$, yielding $h_\kappa(y) = C_{\kappa,1} + \frac{\Phi}{D_e} y + C_{\kappa,2} \exp\left(\frac{y}{\lambda_\ell / D_e}\right)$
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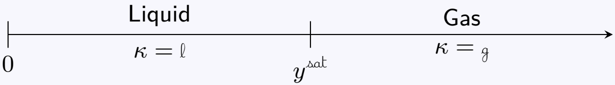


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□

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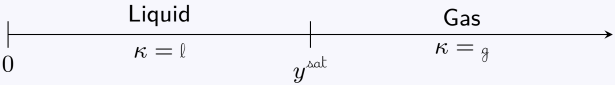


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□

# Solution with $\lambda_m = 0$ and $\lambda_\ell, \lambda_g > 0$ (degenerate diffusion)- II: Liquid/gas (no mixture)

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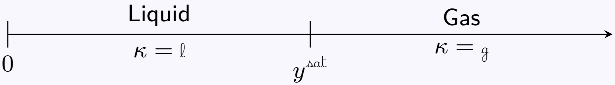


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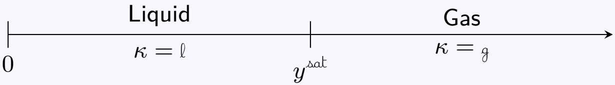
**Proof – Solution on each region.**

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




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

$\square$

# Solution with $\lambda_m = 0$ and $\lambda_\ell, \lambda_g > 0$ (degenerate diffusion)- II: Liquid/gas (no mixture)

**Proof – Liquid/Gas transition.**

This problem is a classic Stefan problem. Thus,

- The jump is fixed and equals the latent heat:
  - Liquid region: $h_\ell(y^{sat}) = h_\ell^{sat} \rightsquigarrow C_{\ell,1}$ is a function of $y^{sat}$
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- The jump relation at $y^{sat}$ is given by:

$$D_e\left(h_g^{sat} - h_\ell^{sat}\right) = \lambda_g h'(y^{sat,+}) - \lambda_\ell h'(y^{sat,-}) \quad \rightsquigarrow \quad \frac{\lambda_\ell}{D_e} h_\ell'(y^{sat,-}) = \frac{\lambda_g}{D_e}\frac{\Phi}{D_e} - (h_g^{sat} - h_\ell^{sat}).$$

This relation provides an **implicit** definition of the position $y^{sat}$ (which can be proven to be unique). $\square$

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# 2. Steady-state model

# Link to the Stationary Stefan Problem - free boundary problem

Find the position $y^{sat}$ such that the over-determinate elliptic problem is satisfied:

**Stationary Stefan problem on enthalpy**

$$\begin{cases} D_e h' - \lambda_\ell h'' = \Phi \\ h(0) = h_e < h_\ell^{sat}, \\ h(y^{sat,-}) = h_\ell^{sat} \end{cases} \quad \text{in } ]0, y^{sat}[$$

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Remark: $[\![h(y^{sat})]\!] = h_g^{sat} - h_\ell^{sat}$

**Stationary Stefan problem on temperature**

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

## Our model

- Diffuse interface framework allowing for mixture.
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Same model when $\frac{\lambda_g}{D_e}\frac{\Phi}{D_e} \geq h_g^{sat} - h_\ell^{sat}$.

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

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# Conclusion on the Steady-State Model

1. In the absence of diffusion, the mixture zone (= diffuse interface) always exists
2. Thermal diffusion in the gas phase reduces the mixture zone and can cause it to vanish if it is high enough:
   - Neglect thermal diffusion in the gas phase if

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*cf.* G.F., C. Galusinski, ESAIM: Proc. 2023, Vol. 72

**Next step:** Time-dependent model

Remark: in a PWR, the ratio $\frac{\lambda_g}{D_e}\frac{\Phi}{D_e}/(h_g^{sat} - h_\ell^{sat})$ is approximately $1.3\ 10^{-6}$ $\rightsquigarrow$ the jump is negligible

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# The Simplified model

$$\begin{cases} \partial_t \varrho + \partial_y(\varrho v) = 0 \\ \partial_t(\varrho h) + \partial_y(\varrho h v) = \left[\Phi + \partial_y\big(\lambda(h)\partial_y h\big)\right] \\ \boxed{h \mapsto \varrho(h) \equiv 1 \text{ for all } h} \end{cases} \quad \rightsquigarrow \quad \begin{cases} \partial_y v = 0 \\ \partial_t h + \partial_y(hv) = \left[\Phi + \partial_y\big(\lambda(h)\partial_y h\big)\right] \end{cases}$$

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$$\partial_t h + v\partial_y h - \partial^2_{yy}(L(h)) = \Phi \quad \text{in } \mathbb{R}^+ \times \mathbb{R}^+$$

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# 3. Simplified Model

# Numerical Time-Dependent Solution

Front Tracking Method $\rightsquigarrow$ benchmark for evaluating the performance of other approaches

## Explicit Scheme

$$\frac{h^{n+1} - h^n}{\delta t} + v\partial_y h^n - \partial^2_{yy}(L(h^n)) = \Phi \quad \text{in } \mathbb{R}^+$$

This is associated with a gradient scheme proposed by Eymard et al. in 2013.

$\rightsquigarrow$ the CFL condition 🐢 🐢 🐢

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This is associated with a gradient scheme as above. Internship by L. Lamerand

$\rightsquigarrow$ Convergence of the fixed point when the jump is generated can be complicated 😅

# Simulations

1. No diffusion: Influence of $\Phi$ on Mixture Zone Width $\Delta x_\kappa^{sat}$ ▸ $\Phi = 2,\ \lambda_\ell = 0,\ \lambda_g = 0$ ▸ $\Phi = 1,\ \lambda_\ell = 0,\ \lambda_g = 0$
2. Diffusion in Liquid Phase: Influence on $y_\ell^{sat}$ and Slope at $y_\ell^{sat}$ ▸ $\Phi = 1,\ \lambda_\ell = 0 \to 2,\ \lambda_g = 0$
3. Diffusion in Gas Phase: Influence on Mixture Zone width $\Delta y_\kappa^{sat}$ and jump at $y_g^{sat}$ ▸ $\Phi = 1,\ \lambda_\ell = 0,\ \lambda_g = 0 \to 1$

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4. Diffusion in Both Phases: Mixture Zone Existence ▸ $\Phi = 1,\ \lambda_\ell = 0 \to 1,\ \lambda_g = 1$
5. Diffusion in Both Phases: Mixture Zone Disappearance ▸ $\Phi = 1,\ \lambda_\ell = 1,\ \lambda_g = 1 \to 2$

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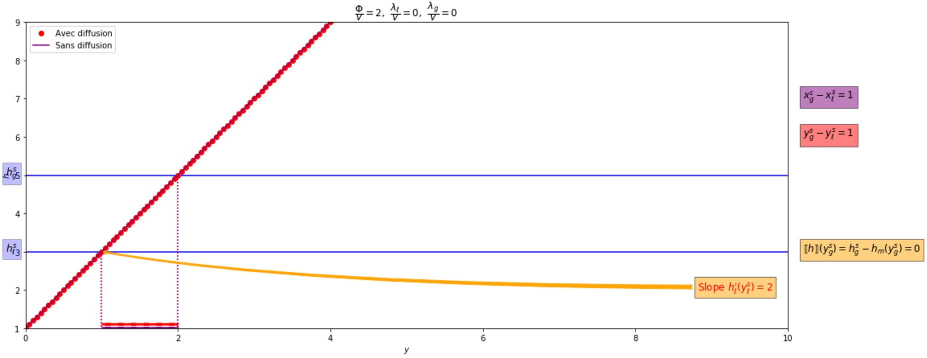
6. Diffusion in Both Phases: No Mixture Zone, Focus on Slope ▸ $\Phi = 1,\ \lambda_\ell = 1,\ \lambda_g = 2 \to 3$ ▸ $\Phi = 1,\ \lambda_\ell = 1,\ \lambda_g = 3 \to 4$
7. Diffusion in Both Phases: No Mixture Zone, Jump in Liquid Phase
   ▸ $\Phi = \frac{1}{2},\ \lambda_\ell = 1,\ \lambda_g = 5$ ▸ $\Phi = \frac{1}{2},\ \lambda_\ell = 0.1,\ \lambda_g = 5$ ▸ $\Phi = \frac{1}{2},\ \lambda_\ell = 0,\ \lambda_g = 5$

◂ Return

$$\frac{\Phi}{v} = 2, \ \frac{\lambda_\ell}{v} = 0, \ \frac{\lambda_g}{v} = 0$$

Case $\dfrac{\lambda_g}{v}\dfrac{\Phi}{v} < h_g^{sat} - h_\ell^{sat}$ : mixture zone at steady state

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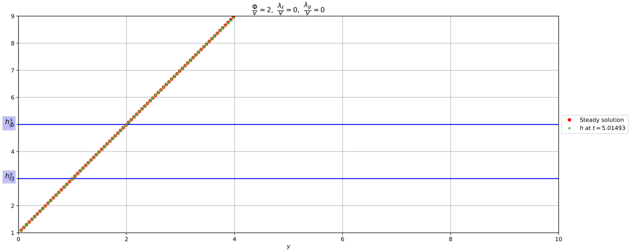


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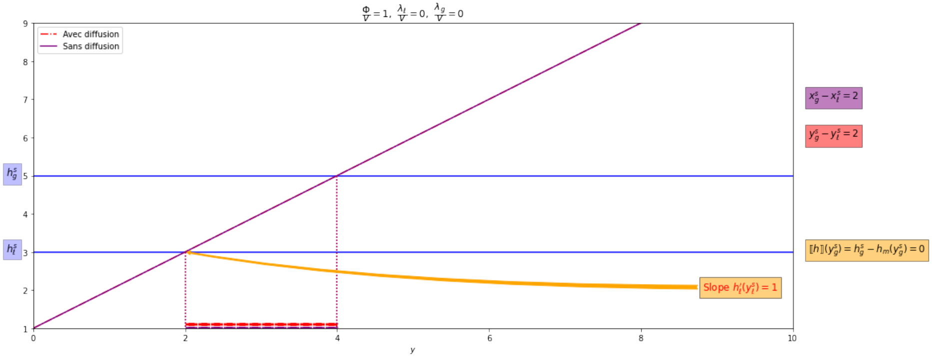


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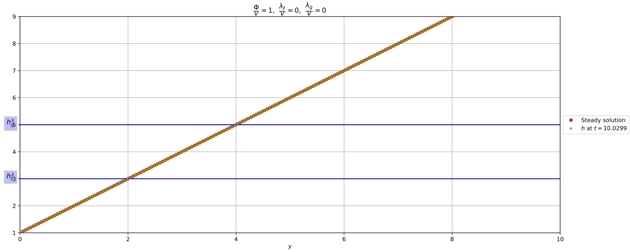
**Case $\dfrac{\lambda_g}{v}\dfrac{\Phi}{v} < h_g^{sat} - h_\ell^{sat}$ : mixture zone at steady state**




No diffusion: influence of $\Phi$ on $\Delta x_\kappa^{sat}$ the width of the mixture zone

Return

$$\frac{\Phi}{v} = 1, \ \frac{\lambda_\ell}{v} = 2, \ \frac{\lambda_g}{v} = 0$$

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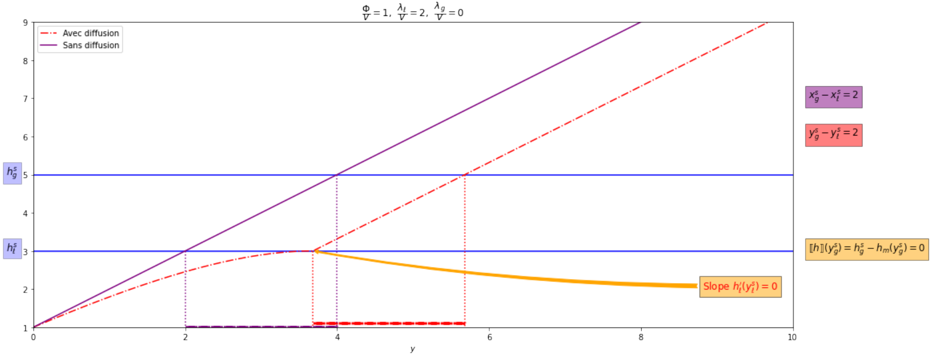


Diffusion Liquid Phase: effect of liquid phase diffusion on $y_\ell^{sat}$ and its associated slope.

Return

$$\frac{\Phi}{v} = 1, \ \frac{\lambda_\ell}{v} = 2, \ \frac{\lambda_g}{v} = 0$$

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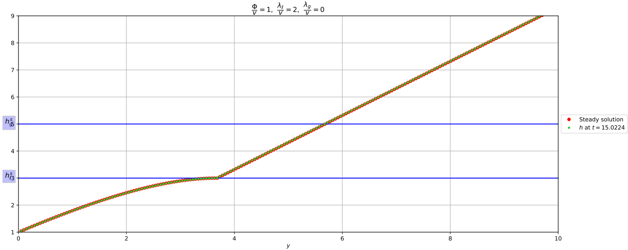


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$$\frac{\Phi}{v} = 1, \ \frac{\lambda_\ell}{v} = 0, \ \frac{\lambda_g}{v} = 1$$

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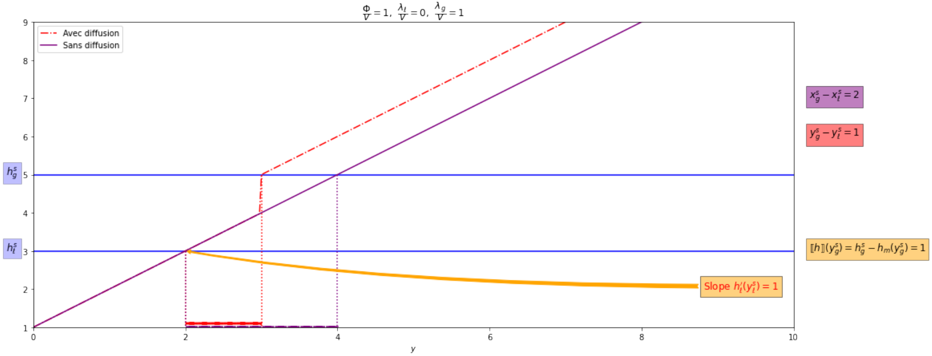


Diffusion in Gas Phase: influence of gas phase diffusion on $\Delta y_\kappa^{sat}$, the width of the mixture zone, and the jump at $y_g^{sat}$.

$$\frac{\Phi}{v} = 1, \ \frac{\lambda_\ell}{v} = 0, \ \frac{\lambda_g}{v} = 1$$

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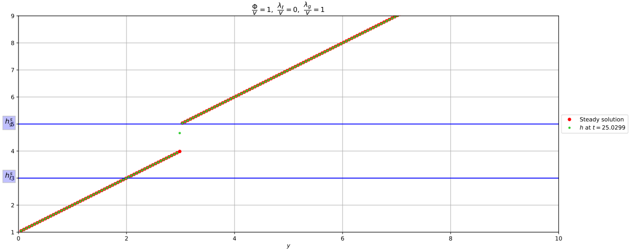


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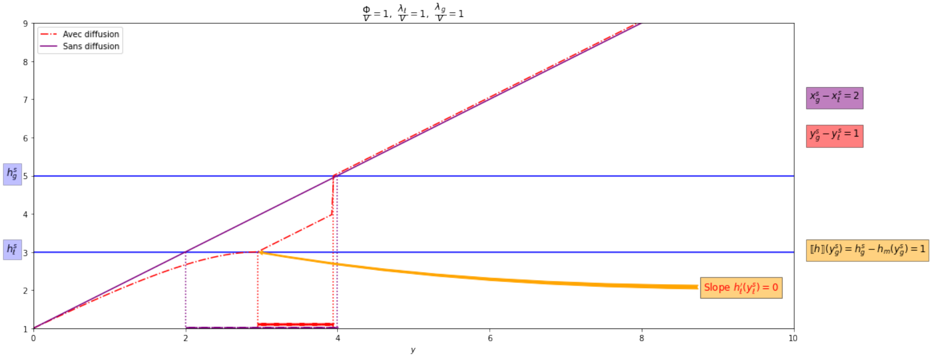


Diffusion in Both Phases: impact on the existence of the mixture zone.

Return

$$\frac{\Phi}{v} = 1, \ \frac{\lambda_\ell}{v} = 1, \ \frac{\lambda_g}{v} = 1$$

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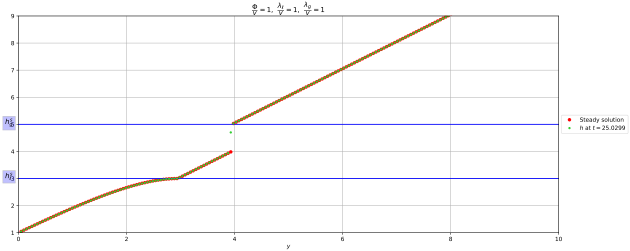
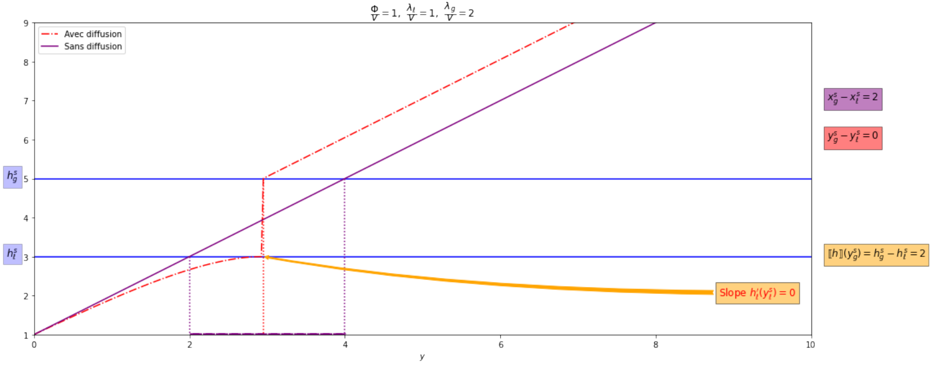



Diffusion in Both Phases: impact on the existence of the mixture zone.

Return

$$\frac{\Phi}{v} = 1,\ \frac{\lambda_\ell}{v} = 1,\ \frac{\lambda_g}{v} = 2$$

Case $\frac{\lambda_g}{v}\frac{\Phi}{v} \geq h_g^{sat} - h_\ell^{sat}$ : no mixture zone at steady state




Diffusion in Both Phases: disappearance of the mixture zone.

Return

$$\frac{\Phi}{v} = 1, \ \frac{\lambda_\ell}{v} = 1, \ \frac{\lambda_g}{v} = 2$$

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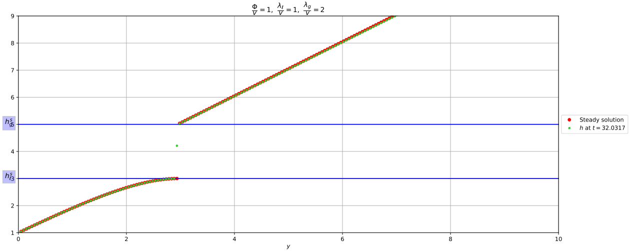
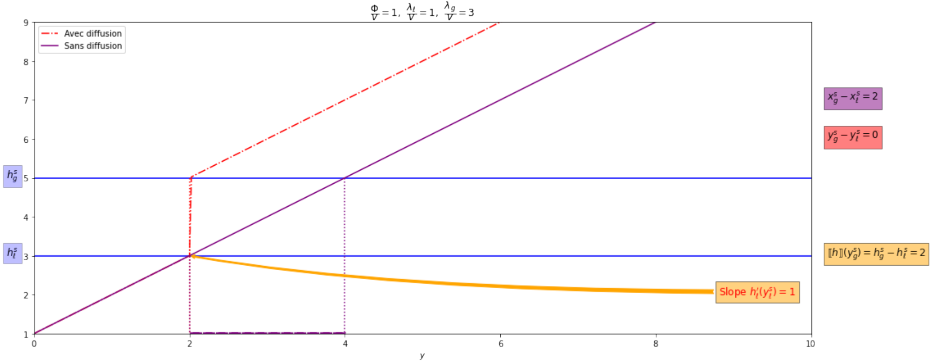



Diffusion in Both Phases: disappearance of the mixture zone.

Return

$$\frac{\Phi}{v} = 1, \ \frac{\lambda_\ell}{v} = 1, \ \frac{\lambda_g}{v} = 3$$

Case $\dfrac{\lambda_g}{v}\dfrac{\Phi}{v} \geq h_g^{sat} - h_\ell^{sat}$ : no mixture zone at steady state




Diffusion in Both Phases – no mixture zone: focus on the slope at $y_\ell^{sat}$.

Return

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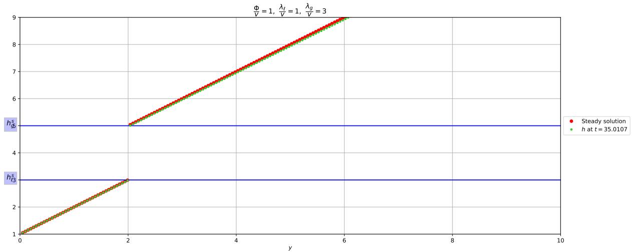
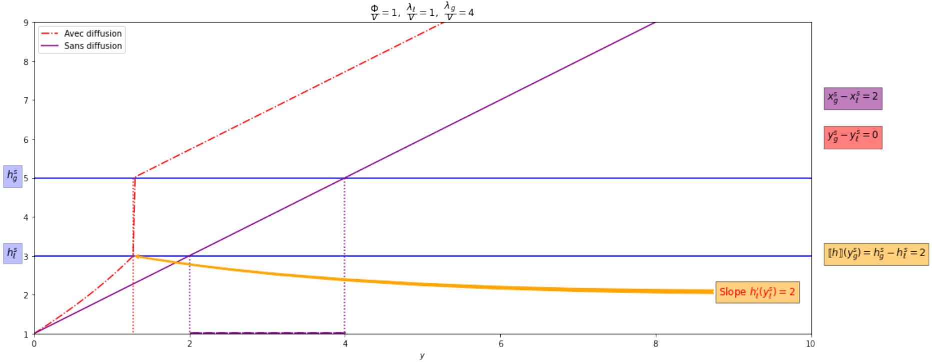



Diffusion in Both Phases – no mixture zone: focus on the slope at $y_\ell^{sat}$.

Return

$$\frac{\Phi}{v} = 1,\ \frac{\lambda_\ell}{v} = 1,\ \frac{\lambda_g}{v} = 4$$

Case $\frac{\lambda_g}{v}\frac{\Phi}{v} \geq h_g^{sat} - h_\ell^{sat}$ : no mixture zone at steady state




Diffusion in Both Phases – no mixture zone: focus on the slope at $y_\ell^{sat}$ that can be $> \frac{\Phi}{v}$

Return

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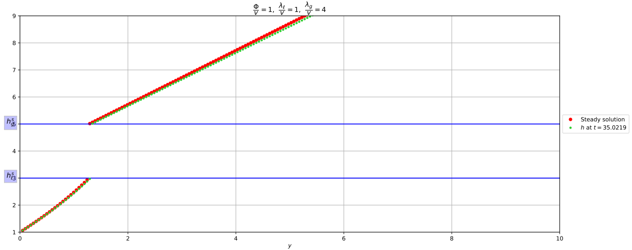
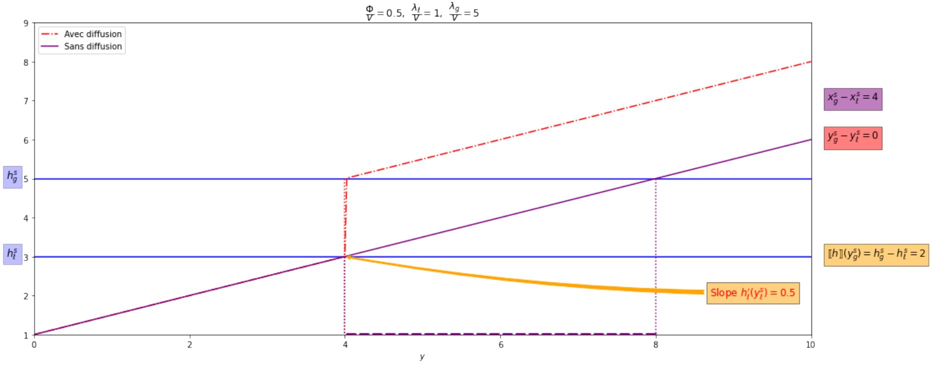



Diffusion in Both Phases – no mixture zone: focus on the slope at $y_\ell^{sat}$ that can be $> \frac{\Phi}{v}$

Return

$$\frac{\Phi}{v} = \frac{1}{2}, \ \frac{\lambda_\ell}{v} = 1, \ \frac{\lambda_g}{v} = 5$$

Case $\frac{\lambda_g}{v}\frac{\Phi}{v} \geq h_g^{sat} - h_\ell^{sat}$ : no mixture zone at steady state




Diffusion in Both Phases – no mixture zone: focus on the slope at $y^{sat,-}$

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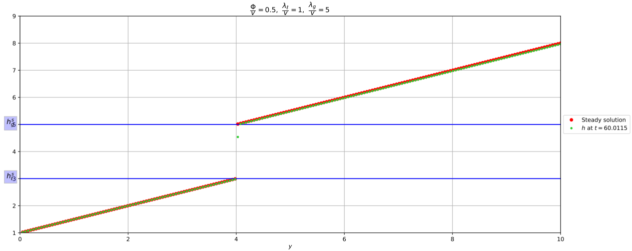
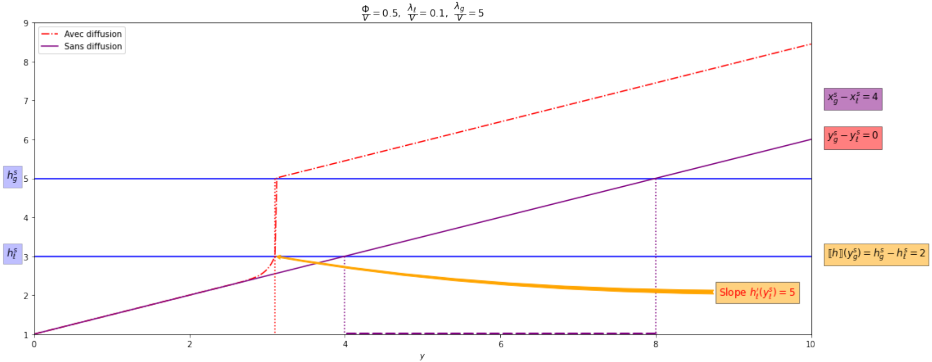



Diffusion in Both Phases – no mixture zone: focus on the slope at $y^{sat,-}$

Return

$$\frac{\Phi}{v} = \frac{1}{2}, \ \frac{\lambda_\ell}{v} = 0.1, \ \frac{\lambda_g}{v} = 5$$

Case $\dfrac{\lambda_g}{v}\dfrac{\Phi}{v} \geq h_g^{sat} - h_\ell^{sat}$ : no mixture zone at steady state




Diffusion in Both Phases – no mixture zone: focus on the slope at $y^{sat,-}$ when $\lambda_\ell \to 0$

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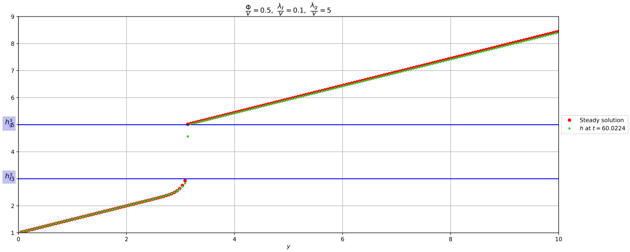


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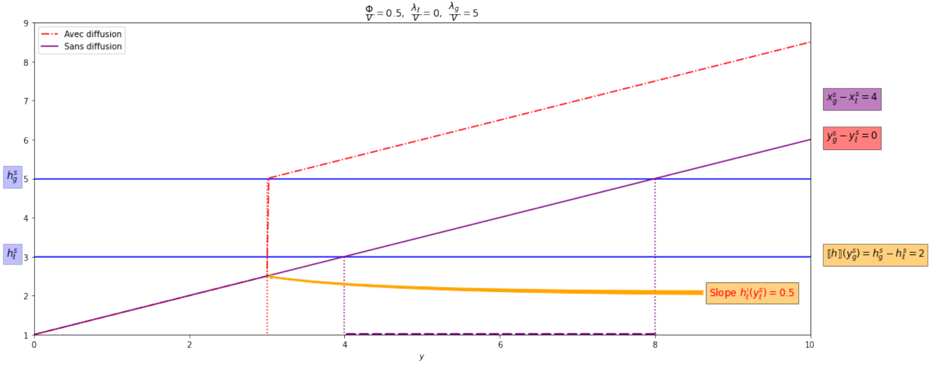


Diffusion only in the Gas – no mixture zone: jump in the liquid phase at $y^{sat}$

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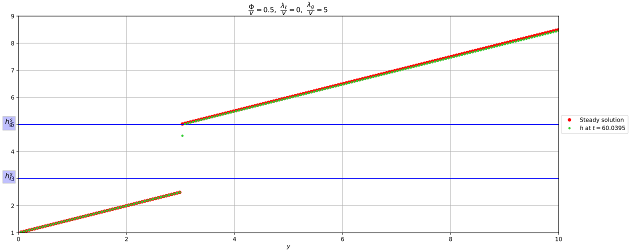
Case $\dfrac{\lambda_g}{v}\dfrac{\Phi}{v} \geq h_g^{sat} - h_\ell^{sat}$ : no mixture zone at steady state

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# 3. Simplified Model

# Validation?

- Asymptotic behavior? ✔
- Transient behavior?
  - Comparison with an interface tracking code? ✔
  - Comparison with an exact solution (in a simplified case) ❓

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Focusing on the jump displacement:

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$$h(t,y) = \begin{cases} h_m^{sat} + \eta(y - y_g^{sat}(t)) & \text{if } y < y_g^{sat}(t) \\ h_g^{sat} + \eta(y - y_g^{sat}(t)) & \text{if } y > y_g^{sat}(t) \end{cases} \qquad \eta \stackrel{\text{def}}{=} \sqrt{\frac{h_g^{sat} - h_m^{sat}}{\lambda_g/\Phi}}$$

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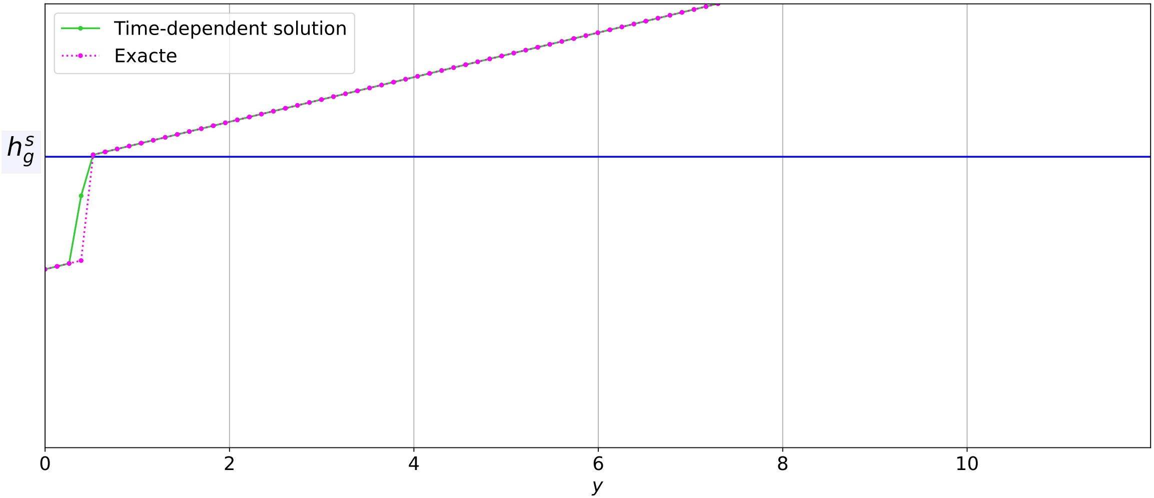
## Validation through Traveling Wave Solution



# 3. Simplified Model

# Conclusion about the Simplified Model

1. Numerical schemes for phase appearance/disappearance and jumps are robust
2. The simulations exhibit precise asymptotic behavior
3. The simulations demonstrate plausible transient behavior
4. Validation of time-dependent jump displacement using analytical solution as traveling waves

**Next step**: Density $\varrho(h) \not\equiv 1 \rightsquigarrow$ complete LMNC model

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$$\varrho(h,p) = \begin{cases} \varrho_\ell(h,p), & \text{if } h \leq h_\ell^{sat}(p) \\ \varrho_m(h,p), & \text{if } h_\ell^{sat}(p) < h < h_g^{sat}(p) \\ \varrho_g(h,p), & \text{if } h \geq h_g^{sat}(p) \end{cases} \qquad \textit{e.g.} \text{ if SG} \quad \varrho_\kappa(h,p) = \frac{\zeta_\kappa(p)}{h - q_\kappa}$$

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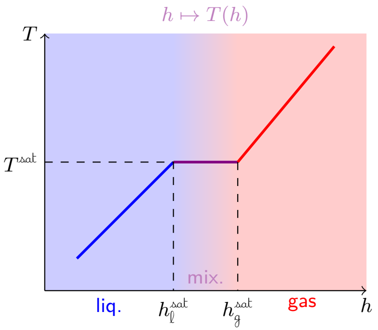


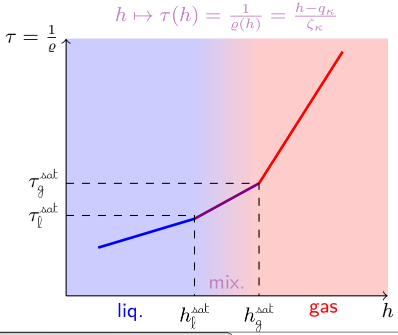

# 4. Full Model

# The Full Model with Degenerating Diffusion

When $\lambda_m = 0$, the steady solution exhibits...

$$\text{a jump in } h \rightsquigarrow \text{a jump in } \varrho(h) \rightsquigarrow \text{a jump in } v = \frac{D_e}{\varrho(h)}$$

$$\Downarrow$$

**We cannot work with the non-conservative form as in the simplified model**

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

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How can we compute $h^{n+1}$ and $v^{n+1}$ from $h^n$ and $v^n$?

Direct Explicit schemes are as there is no explicit time derivative of $v$ (the system is not hyperbolic):

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   ($\simeq$ one step of a fixed point for an implicit scheme)

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# ② Predictor-Corrector Approach

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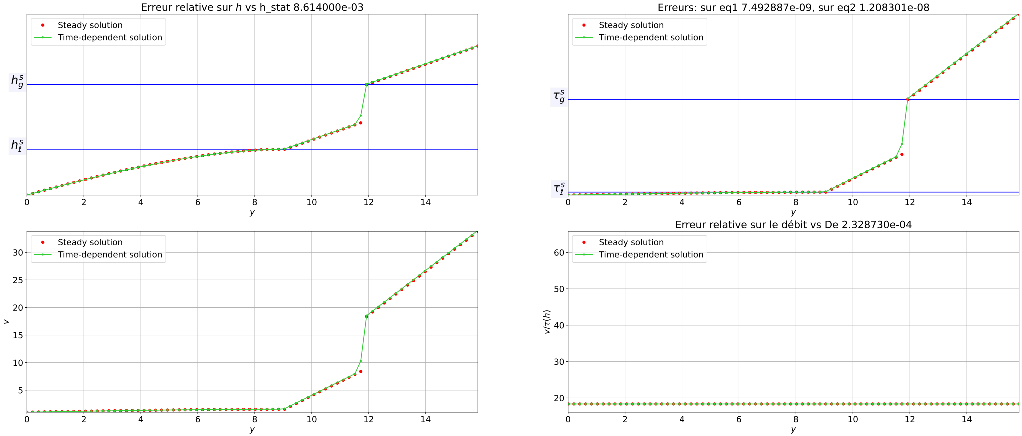
2. Corrector step:

$$\begin{cases} \partial_t \varrho_i + \partial_y (\varrho v)^{n+1} = 0 \\ \partial_t (\varrho h)_i + \partial_y (\varrho h v)^{n+1} - \partial_{yy} L(h^{n+1}) = \Phi \end{cases} \quad \rightsquigarrow v^{n+1} \text{ (overdetermined)}$$

# ② Predictor-Corrector Approach



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Focus on an exact transient solution in the form of a traveling wave:

- Focusing on the jump displacement (thermal diffusion only in the gas)
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- If $h_e(t) = h_m^{sat} - \eta y_g^{sat}(t)$, the solution (which does not exhibit asymptotic behavior) is given by $h$ and $\eta$ as in the simplified model and $v$ as a function of $h$:

$$v(h) = \begin{cases} c + \frac{\Phi}{\eta \varrho(h_m^s)} + \frac{\Phi}{\eta \zeta_m}(h - h_m^{sat}(t)) & \text{if } h < h_m^{sat}(t) \\ c + \frac{\Phi}{\eta \varrho(h_g^s)} + \frac{\Phi}{\eta \zeta_g}(h - h_g^{sat}(t)) & \text{if } h > h_g^{sat}(t) \end{cases} \qquad v_e(t) = v(h_e(t))$$

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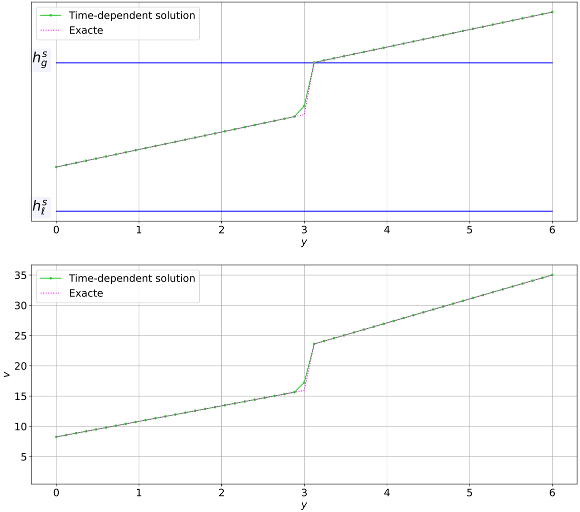
- If $h_e(t) = h_m^{sat} - \eta y_g^{sat}(t)$, the solution (which does not exhibit asymptotic behavior) is given by $h$ and $\eta$ as in the simplified model and $v$ as a function of $h$:

$$v(h) = \begin{cases} c + \frac{\Phi}{\eta\varrho(h_m^s)} + \frac{\Phi}{\eta\zeta_m}(h - h_m^{sat}(t)) & \text{if } h < h_m^{sat}(t) \\ c + \frac{\Phi}{\eta\varrho(h_g^s)} + \frac{\Phi}{\eta\zeta_g}(h - h_g^{sat}(t)) & \text{if } h > h_g^{sat}(t) \end{cases} \qquad v_e(t) = v(h_e(t))$$

# ② Predictor-Corrector Approach



# ③ Relaxation Approach

4-LMNC

$$
\begin{cases}
\partial_t \varrho_\varepsilon + \partial_y(\varrho_\varepsilon v_\varepsilon) = 0\\
\partial_t(\varrho_\varepsilon h_\varepsilon) + \partial_y(\varrho_\varepsilon h_\varepsilon v_\varepsilon) = \Phi + \partial_y(\omega_\varepsilon \partial_y T_\varepsilon)\\
\partial_t(\varrho_\varepsilon \varphi_\varepsilon) + \partial_y(\varrho_\varepsilon \varphi_\varepsilon v_\varepsilon) = \frac{1}{\varepsilon}\varrho_\varepsilon\left(\varphi^{\text{sat}}(h_\varepsilon) - \varphi_\varepsilon\right)
\end{cases}
$$

- Unknowns: $h_\varepsilon$, $v_\varepsilon$, $\varphi_\varepsilon$ (mass fraction)
- EoS iso-$Tp$: $(h_\varepsilon, \varphi_\varepsilon) \mapsto \varrho_\varepsilon$ and $(h_\varepsilon, \varphi_\varepsilon) \mapsto T_\varepsilon$
- Diffusion:

$$
\omega_\varepsilon \partial_y T_\varepsilon = \frac{\omega_\varepsilon}{c_p(\varphi_\varepsilon)}\partial_y h_\varepsilon + \omega_\varepsilon \frac{\partial T_\varepsilon}{\partial \varphi}\partial_y \varphi_\varepsilon
$$

non degenerated

mixture always present!

(3)-LMNC

$$
\begin{cases}
\partial_t \varrho + \partial_y(\varrho v) = 0\\
\partial_t(\varrho h) + \partial_y(\varrho h v) = \Phi + \partial_y(\omega \partial_y T)
\end{cases}
$$

- Unknowns: $h$, $v$
- EoS iso-$Tp\mu$: $h \mapsto \varrho$ and $h \mapsto T$ $\rightsquigarrow$ mass fraction

$$
\varphi^{\text{sat}}(h) \stackrel{\text{def}}{=}
\begin{cases}
0 & \text{if } h \le h_\ell^{\text{sat}}\\
\frac{h - h_\ell^{\text{sat}}}{h_g^{\text{sat}} - h_\ell^{\text{sat}}} & \text{if } h_\ell^{\text{sat}} < h < h_g^{\text{sat}}\\
1 & \text{if } h \ge h_g^{\text{sat}}
\end{cases}
$$

- Diffusion:

$$
\omega \partial_y T =
\begin{cases}
\lambda_\ell \partial_y h & \text{if } h \le h_\ell^{\text{sat}}\\
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\end{cases}
$$

- Since $\varrho_\varepsilon(h, \varphi^{\text{sat}}(h)) = \varrho(h)$ and $T_\varepsilon(h, \varphi^{\text{sat}}(h)) = T^{\text{sat}}$, formally 4-LMNC $\xrightarrow[\varepsilon \to 0]{}$ (3)-LMNC
- In the 4-LMNC model the phase is not identified by the value of $h_\varepsilon$ but $\varphi_\varepsilon$: we can have a mixture even if $h_\varepsilon > h_g^{\text{sat}}$.

# ③ Relaxation Approach

4-LMNC

$$\begin{cases}\partial_t \varrho_\varepsilon + \partial_y(\varrho_\varepsilon v_\varepsilon) = 0\\ \partial_t(\varrho_\varepsilon h_\varepsilon) + \partial_y(\varrho_\varepsilon h_\varepsilon v_\varepsilon) = \Phi + \partial_y(\omega_\varepsilon \partial_y T_\varepsilon)\\ \partial_t(\varrho_\varepsilon \varphi_\varepsilon) + \partial_y(\varrho_\varepsilon \varphi_\varepsilon v_\varepsilon) = \frac{1}{\varepsilon}\varrho_\varepsilon\left(\varphi^{sat}(h_\varepsilon) - \varphi_\varepsilon\right)\end{cases}$$

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- Since $\varrho_\varepsilon(h, \varphi^{sat}(h)) = \varrho(h)$ and $T_\varepsilon(h, \varphi^{sat}(h)) = T^{sat}$, formally 4-LMNC $\xrightarrow[\varepsilon \to 0]{}$ (3)-LMNC
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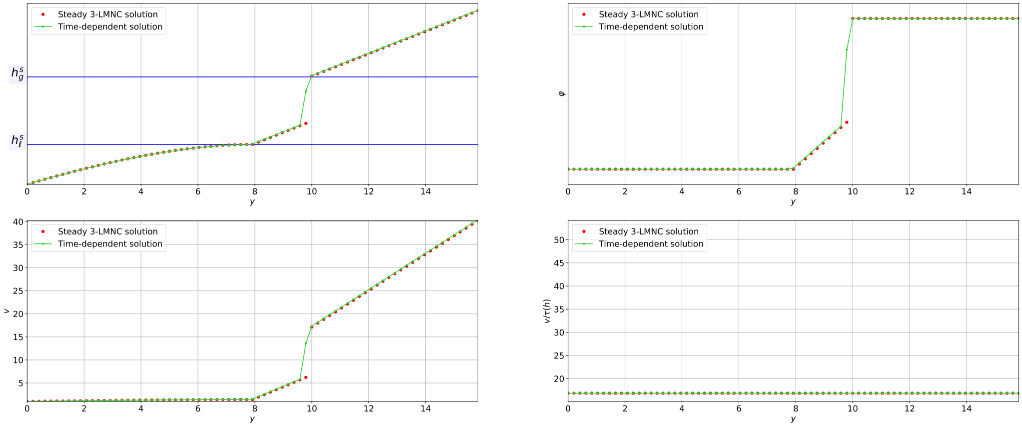
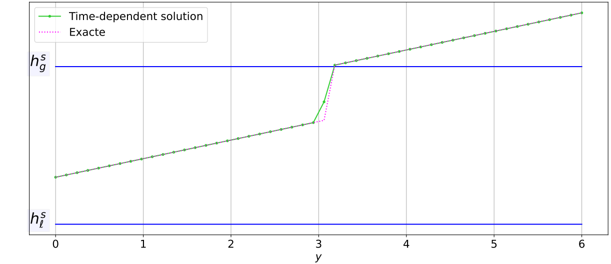
# ③ Relaxation Approach – $\varepsilon = 10^{-12}$

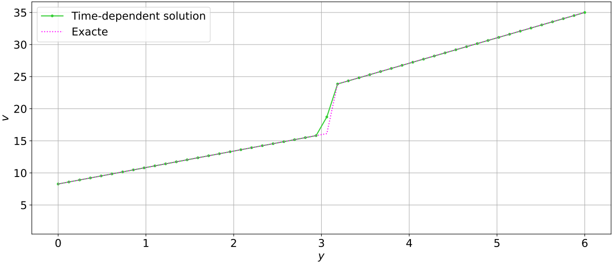


# ③ Relaxation Approach – Validation?

- Asymptotic behavior? ✔️
- Transient behavior?
  - Plausible? ✔️
  - Comparison with an exact solution (in a simplified case) ❓

    ⇝ focus on the exact transient solution in the form of a traveling wave as in Predictor-Corrector Approach



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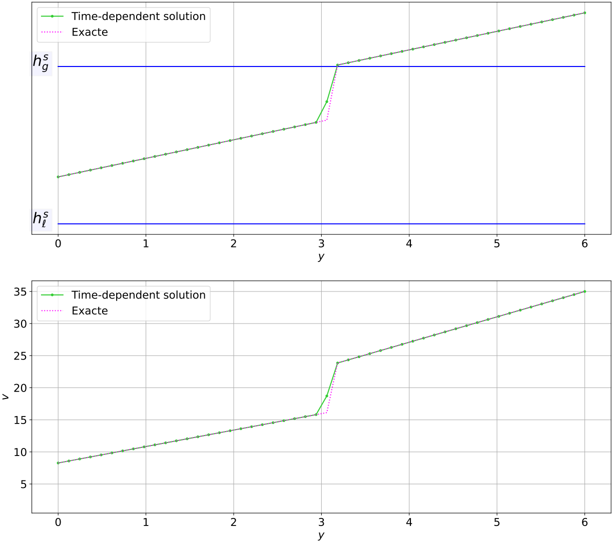

# 4. Full Model

# Concluding Remarks on the Full Model

1. Without diffusion or with non-degenerate diffusion: approaches as for Navier-Stokes equations

2. Degenerated diffusion poses challenges:

   - Jumps in $h$, $\varrho$, and $u$ necessitate schemes based on conservative formulation...
   - ...but the system is not a classic hyperbolic system of conservation laws (no explicit time-derivative $v$)

   - Explored three strategies with precise asymptotic behavior and satisfactory conservation properties, but...

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       conservation;
       the CFL condition and potential splitting errors
     - Regularization via relaxation:
       WB scheme based on a non-conservative formulation can be direct generalized in 3D
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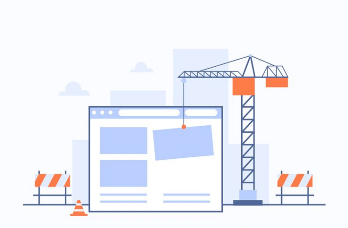

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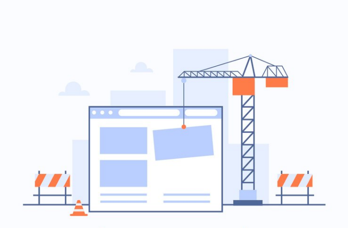

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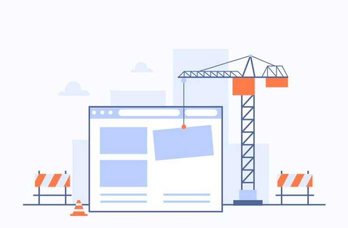

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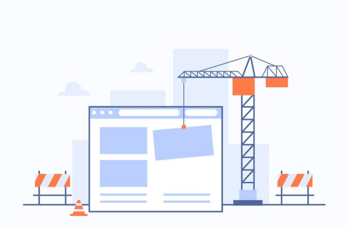

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# 5. Summary

1 The LMNC Model

- Diffusive interface framework: two pure phases + mixture
- Hyperbolic conservation laws:
  HEM (mixture at saturation with phase transition)
- Low Mach Hypothesis: $p(t,\mathbf{x}) = p_* + M^2\bar{p}(t,\mathbf{x})$ with $M \ll 1$

$\rightsquigarrow$ Low Mach Nuclear Core Model

- **Not a hyperbolic system**
- **Thermal diffusion vanishes in mixture**

2 Steady-state model

- Mixture zone always exists without thermal diffusion
- **Thermal diffusion in gas phase** reduces the mixture zone, potentially causing it to vanish
- Connection to the Stefan problem (sharp interface)

3 Simplified model (constant density)

- Robust numerical schemes for enthalpy jump
- Precise asymptotic and plausible transient behavior observed in simulations
- Validation through traveling wave solution

4 Full model

- Numerical approaches similar to NS with or without non-degenerate thermal diffusion
- Challenges with degenerate diffusion, requiring conservative formulation despite it not being a hyperbolic system
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IT'S THE END
THANK FOR YOUR ATTENTION

# Appendix

6. Dimensionless Transformation

7. How to compute the traveling wave

# 6. Dimensionless Transformation

# Dimensionless Transformation

- Define fixed reference values $h^r$ and $\varrho^r$. We choice $h^r = q_m$ and $\varrho^r = \zeta_m / h^r$.
- Introduce dimensionless variables: $\bar{h} = \frac{h}{h^r}$ and $\bar{\Phi} = \frac{\Phi}{h^r \varrho^r}$
- Define dimensionless functions: $\bar{\varrho}(\bar{h}) = \frac{1}{\varrho^r}\varrho(h(\bar{h})) = \frac{1}{\varrho^r}\varrho(h^r\bar{h})$ and $\bar{\lambda}(\bar{h}) = \frac{1}{\varrho^r}\lambda(h(\bar{h})) = \frac{1}{\varrho^r}\lambda(h^r\bar{h})$

This yields transformed equations:

- $\partial_t(\varrho(h)) + \partial_y(\varrho(h)v) = 0 \rightsquigarrow \partial_t(\varrho(h^r\bar{h})) + \partial_y(\varrho(h^r\bar{h})v) = 0 \rightsquigarrow$

$$\partial_t \bar{\varrho} + \partial_y(\bar{\varrho}v) = 0$$

- $\partial_t(\varrho(h)h) + \partial_y(\varrho(h)hv) = [\Phi + \partial_y(\lambda(h)\partial_y h)] \rightsquigarrow$
  $\partial_t(h^r\bar{h}\varrho(h^r\bar{h})) + \partial_y(h^r\bar{h}\varrho(h^r\bar{h})v) = \left[\Phi + \partial_y(\lambda(h^r\bar{h})\partial_y(h^r\bar{h}))\right] \rightsquigarrow$

$$\partial_t(\bar{\varrho}\bar{h}) + \partial_y(\bar{\varrho}\bar{h}v) = \bar{\Phi} + \partial_y\left(\bar{\lambda}(\bar{h})\partial_y\bar{h}\right)$$

# 7. How to compute the traveling wave

# How to compute the traveling wave – I

Consider only mixture/gas transition $(h_e(t) > h_\ell^{sat})$

- The EoS is

$$\tau(h) = \frac{1}{\varrho}(h) = \begin{cases} \dfrac{h - q_g}{\zeta_g} & \text{if } h > h_g^{sat} \\ \dfrac{h - q_m}{\zeta_m} & \text{otherwise} \end{cases}$$

- Constants given: $\lambda_m = 0$, $\lambda_g > 0$, $q_m$, $q_g$, $\zeta_m$, $\zeta_g$, $h_g^{sat}$
- Constants chosen:
  - $c$ as the speed of the traveling wave
  - $y_g^{sat}(0)$ as the initial jump position
  - $h_m^{sat} < h_g^{sat}$ as the bottom of jump
- Jump position displacement imposed: $y_g^{sat}(t) = y_g^{sat}(0) - ct$
- Constant jump amplitude: $[\![h]\!] = h_g^{sat} - h_m^{sat}$ for all $t$

# How to compute the traveling wave – II

We seek a solution in the form

Enthalpy

$$\boxed{h(t,y) = \begin{cases} p_g(y - y_0(t)) + h_g^{sat} & \text{if } y > y_0(t) \\ p_m(y - y_0(t)) + h_m^{sat} & \text{otherwise} \end{cases} \quad \leadsto \quad h_e(t) = -p_m y_0(t) + h_m^{sat}.}$$

Velocity (as a function of the enthalpy!)

$$\boxed{v(h) = \begin{cases} a_g(h - h_g^{sat}) + v_g^{sat} & \text{if } h > h_s^{sat} \\ a_m(h - h_m^{sat}) + v_m^{sat} & \text{otherwise} \end{cases} \quad \leadsto \quad v_e(t) = v(h_e(t)).}$$

- We denoted
  - $\star_g^{sat} = \star(h_g^{sat,+})$ as the value of $\star$ at the top of jumps
  - $\star_m^{sat} = \star(h_g^{sat,-}) = \star_g^{sat} - [\![\star]\!]$ as the value of $\star$ at the bottom of jumps
- Initialization: we define $h_0(y) = h(t = 0, y)$ and $v_0(y) = v(h_0(y))$
- Constants to be determined: $p_k$, $a_k$, $v_k^{sat}$

# How to compute the traveling wave – In Each Region

In each region, the functions are regular, and we can expand the partial derivatives:

$$\begin{cases} \partial_t \varrho + \partial_y(\varrho v) = 0 \\ \partial_t(\varrho h) + \partial_y(\varrho h v) = [\Phi + \partial_y(\lambda_k \partial_y h)] \end{cases} \iff \begin{cases} \partial_t \tau + v\partial_y \tau = \tau \partial_y v \\ \partial_t h + v\partial_y h = \tau\,[\Phi + \partial_y(\lambda_k \partial_y h)] \end{cases}$$

$$\iff \begin{cases} \tau'(h)\,[\Phi + \partial_y(A_k \partial_y h)] = \partial_y v \\ \partial_t h + v\partial_y h = \tau\,[\Phi + \partial_y(\lambda_k \partial_y h)] \end{cases}$$

In each phase, $h$ is affine, so the diffusion term is zero:

$$\begin{cases} \partial_y v = \Phi \tau'(h) \\ \partial_t h + v\partial_y h = \Phi \tau(h) \end{cases}$$

# How to compute the traveling wave – Traveling Wave

We seek a solution of the form $h(t,y) = h_0(y-ct)$ and $v(t,y) = v_0(y-ct)$.
The first equation $\partial_y v = \Phi\tau'(h)$ gives

$$a_k p_k = \Phi \frac{1}{\zeta_k}$$

As $\partial_t h = -c\partial_y h$, the second equation gives

$$(a_k(h - h_k^{\mathrm{sat}}) + v_k^{\mathrm{sat}} - c)p_k = \Phi \frac{h - q_k}{\zeta_k}$$

We express the velocity parameters $a_k$ and $v_k^{\mathrm{sat}}$ in terms of the enthalpy parameters

$$\begin{cases} a_k = \dfrac{\Phi}{p_k \zeta_k} \\ v_k^{\mathrm{sat}} = c + \dfrac{\Phi}{p_k} \dfrac{(h_k^{\mathrm{sat}} - q_k)}{\zeta_k} = c + \Phi \dfrac{\tau_k^{\mathrm{sat}}}{p_k} \end{cases}$$

and we still need to fix the $p_k$.

# How to compute the traveling wave – Jump relations

$$\begin{cases} -c[\![\varrho]\!] + [\![\varrho v]\!] = 0 \\ -c[\![\varrho h]\!] + [\![\varrho v h]\!] = p_g A_g \end{cases}$$

The first jump relation becomes

$$(v_g^{sat} - c)\varrho_g^{sat} = (v_m^{sat} - c)\varrho_m^{sat}$$

and using the expression $v_k^{sat} = c + \frac{\Phi}{p_k \varrho_k^{sat}}$,

$$\frac{1}{p_g} = \frac{1}{p_m} \quad \Rightarrow \quad p_m = p_g$$

The second relation gives

$$(v_g^{sat} - c)\varrho_g^{sat} h_g^{sat} - (v_m^{sat} - c)\varrho_m^{sat} h_m^{sat} = p_g A_g$$

and using the expression $v_k^{sat} = c + \frac{\Phi}{p_k \varrho_k^{sat}}$ and the equality of slopes $p_m = p_g$,

$$p_g = p_m = \sqrt{\frac{(h_g^{sat} - h_m^{sat})\Phi}{A_g}}$$

# How to compute the traveling wave – Conclusion

Let's define $\eta \stackrel{\text{def}}{=} \sqrt{\frac{h_g^{sat} - h_m^{sat}}{\lambda_g / \Phi}}$.

If $h_e(t) = h_m^{sat} - \eta y_g^{sat}(t)$ and $v_e(t) = v(h_e(t))$, the solution is given by

$$h(t,y) = \begin{cases} h_m^{sat} + \eta(y - y_g^{sat}(t)) & \text{if } y < y_g^{sat}(t) \\ h_g^{sat} + \eta(y - y_g^{sat}(t)) & \text{if } y > y_g^{sat}(t) \end{cases}$$

$$v(h) = \begin{cases} c + \dfrac{\Phi}{\eta \varrho(h_m^s)} + \dfrac{\Phi}{\eta \zeta_m}(h - h_m^{sat}(t)) & \text{if } h < h_m^{sat}(t) \\ c + \dfrac{\Phi}{\eta \varrho(h_g^s)} + \dfrac{\Phi}{\eta \zeta_g}(h - h_g^{sat}(t)) & \text{if } h > h_g^{sat}(t) \end{cases}$$