Workshop on PDEs and Control 2025 (PKM-60)-Celebrating the 60th birthday of Kisko and Manolo

Non-residual-based stabilization formulation for liquid-solid phase-change flows including macrosegregation scenarios

Roberto Cabrales
Depto. de Matemática
U. de Tarapacá, Chile.
rccabrales@academicos.uta.cl

Ernesto Castillo
Depto. de Ing. Mecánica
U. de Santiago de Chile, Chile
ernesto.castillode@usach.cl

Ramón Codina
Depto. Ing. Civil y Ambiental
U. Politècnica de Catalunya, Spain
ramon.codina@upc.edu

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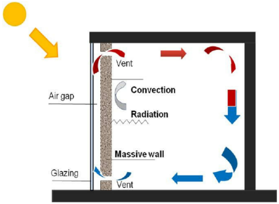
Plan

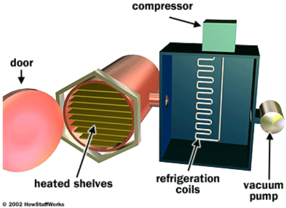
- Motivation.
- Mathematical model.
- Variational and Galerkin formulation.
- VMS approximation.
- Numerical results.
- Conclusions.
- Future work.

Route 5, far, far north of Chile



House climatization

Water freezing.



Food freezing/drying.

Alloy solidification.

Macrosegregation refers to the **nonuniform distribution** of alloying elements on a macroscopic scale, **usually occurring during a solidification process**

Causes

- Solute rejection during solidification.
- Convection effects.
- Solidification shrinkage or sedimentation.

Consequences

- Poor mechanical properties (e.g., weakness, brittleness).
- Inhomogeneous microstructure.
- Defects in critical applications.

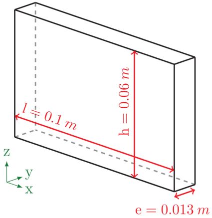
Numerical difficulties:

1. Multi-physical problem.
2. Highly Coupled.
3. Dynamic and non-linear.
4. Conductive and convective heat transfer.
5. Two-phase problem.

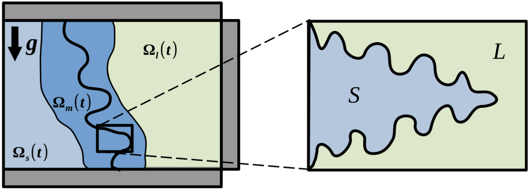
Liquid alloy of Pb-48 %Sn initially homogeneus, motionless and uniform temperature in a mould.

On $x = 0$ we decrease the temperature with null heat flux on the others sides.

The velocity and mass flux are zero on all sides.



Domain of the experiment.



Schematic of solidification for a time $t > 0$.

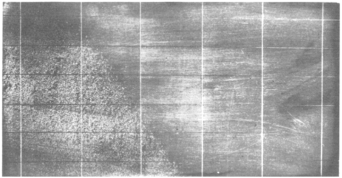


Photo in the Hebditch and Hunt paper.

[1] D.J. Hebditch & J.D. Hunt, *Observations of ingot macrosegregation on model systems*. Metallurgical Transactions 5. 1974.

Let $\Omega \subset \mathbb{R}^d$, $d = 2, 3$ a domain with boundary $\partial\Omega$. The regularized coupled system of PDEs in $\Omega \times (0, t_f)$ for the velocity $\boldsymbol{u}$, pressure p, temperature T, and concentration c considering the Carman-Kozeny model and the Boussinesq approximation, is

$$
\begin{aligned}
\rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho(\boldsymbol{u} \cdot \nabla)\boldsymbol{u} - \nabla \cdot (2\mu \nabla^s \boldsymbol{u}) + \nabla p + \mathcal{K}_\varepsilon(f_s)\boldsymbol{u} &= \rho \boldsymbol{g} \left(1 - \beta_T(T - T_r) - \beta_c(c_l - c_r)\right), \\
\mathcal{K}_\varepsilon(f_s, \boldsymbol{u}) &= \frac{C_0 \mu}{\lambda^2} \cdot \frac{f_s^2}{[(1 - f_s)^3 + \varepsilon]}, \\
\nabla \cdot \boldsymbol{u} &= 0, \\
\frac{\partial \mathcal{H}}{\partial t} + \rho C_p \boldsymbol{u} \cdot \nabla T - \kappa \Delta T &= 0, \\
\frac{\partial c}{\partial t} + \boldsymbol{u} \cdot \nabla c_l &= 0,
\end{aligned}
$$

with properly initial and boundary conditions. The enthalpy $\mathcal{H}$, solid fraction f_s, and concentration of liquid species c_l are determined as

$$
\begin{aligned}
\mathcal{H} &= \rho C_p T + (1 - f_s)\rho L. \\
f_s(c, T) &= \frac{a}{a + b}, \\
c_l &= \frac{c}{1 - (1 - r) f_s}.
\end{aligned}
$$

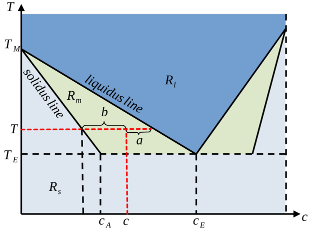


Figura 1: Phase diagram for a binary alloy.

Variational and Galerkin formulation

Let $\boldsymbol{\mathcal{V}} = H^1_0(\Omega)^d$, $\mathcal{Q} = L^2_0(\Omega)$, $\Theta = H^1_0(\Omega)$ and $\Psi = H^1(\Omega)$ the spaces for $\boldsymbol{u}$, p, T, and c.

The weak formulation consists of finding $\boldsymbol{U} = [\boldsymbol{u}, p, T, c] : (0, t_{\mathrm{f}}) \to \boldsymbol{\mathcal{X}} := \boldsymbol{\mathcal{V}} \times \mathcal{Q} \times \Theta \times \Psi$ such that

$$
\begin{aligned}
\left(\rho \frac{\partial \boldsymbol{u}}{\partial t}, \boldsymbol{v}\right) + \mathcal{B}([\boldsymbol{u}, p], [\boldsymbol{v}, q]) &= \langle \boldsymbol{f}, \boldsymbol{v} \rangle \,, \\
\rho C_p \left(\frac{\partial T}{\partial t}, \theta\right) + b(\boldsymbol{u}, T, \theta) &= \left\langle L \frac{\partial f_s}{\partial t}, \theta \right\rangle , \\
\left(\frac{\partial c}{\partial t}, \psi\right) + \langle \boldsymbol{u} \cdot \nabla c_l, \psi \rangle + \alpha \left(\nabla c_l, \nabla \psi\right) &= 0,
\end{aligned}
$$

for all $\boldsymbol{V} = [\boldsymbol{v}, q, \theta, \psi] \in \boldsymbol{\mathcal{X}}$, considering that $\boldsymbol{f} \in (H^{-1}(\Omega))^d$, and with

$$
\begin{aligned}
\mathcal{B}([\boldsymbol{u}, p], [\boldsymbol{v}, q]) &= \rho \langle \boldsymbol{u} \cdot \nabla \boldsymbol{u}, \boldsymbol{v} \rangle + (2\mu \nabla^s \boldsymbol{u}, \nabla^s \boldsymbol{v}) - (p, \nabla \cdot \boldsymbol{v}) + \langle \mathcal{K}_\varepsilon(f_s, \boldsymbol{u}), \boldsymbol{v} \rangle + (\nabla \cdot \boldsymbol{u}, q), \\
b(\boldsymbol{u}, T, \theta) &= \rho C_p \langle \boldsymbol{u} \cdot \nabla T, \theta \rangle + \kappa \left(\nabla T, \nabla \theta\right) .
\end{aligned}
$$

The Galerkin problem is obtained by approximating each variable by conforming finite elements $\boldsymbol{\mathcal{V}}_h \subset \boldsymbol{\mathcal{V}}$, $\mathcal{Q}_h \subset \mathcal{Q}$, $\Theta_h \subset \Theta$, and $\Psi_h \subset \Psi$.

The time discretization is performed using a q-order BDF scheme:

$$
\left.\frac{\partial \phi^n}{\partial t}\right|_{t^n} \approx \frac{1}{\delta t} \left(\gamma_q \phi^n - \sum_{s=1}^{q} \gamma_s \phi^{n-s} \right)
$$

The VMS approximation

VMS methods [2] decompose the space $\mathcal{X}$ into the direct sum of the finite element space $\mathcal{X}_h$ and the *sub-scale space* $\widetilde{\mathcal{X}}$:

$$\mathcal{X} = \mathcal{X}_h \oplus \widetilde{\mathcal{X}}$$

Then, for each $t \in (0, t_{\mathrm{f}})$ we can uniquely write

$$\boldsymbol{u} = \boldsymbol{u}_h + \tilde{\boldsymbol{u}} = \boldsymbol{u}_h + \tilde{\boldsymbol{u}}_1 + \tilde{\boldsymbol{u}}_2, \quad p = p_h + \tilde{p}, \quad T = T_h + \tilde{T} \text{ and } c = c_h + \tilde{c}.$$

The VMS method used is non-residual, orthogonal, dynamic-term-by-term, allowing:

1. the simulation of laminar and turbulent flows
2. the use of anisotropic space-time discretizations.
3. stability for highly convective flows,
4. the avoid the compatibility condition imposed by the inf-sup condition, and
5. the reduction of the non-linear iterations needed to converge to the solution.

The five subescales $\tilde{\boldsymbol{u}}_1$, $\tilde{\boldsymbol{u}}_2$, $\tilde{p}$, $\tilde{T}$ and $\tilde{c}$ are approximated in terms of the FEM variables $\boldsymbol{u}_h, p_h, T_h, c_h$ by dynamic equations.

[2] Codina, Badia, Baiges & Principe. Encyclopedia of Computational Mechanics, 2017

Let us define the stabilizing form

$$B_{\mathrm{VMS}}(\boldsymbol{u};[\boldsymbol{v},q],[\tilde{\boldsymbol{u}},\tilde{p}]) = \sum_K (\rho(\boldsymbol{u}\cdot\nabla)\boldsymbol{v},\tilde{\boldsymbol{u}}_1)_K + \sum_K (\nabla q,\tilde{\boldsymbol{u}}_2)_K + \sum_K (\nabla\cdot\boldsymbol{v},\tilde{p})_K,$$

The (non-linear) VMS stabilized formulation is

$$(\rho\partial_t\boldsymbol{u}_h,\boldsymbol{v}_h) + B(\boldsymbol{u}_h;[\boldsymbol{u}_h,p_h],[\boldsymbol{v}_h,q_h]) - B_{\mathrm{VMS}}(\boldsymbol{u}_h;[\boldsymbol{v}_h,q_h],[\tilde{\boldsymbol{u}},\tilde{p}]) = (\boldsymbol{f}_h,\boldsymbol{v}_h), \tag{1}$$

$$(\rho C_p\partial_t T_h,\theta_h) + b(\boldsymbol{u}_h;T_h,\theta_h) - \sum_K (\rho C_p\boldsymbol{u}_h\cdot\nabla\theta_h,\tilde{T})_K = \left\langle \rho L\partial_t f_{s,h},\theta\right\rangle, \tag{2}$$

$$(\partial_t c_h,\psi_h) + \langle \boldsymbol{u}_h\cdot\nabla c_l,\psi_h\rangle - \sum_K (\boldsymbol{u}_h\cdot\psi_h,\tilde{c}) = 0, \tag{3}$$

and the equations for the subescales $\tilde{\boldsymbol{u}}_1$, $\tilde{\boldsymbol{u}}_2$, $\tilde{p}$, $\tilde{T}$ and $\tilde{c}$ are

$$\rho\partial_t\tilde{\boldsymbol{u}}_1 + \tau_{\boldsymbol{u}}^{-1}\tilde{\boldsymbol{u}}_1 = -\boldsymbol{\mathcal{P}}_h^{\perp}\left[(\rho\boldsymbol{u}_h\cdot\nabla)\boldsymbol{u}_h\right], \quad \rho\partial_t\tilde{\boldsymbol{u}}_2 + \tau_{\boldsymbol{u}}^{-1}\tilde{\boldsymbol{u}}_2 = -\boldsymbol{\mathcal{P}}_h^{\perp}(\nabla p_h), \quad \tau_p^{-1}\tilde{p} = -\mathcal{P}_h^{\perp}\left(\nabla\cdot\boldsymbol{u}_h\right),$$

$$\rho C_p\partial_t\tilde{T} + \tau_T^{-1}\tilde{T} = -\mathcal{P}_h^{\perp}\left(\rho C_p\boldsymbol{u}_h\cdot\nabla T_h\right), \quad \partial_t\tilde{c} + \tau_c^{-1}\tilde{c} = -\mathcal{P}_h^{\perp}\left(\boldsymbol{u}_h\cdot\nabla c_h\right),$$

with $\mathcal{P}_h^{\perp}$ the L^2-ortogonal projection on the corresponding FE space and the stabilization parameters (ensuring dimensional consistency and optimal convergence rates) are

$$\tau_{\boldsymbol{u}}^{-1} = \frac{4k^4\mu}{|K|} + \frac{2k\rho|\boldsymbol{u}_h|}{h_2}, \quad \tau_p^{-1} = \frac{4k^4\tau_1}{|K|}, \quad \tau_T^{-1} = \frac{4k^4\kappa}{|K|} + \frac{2k\rho C_p|\boldsymbol{u}_h|}{h}, \quad \tau_c^{-1} = \frac{4k^4\alpha}{|K|} + \frac{2k|\boldsymbol{u}_h|}{h}.$$

Step 0. Define initial conditions.

Step 1. Compute the velocity $\boldsymbol{u}_h^{n_j}$ and pressure $p_h^{n_j}$.

Step 2. Compute the temperature $T_h^{n_j}$.

Step 3. Compute the concentration $c_h^{n_j}$.

Step 4. Calculate the solid fraction $f_{s,h}^{n_j}$.

Step 5. Compute the liquid concentration $c_{l,h}^{n_j}$.

Step 6. Check convergence.

al-go-rithm
(noun)

word used by programmers when they do not want to explain what they did

Steps 1 to 5 are solved iteratively to take into account non-linearities and coupling.

We present the following results:

Convergence tests

- Error in time.
- Error in space.

Pb-48 %Sn solidification

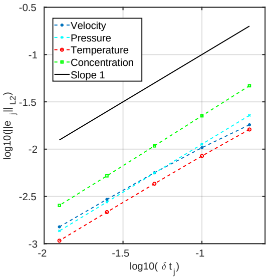
- Lateral freezing.
- Bottom freezing.

Domains, time interval, and expressions defining the functions for the time and space error convergence study.

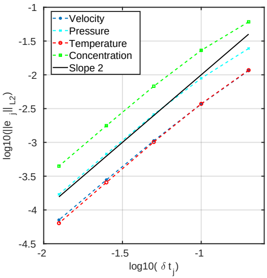
	Parameters for time-error		Parameters for space-error	
Domains	$\Omega = (-\frac{1}{2}, \frac{1}{2}) \times (-\frac{1}{2}, \frac{1}{2})$		$\Omega = (0,1) \times (0,1)$	
Time interval	$(0, t_{\mathrm{f}}) = (0, 0{,}01)$		$(0, t_{\mathrm{f}}) = (0, 0{,}2)$	
	$h(\boldsymbol{x})$	$g(t)$	$h(\boldsymbol{x})$	$g(t)$
$\boldsymbol{u} = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$	$\begin{bmatrix} -y \\ x \end{bmatrix}$	$\cos(\pi t)e^{-t}$	$\begin{bmatrix} 200x^2(x-1)^2y(y-1)(2y-1) \\ -200(x-1)(2x-1)y^2(y-1)^2x \end{bmatrix}$	$1-t$
p	$x+y$	1	$100(2x-1)(2y-1)$	1
T	$1+x-y$	$\cos(\pi t)e^{-t}$	$1-x+\sin(\pi x)\cos(\pi y)$	$1-t$
c	$1-x-y$	$\cos(2\pi t)e^{-t}$	$1-x-\sin(\pi x)\cos(\pi y)$	$1-2t$

Error in time

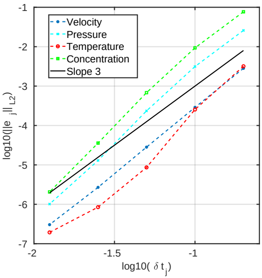
Errors for $t_{\mathrm{f}} = 0{,}2$ in L^2-norm of the velocity, pressure, temperature and concentration for each BDFq, $q = 1, 2, 3$ as a function of the time step. The mesh size is $h = \sqrt{2}/16$ and the time steps considered are $\delta t_j = 0{,}2 \times 2^{1-j}, j = 1, 2, 3, 4, 5$.



2.1 Errors for BDF1.



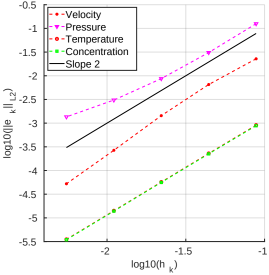
2.2 Errors for BDF2.



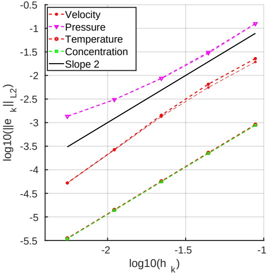
2.3 Errors for BDF3.

Error in space

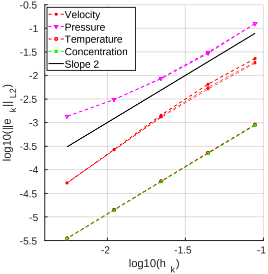
Errors for $t_{\mathrm{f}} = 0{,}01$ in L^2-norm for velocity, pressure, temperature and concentration using the time step $\delta t = 10^{-3}$ and the mesh sizes considered are $h_k = \sqrt{2} \times 2^{1-j}, j = 4, 5, 6, 7, 8$.



2.4 Errors for BDF1 with $\mathbb{P}_1$.



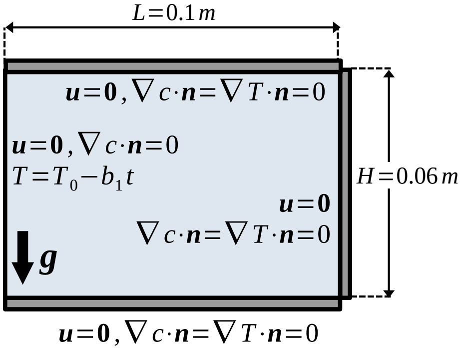
2.5 Errors for BDF2 with $\mathbb{P}_1$.



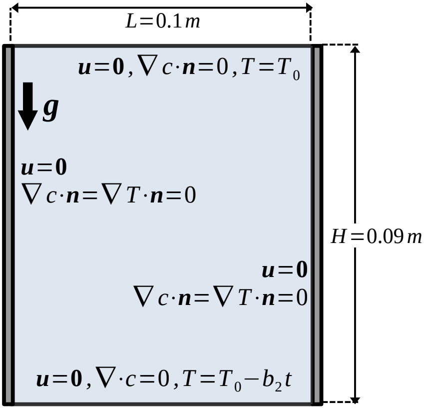
2.6 Errors for BDF3 with $\mathbb{P}_1$.

Two situations implemented in `FreeFem++` on a rectangular cavity with initial conditions

$$\boldsymbol{u} = \boldsymbol{0}, \quad T = 216^\circ C, \quad c = 48, \quad f_s = 0.$$



Lateral freezing (Hebditch-Hunt).



Bottom freezing.

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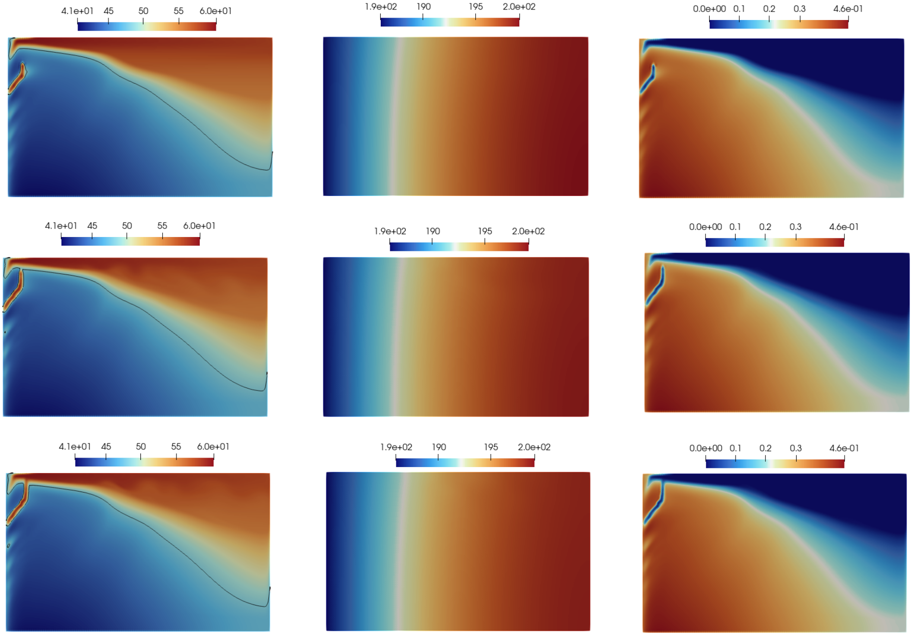

Concentration c, temperature T and solid fraction f_s for $t = 600$s obtained with BDF1, 2 and 3.

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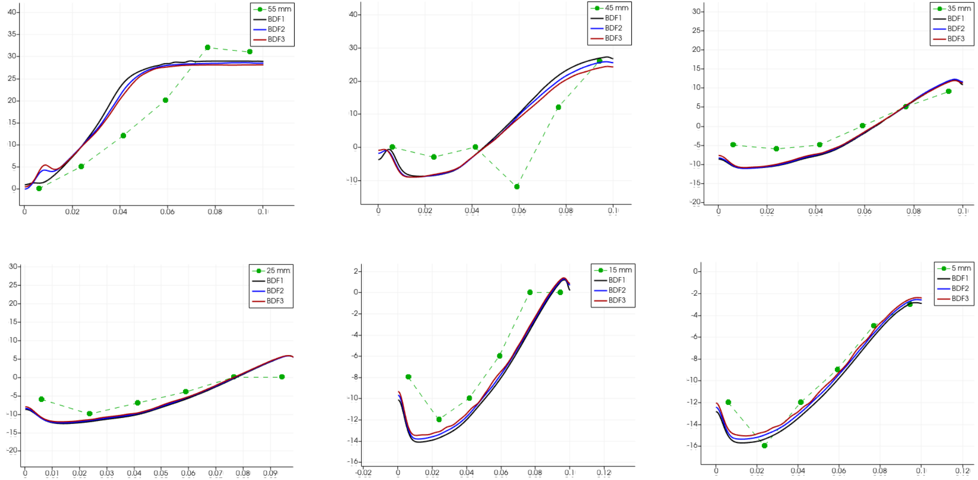
Comparison of concentration percent deviation after full solidification of Pb-48Sn alloy with experimental values reported by Hebditch and Hunt with numerical values obtained with BDF1, 2 and 3 mesh size $h = 5{,}8926 \times 10^{-4}$



Numerical results | Bottom freezing of Pb-48 %Sn solidification

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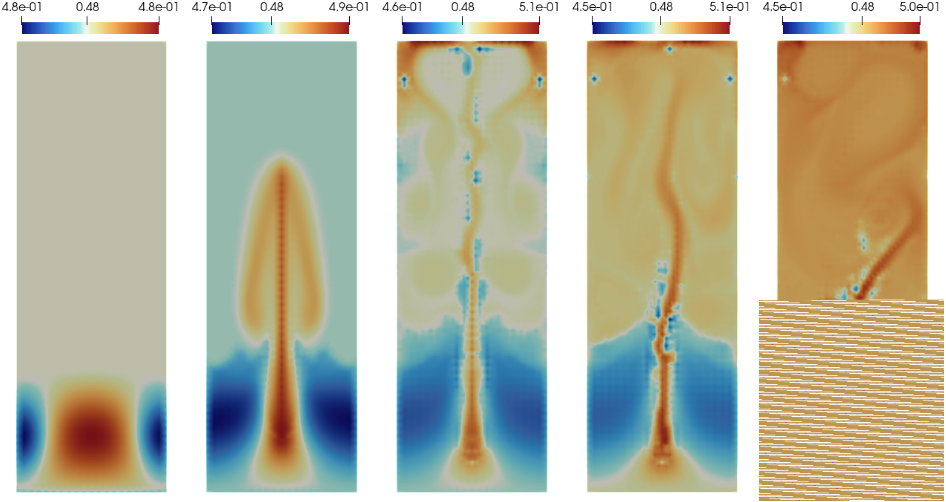

Concentration field obtained with BDF3 and $\mathbb{P}_1$ for $t = 15$s, $t = 22$s, $t = 29$s, $t = 33$s and $t = 36$s.

Drawings made by Gabriela Cabrales Lefimil.

Kisko & Manolo:

Feliz cumpleaños!
Muchas gracias por los grandes momentos!