



HAL
open science

Comparison of numerical approaches for the modeling of mass transfer across resolved interfaces

Nour Elhouda Djaballah, Stéphane Vincent, Eric Chénier, Benoît Trouette,
Can Selçuk

► To cite this version:

Nour Elhouda Djaballah, Stéphane Vincent, Eric Chénier, Benoît Trouette, Can Selçuk. Comparison of numerical approaches for the modeling of mass transfer across resolved interfaces. 22nd IACM Computational Fluids Conference, Apr 2023, Cannes, France. hal-04166378

HAL Id: hal-04166378

<https://hal.science/hal-04166378>

Submitted on 19 Jul 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Comparison of numerical approaches for the modeling of mass transfer across interfaces

N. E. DJABALLAH *

* Nour-el-houda.djaballah@univ-eiffel.fr

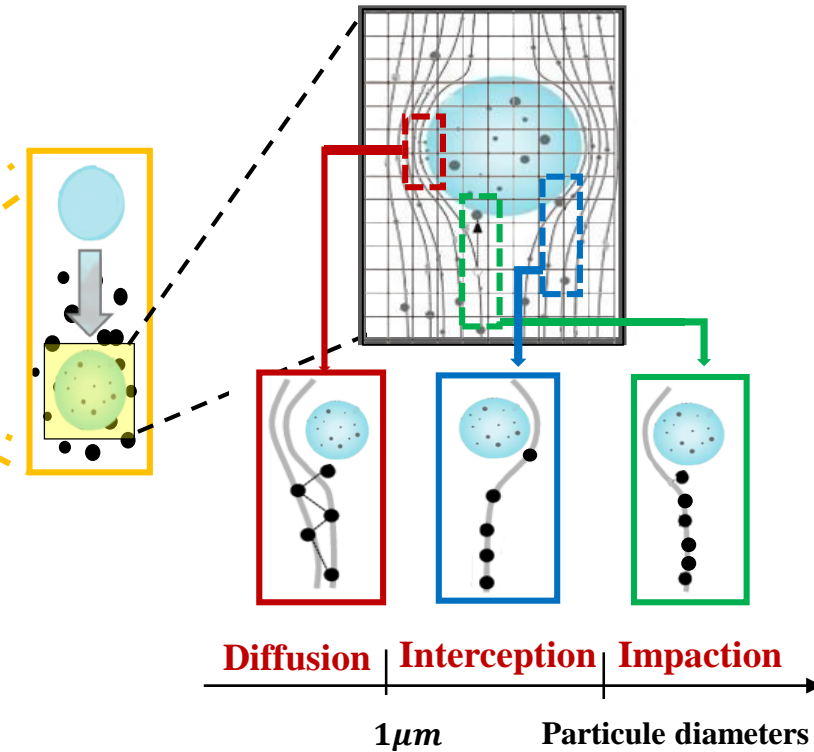
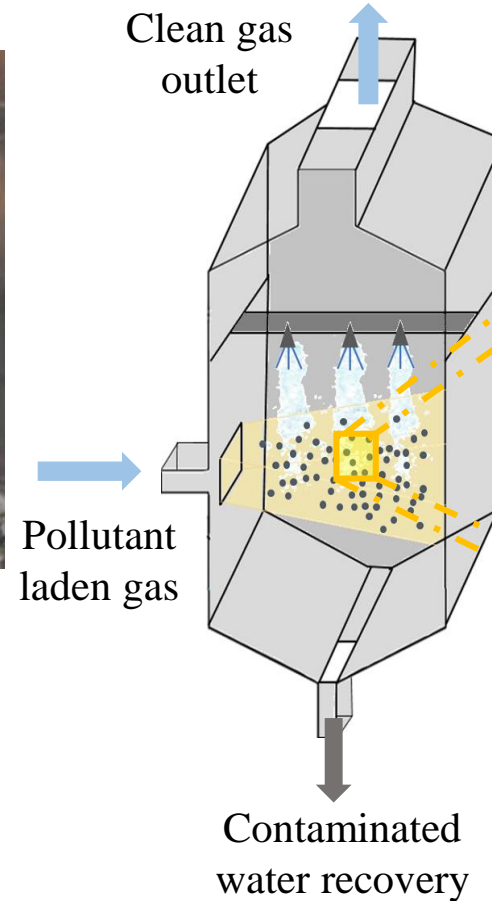
S. VINCENT, E. CHENIER, B. TROUETTE, C. SELCUK

**MSME laboratory
Gustave Eiffel University**

Introduction

- **Air washout:** use of spray droplets for the collect of air impurities.

Physical phenomena involved during captures



- **Objectives**

- ✓ Prevention
- ✓ Optimization of collection processes by developing numerical models

Outline

1. Presentation of three numerical methods for studying the diffusion mechanism across a resolved gas-liquid interface with discontinuities

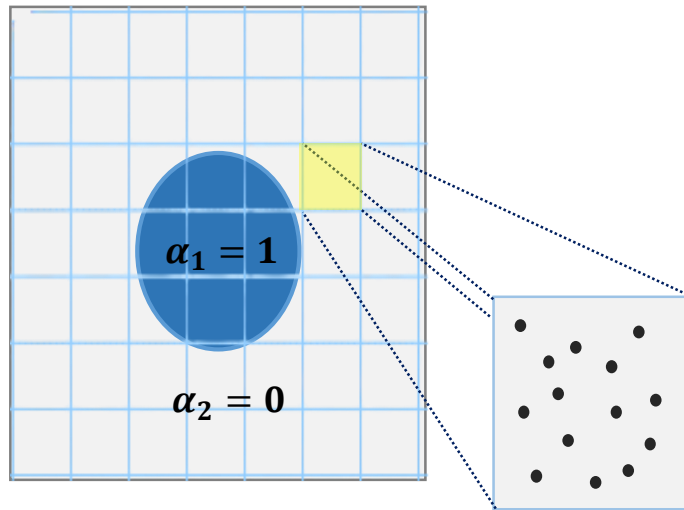
- Single field formulation involving a specific source-term
- Ghost-Fluid Method (GFM)
- Directional Cut-Cell method (D-CCM)

2. Comparison of the presented approaches on different static test cases

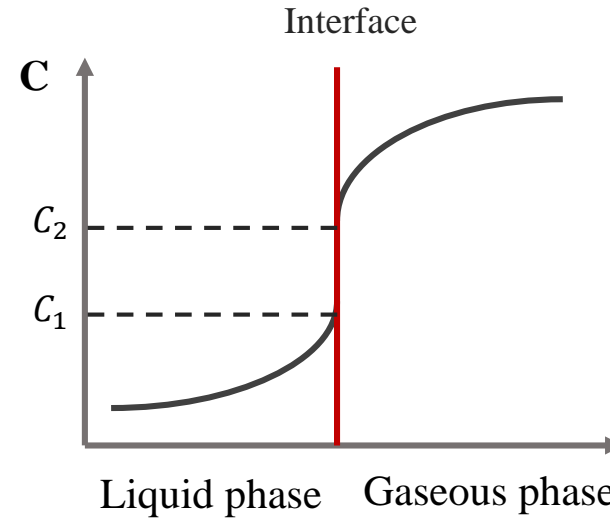
- One-dimensional steady diffusion
- Three-dimensional steady diffusion
- Three-dimensional unsteady diffusion

Modeling of the diffusion part

Jump conditions at the interface



- Gaseous phase
- Liquid phase
- Impurities



$$\frac{C_2}{C_1} = He$$

$$\beta_1 \nabla C_1 \Big|_I - \beta_2 \nabla C_2 \Big|_I = 0$$

Two-fluid approach

$$\frac{\partial C_k}{\partial t} = \nabla \cdot (\beta_k \nabla C_k)$$

$k \in [1,2] : (1)=\text{liquid}, (2)=\text{gas}$

Single-fluid approach

- Introducing the phase indicator function, χ_k
- Using the spatial volume averaging filter

$$\sum_{k=1}^2 \overline{\chi_k \frac{\partial C_k}{\partial t}} = \sum_{k=1}^2 \overline{\chi_k \nabla \cdot (\beta_k \nabla C_k)} \quad [1]$$

$$\frac{\partial C}{\partial t} = \nabla \cdot (\beta \nabla C - \phi) \quad [2]$$

Where

$$\phi = \frac{\beta(1 - He)C \nabla \alpha}{\alpha He + (1 - \alpha)}$$

$$\beta = \frac{\beta_1 \beta_2}{\beta_2(1 - \alpha) + \beta_1 \alpha}$$

[1] I. Kataoka. November 1985. Local instant formulation of two-phase flow

[2] Y. Haroun , D. Legendre, L. Raynal .January 2010. Volume of fluid method for interfacial reactive mass transfer: Application to stable liquid film.

1. Single-field formulation

One-fluid model

$$\frac{\partial C}{\partial t} = \nabla \cdot (\beta \nabla C - \phi)$$

Where $k \in [1,2] : (1)=\text{liquid}, (2)=\text{gas}$

$$\phi = \frac{\beta(1 - He)C \nabla \alpha}{\alpha He + (1 - \alpha)}$$

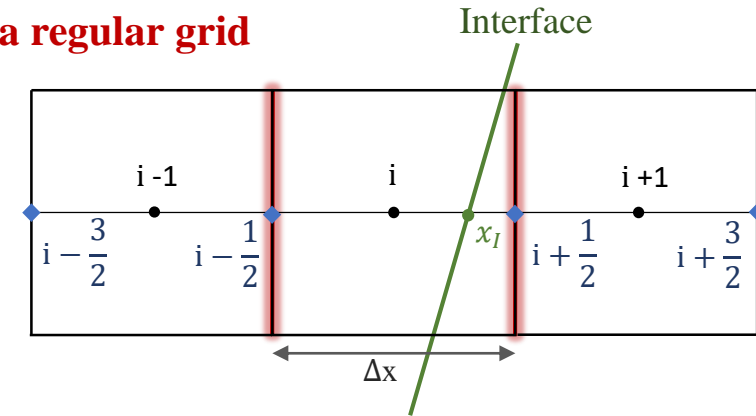
$$\beta = \frac{\beta_1 \beta_2}{\beta_2(1 - \alpha) + \beta_1 \alpha}$$

C , the filtered concentration
 β , the diffusion coefficient
 He , the jump constant.
 α , the volume fraction.

Numerical scheme

- Finite volume discretization on a regular grid

$$\sum_f \int_f (\beta \nabla C - \phi) \cdot \mathbf{n} = V \frac{\partial C}{\partial t}$$



- Flux on the face $i + \frac{1}{2}$

$$\int_{i+\frac{1}{2}} (\beta \nabla C - \phi) \cdot \mathbf{n} = \beta_{i+\frac{1}{2}} \left(\frac{C_{i+1} - C_i}{\Delta x} - \frac{1 - He}{\alpha_{i+\frac{1}{2}} + (1 - \alpha_{i+\frac{1}{2}})He} C_{i+\frac{1}{2}} \nabla \alpha_{i+\frac{1}{2}} \right)$$

Where

$$\alpha_{i+\frac{1}{2}} = \frac{\alpha_{i+1} + \alpha_i}{2} \quad C_{i+\frac{1}{2}} = \frac{C_{i+1} + C_i}{2} \quad \nabla \alpha_{i+\frac{1}{2}} = \frac{\alpha_{i+1} - \alpha_i}{\Delta x}$$

2. Ghost Fluid Method (GFM)

Two-fluid model

$$\frac{\partial C_k}{\partial t} = \nabla \cdot (\beta_k \nabla C_k)$$

Where $k \in [1,2]$: (1)=liquid, (2)= gas

➤ **1D per direction** $\frac{d}{dx} \left(\beta \frac{dc}{dx} \right) = \frac{\partial c}{\partial t}$

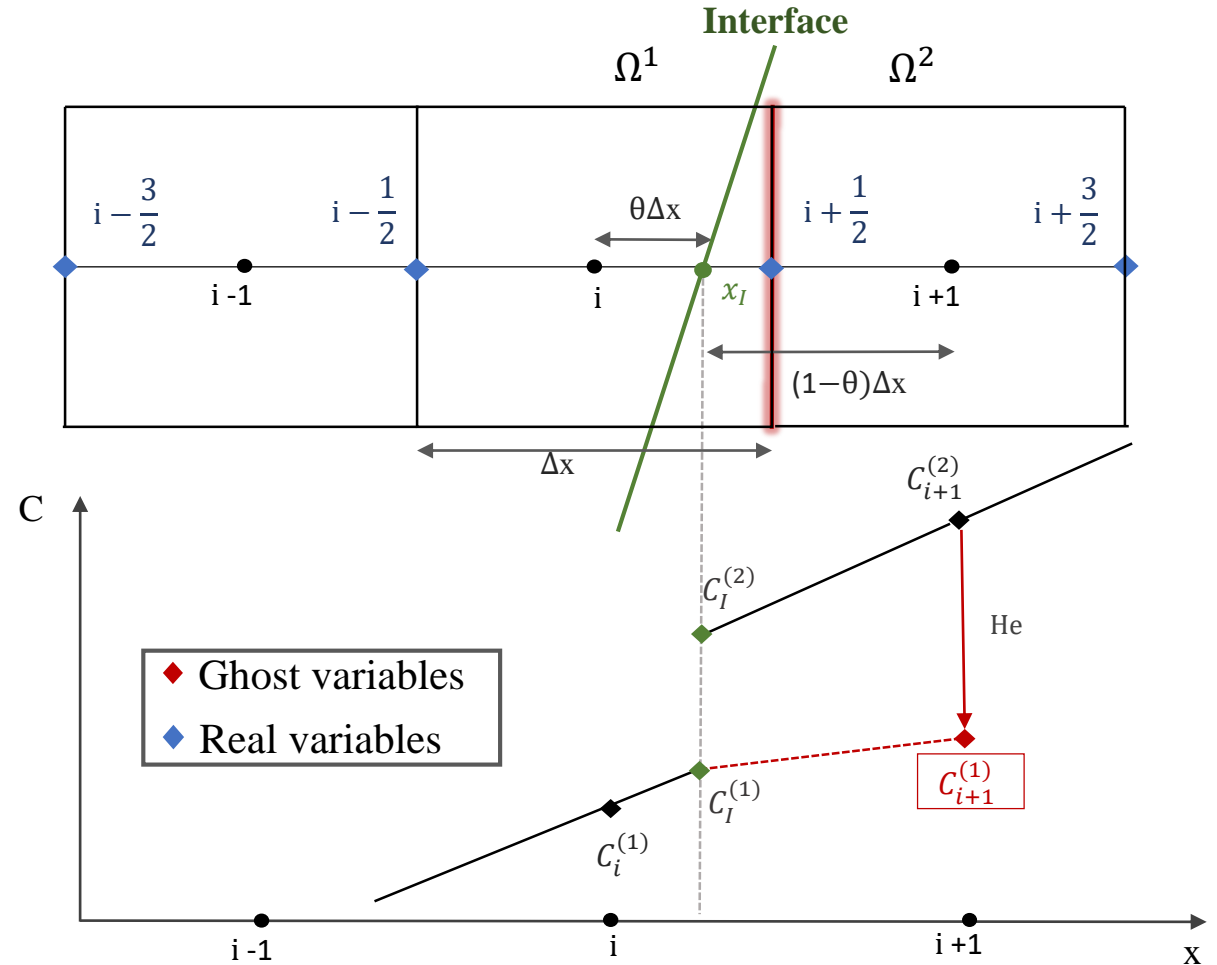
Numerical scheme

- Flux balance in the cell centred at i

$$\int_{x_{i-1/2}}^{x_{i+1/2}} \frac{d}{dx} \left(\beta \frac{dc}{dx} \right) dx = \hat{\beta} \frac{c_{i+1}^{(2)} - c_i^{(1)}}{\Delta x} - \beta_1 \frac{c_i^{(1)} - c_{i-1}^{(1)}}{\Delta x}$$

Where $\hat{\beta} = \frac{\beta_2 \beta_1}{\theta \beta_2 + (1 - \theta) \beta_1}$

Finite volume discretization on a regular grid



Principle of the ghost-fluid method [3]

3. Directional Cut–Cell Method (D-CCM)

Two-fluid model

$$\frac{\partial C_k}{\partial t} = \nabla \cdot (\beta_k \nabla C_k)$$

Where $k \in [1,2] : (1)=\text{liquid}, (2)=\text{gas}$

➤ **1D per direction** $\frac{d}{dx} \left(\beta \frac{dc}{dx} \right) = \frac{\partial c}{\partial t}$

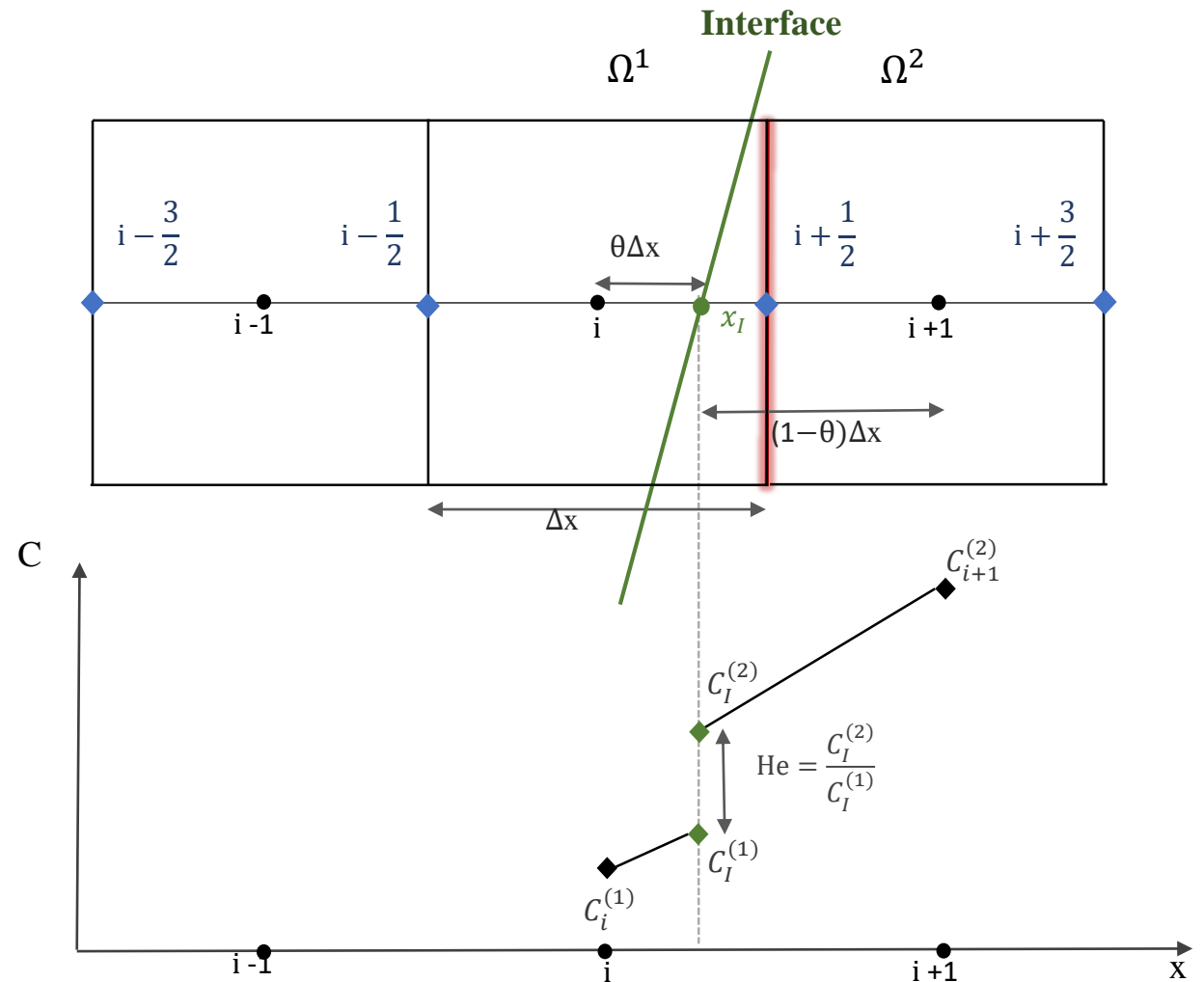
Numerical scheme

- Flux balance in the cell centred at i

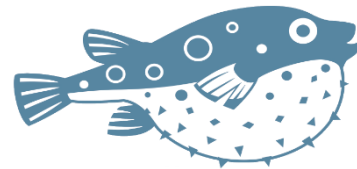
$$\int_{x_{i-1/2}}^{x_{i+1/2}} \frac{d}{dx} \left(\beta \frac{dc}{dx} \right) dx = \hat{\beta} \frac{c_{i+1}^{(2)} - c_i^{(1)}}{\Delta x} - \beta_1 \frac{c_i^{(1)} - c_{i-1}^{(1)}}{\Delta x}$$

Where $\hat{\beta} = \frac{He \beta_2 \beta_1}{He \times \theta \beta_2 + (1 - \theta) \beta_1}$

Finite volume discretization on a regular grid



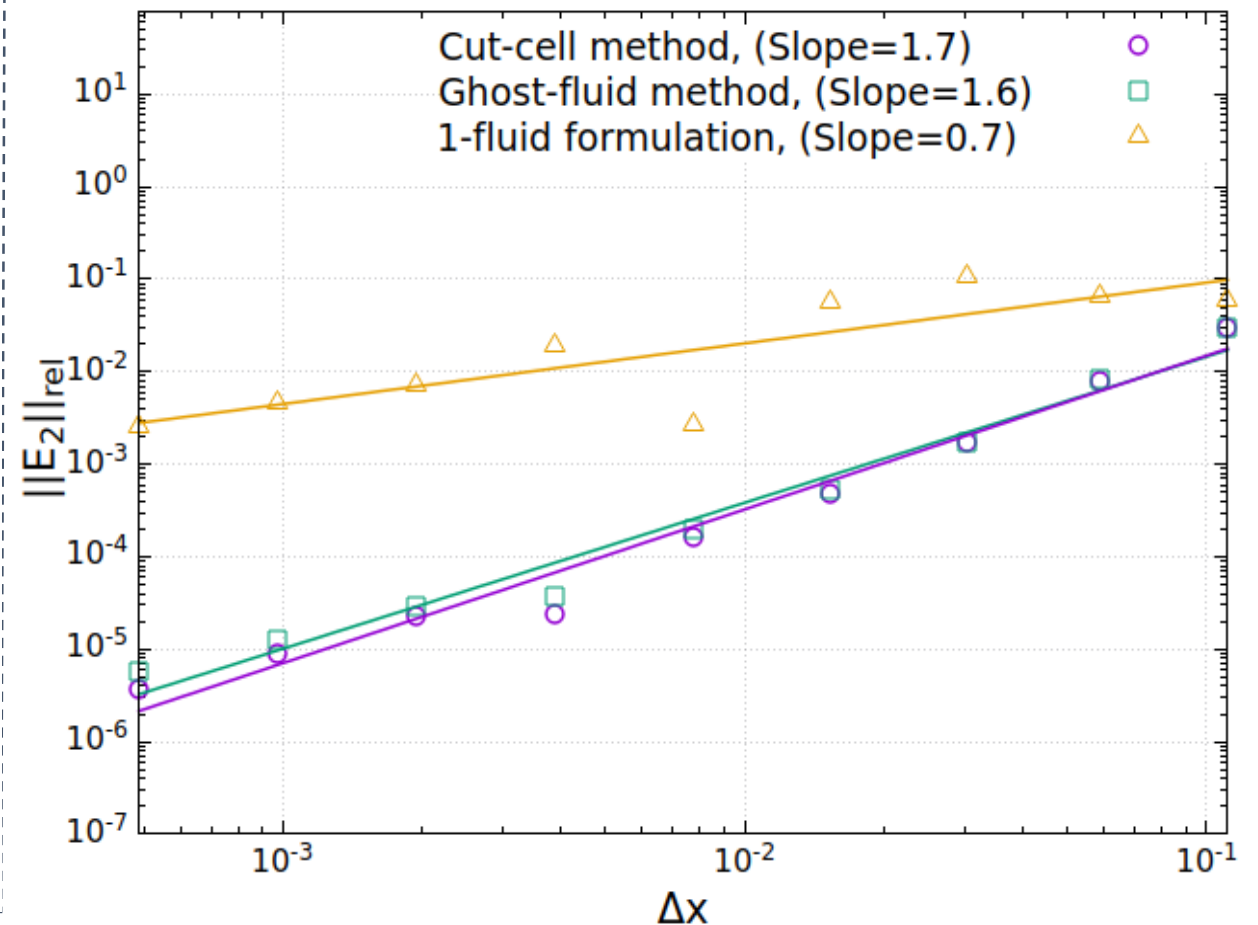
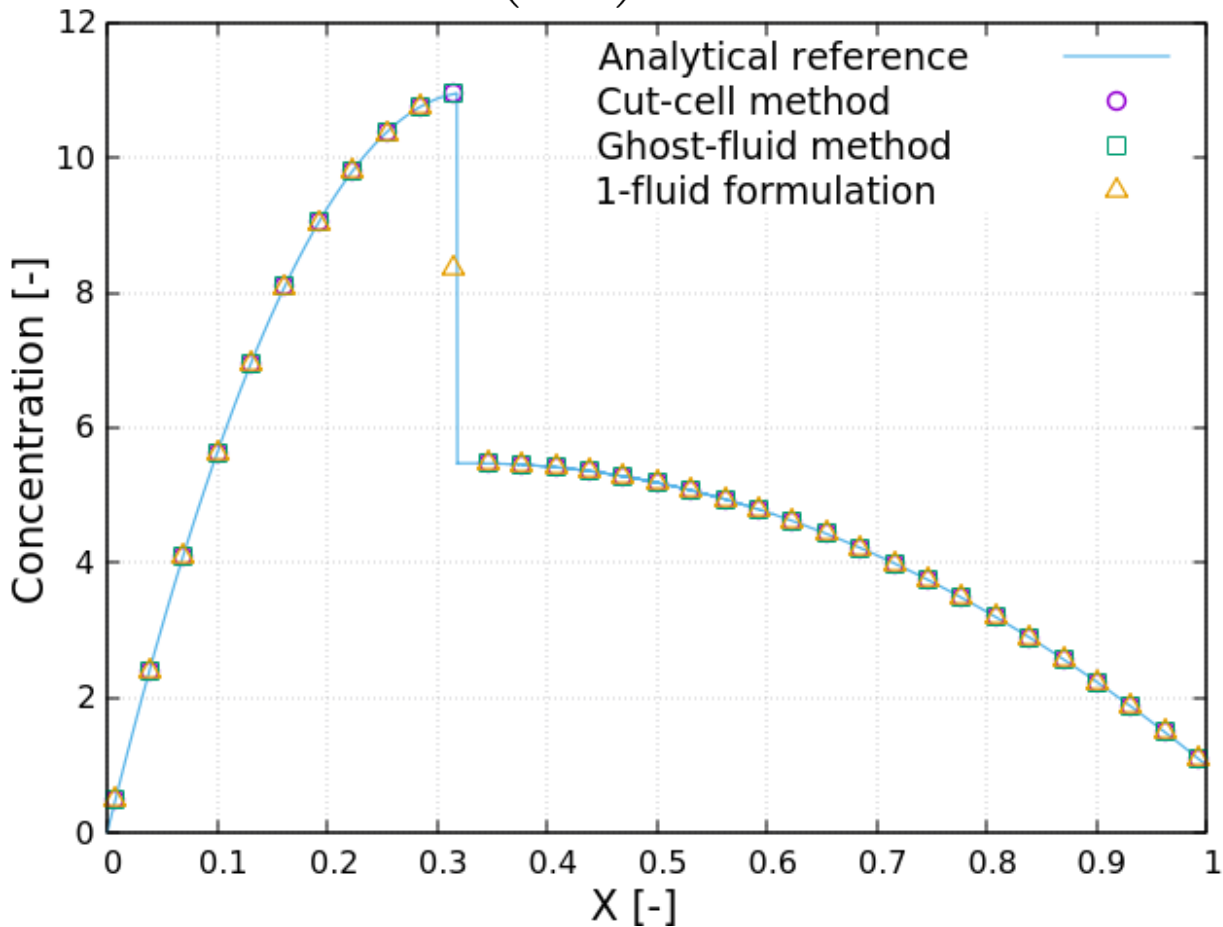
Results and discussion



Test cases: Steady 1D diffusion across a flat interface

Physical problem parameters: $He = C_1^1/C_1^2 = 0,5$; $\beta_2/\beta_1 = 10$; $\omega = 200$

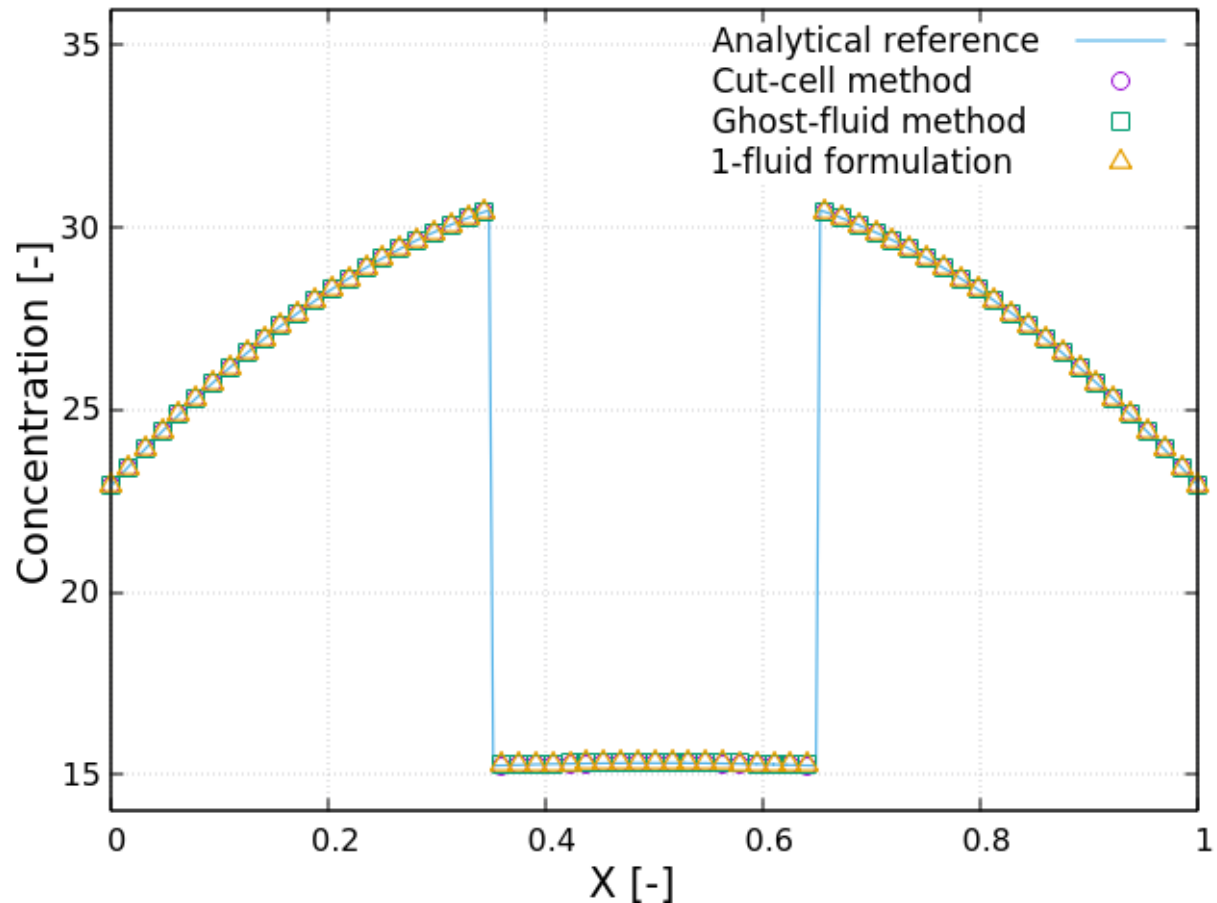
$$\frac{d}{dx} \left(\beta \frac{dc}{dx} \right) + \omega = 0$$



Test cases: Steady 3D diffusion across a spherical interface

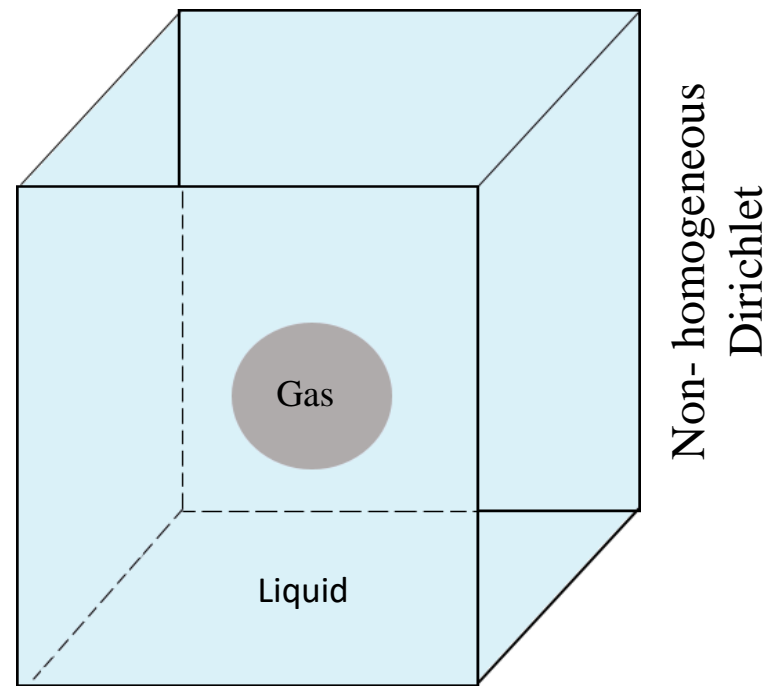
- Numerical model**

$$\frac{\partial}{\partial x} \left(\beta \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left(\beta \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left(\beta \frac{\partial c}{\partial z} \right) + \omega = 0$$



- Physical and geometrical parameters**

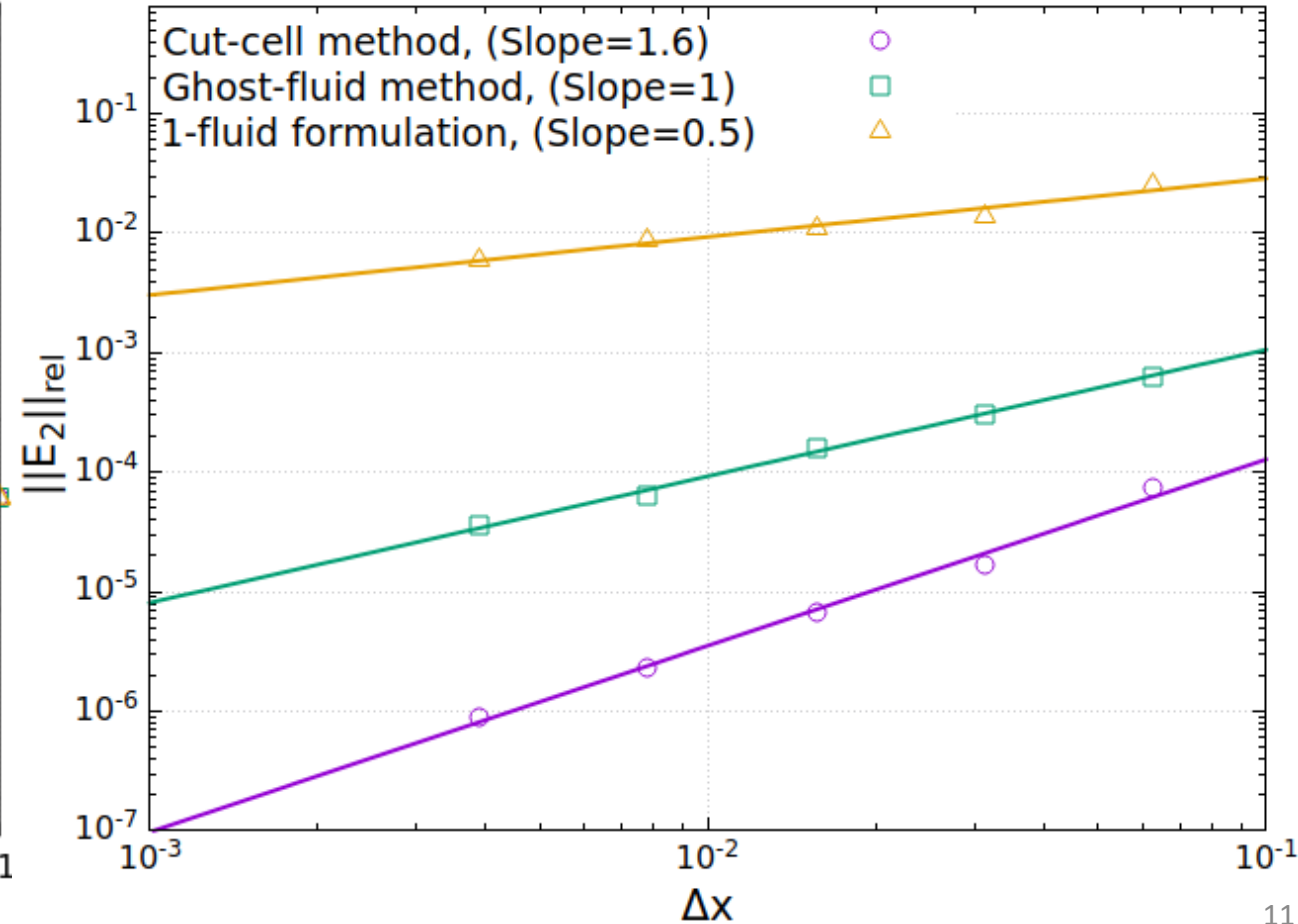
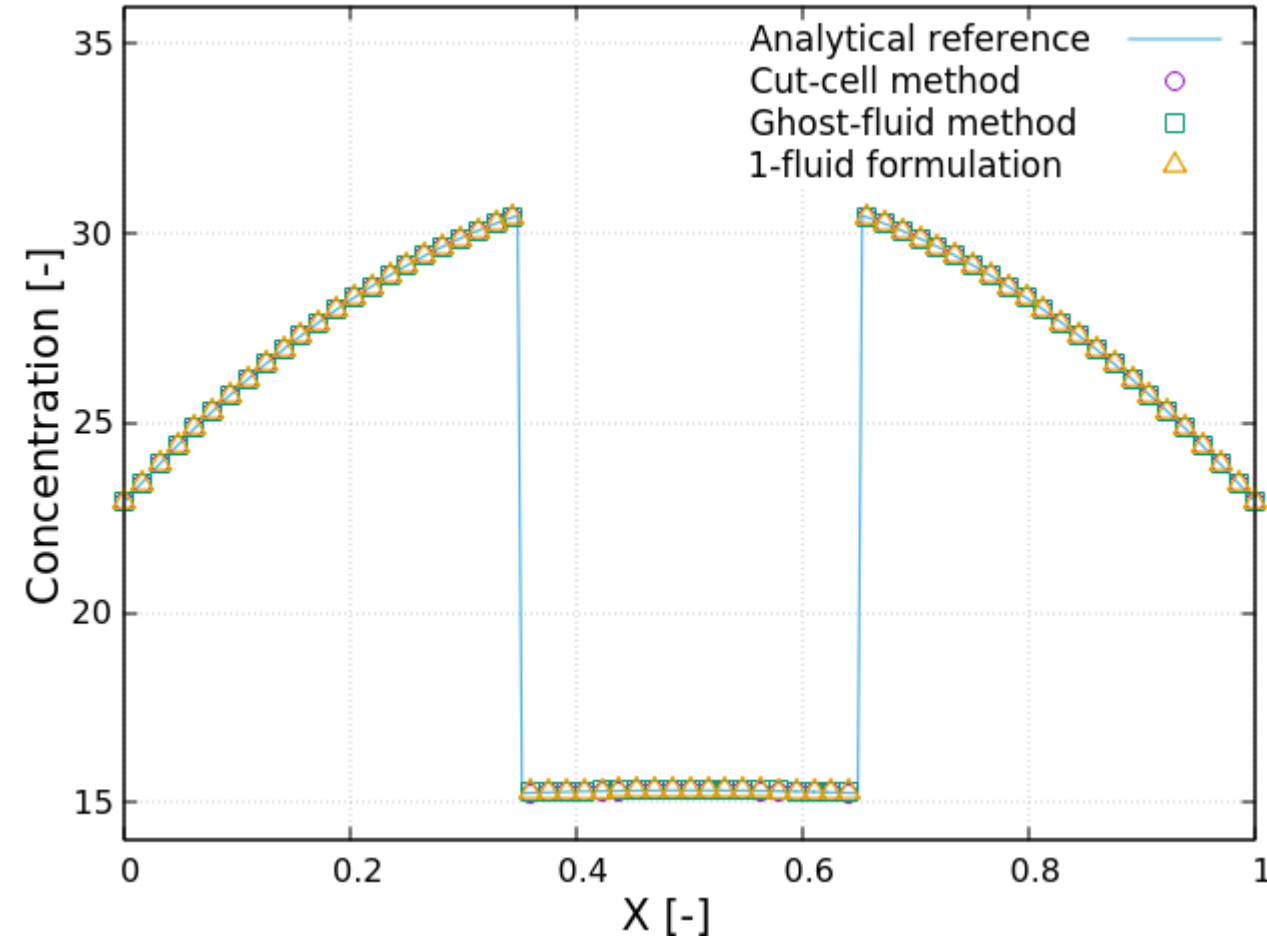
- ✓ $He = C_l^1/C_l^2 = 0,5$
- ✓ $\beta_2/\beta_1 = 10$
- ✓ $d_0/L = 0,3$
- ✓ $\omega = 200$
- ✓ BC : Non-homogeneous Dirichlet



Test cases: Steady 3D diffusion across a spherical interface

Spatial evolution of the numerical solution

Physical problem parameters: $He = 0,001$; $\beta_1/\beta_2 = 10$; $d_0/L = 0,3$; $\omega = 200$



Test cases: Unsteady 3D diffusion across a spherical interface

- Numerical model solved on 3D cartesian domain

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left(\beta \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left(\beta \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left(\beta \frac{\partial c}{\partial z} \right)$$

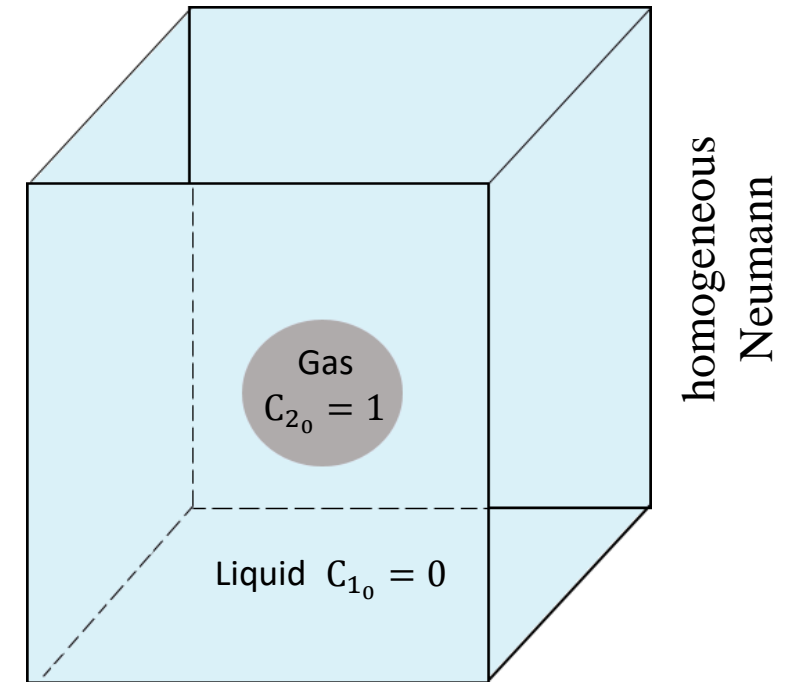
- Analytical reference (spherical symmetry solution [4])

$$C_2(t, r) = -\frac{2C_{2_0}}{\pi r} \int_0^\infty \frac{1}{x} \text{Im} \left(\frac{\sinh(\lambda_2(-x)r)}{\xi(-x)} \right) \exp(-xt) dx$$

$$C_1(t, r) = \frac{C_{2_0}}{\pi r} \int_0^\infty \frac{1}{x} \text{Im} \left(\frac{\xi(-x)}{\xi(-x)} \exp(-\lambda_1(-x)r) \right) \exp(-xt) dx$$

- Physical and geometrical parameters

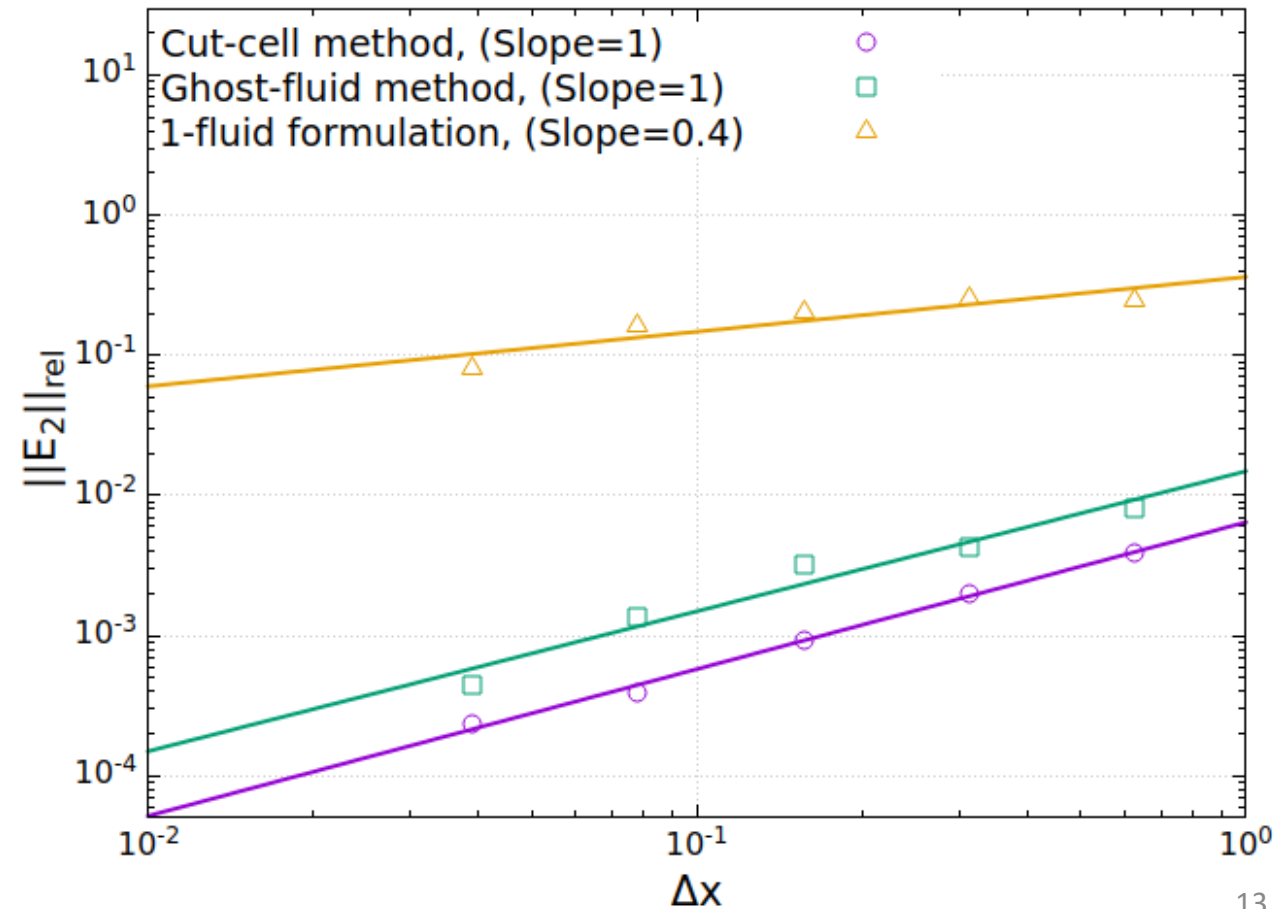
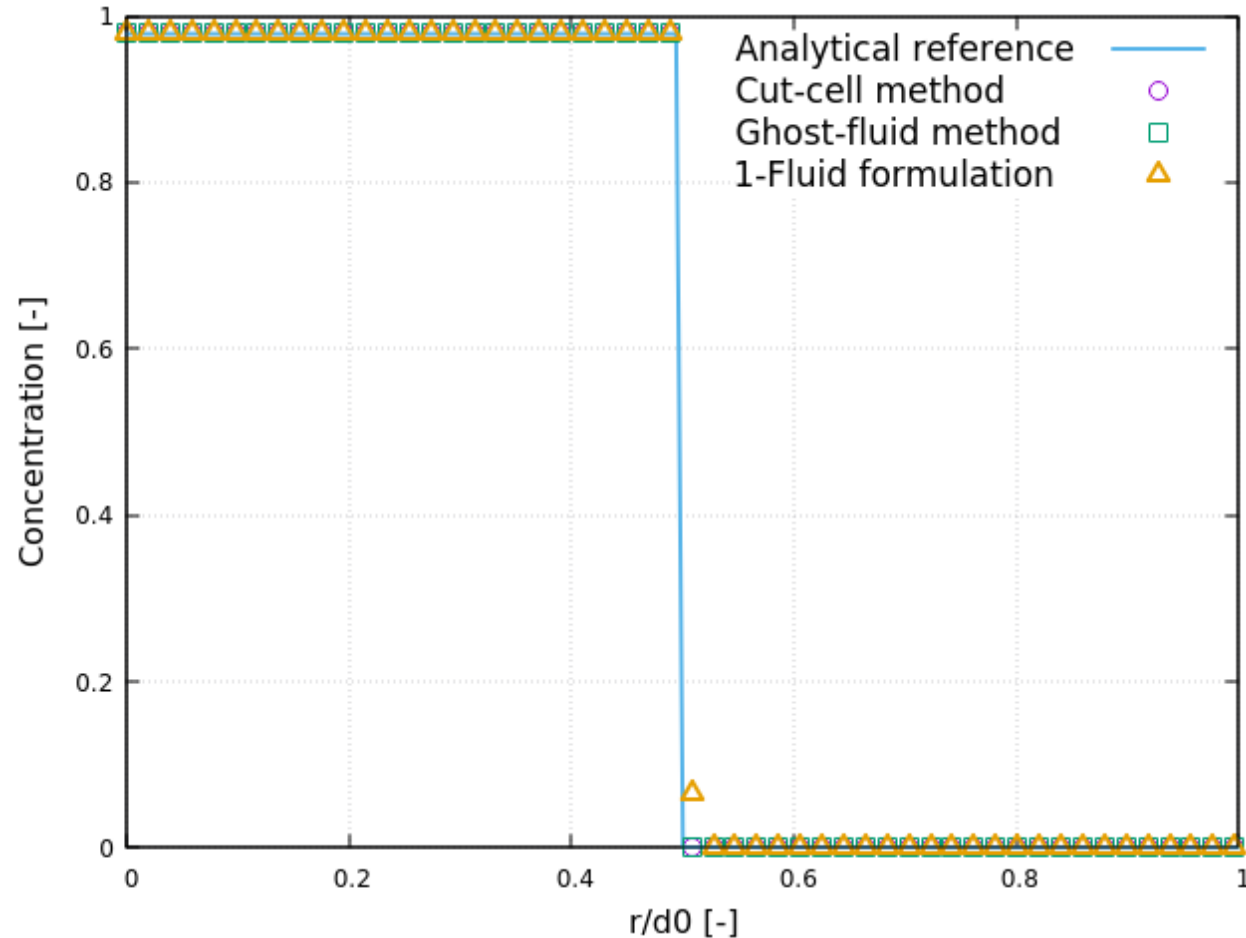
- ✓ $He = C_I^1 / C_I^2 = 10^{-3}$
- ✓ $\beta_2 / \beta_1 = 10$
- ✓ $d_0 / L = 0,2$
- ✓ BC : Homogeneous Neumann



Test cases: Unsteady 3D diffusion across a spherical interface

Spatial evolution at a fixed simulation time: at final non-dimensional time, $t^* \approx 1$

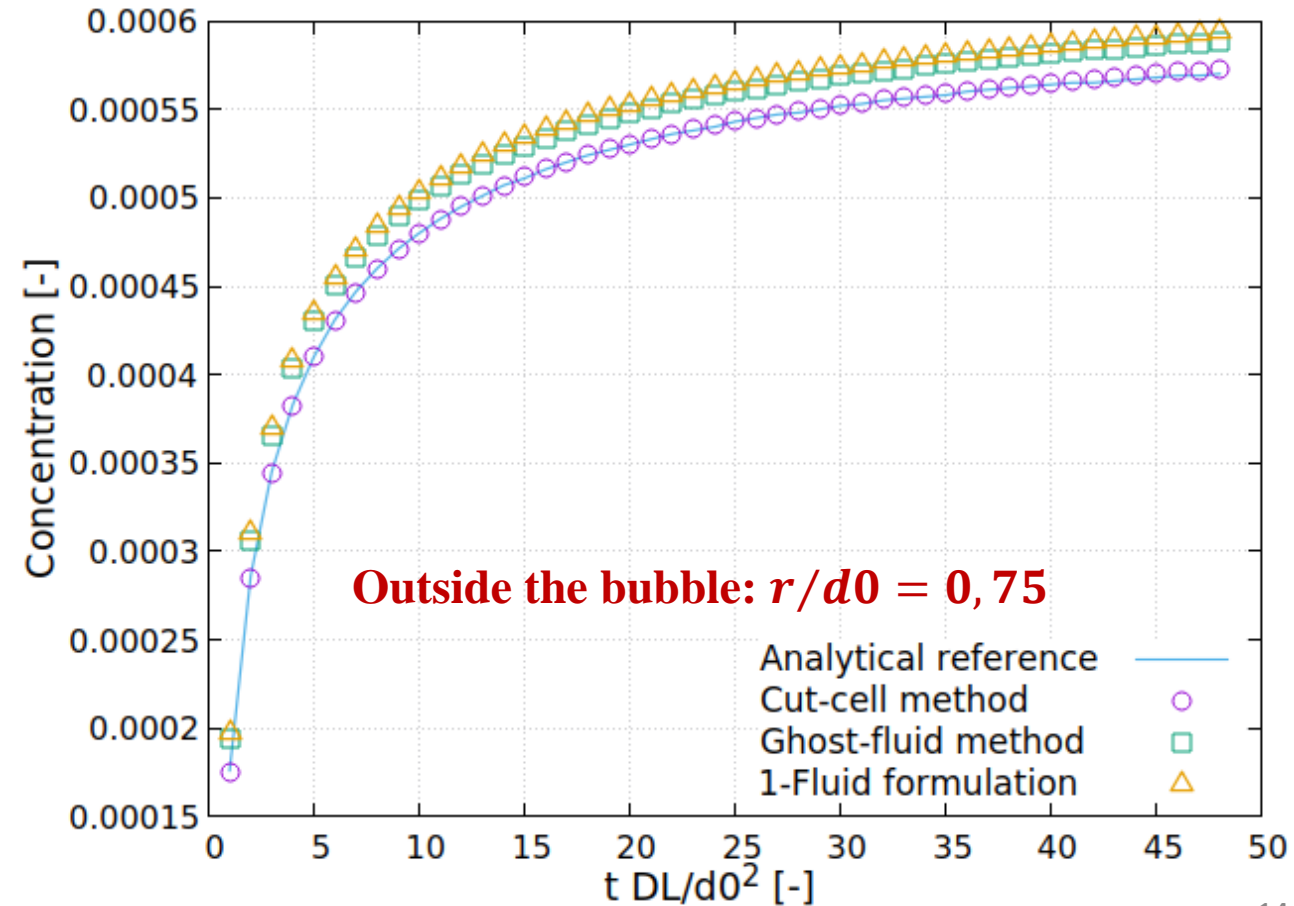
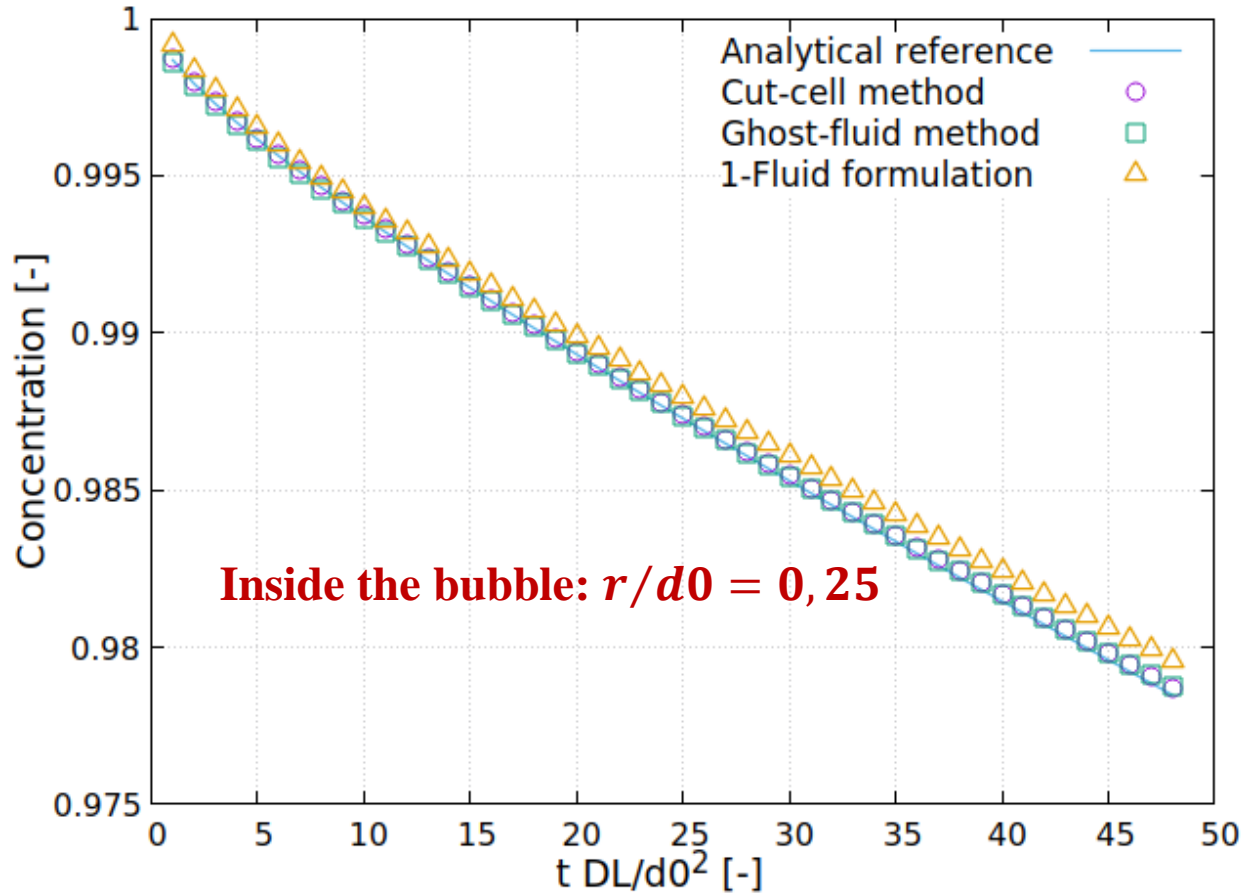
Physical problem parameters: $He = 0,001$; $\beta_1/\beta_2 = 10$; $d_0/L = 0,2$



Test cases: Unsteady 3D diffusion across a spherical interface

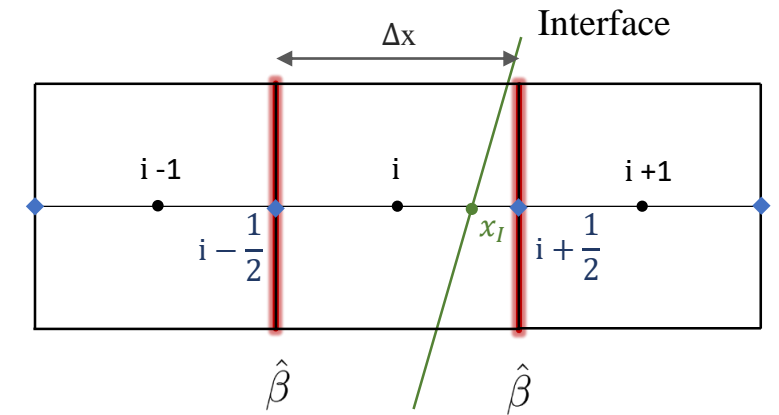
Temporal evolution at a two fixed positions

Physical problem parameters: $He = 0,001$; $\beta_1/\beta_2 = 10$; $d_0/L = 0,2$



Summary

Method	Discretisation on the cell centred at i	$\hat{\beta}$
Single-Field formulation	$\hat{\beta} \left(\frac{C_i - C_{i-1}}{\Delta x} - \frac{1 - He}{\alpha_{i-\frac{1}{2}} + (1 - \alpha_{i-\frac{1}{2}})He} C_{i-\frac{1}{2}} \nabla \alpha_{i-\frac{1}{2}} \right)$ $+ \hat{\beta} \left(\frac{C_{i+1} - C_i}{\Delta x} - \frac{1 - He}{\alpha_{i+\frac{1}{2}} + (1 - \alpha_{i+\frac{1}{2}})He} C_{i+\frac{1}{2}} \nabla \alpha_{i+\frac{1}{2}} \right)$	$\hat{\beta} = \frac{\beta_1 \beta_2}{\beta_2 (1 - \alpha) + \beta_1 \alpha}$
GFM	$\hat{\beta} \frac{c_{i+1}^{(2)} - c_i^{(1)}}{\Delta x} - \beta_1 \frac{c_i^{(1)} - c_{i-1}^{(1)}}{\Delta x}$	$\hat{\beta} = \frac{\beta_2 \beta_1}{\theta \beta_2 + (1 - \theta) \beta_1}$
D-CCM	$\hat{\beta} \frac{c_{i+1}^{(2)} - c_i^{(1)}}{\Delta x} - \beta_1 \frac{c_i^{(1)} - c_{i-1}^{(1)}}{\Delta x}$	$\hat{\beta} = \frac{He \beta_2 \beta_1}{He \times \theta \beta_2 + (1 - \theta) \beta_1}$



- **The normalized distance function**

$$\theta = \frac{|\phi_i|}{|\phi_i| + |\phi_{i+1}|} \quad \phi_i = x_i - x_I$$

THANKS

APPENDIX