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

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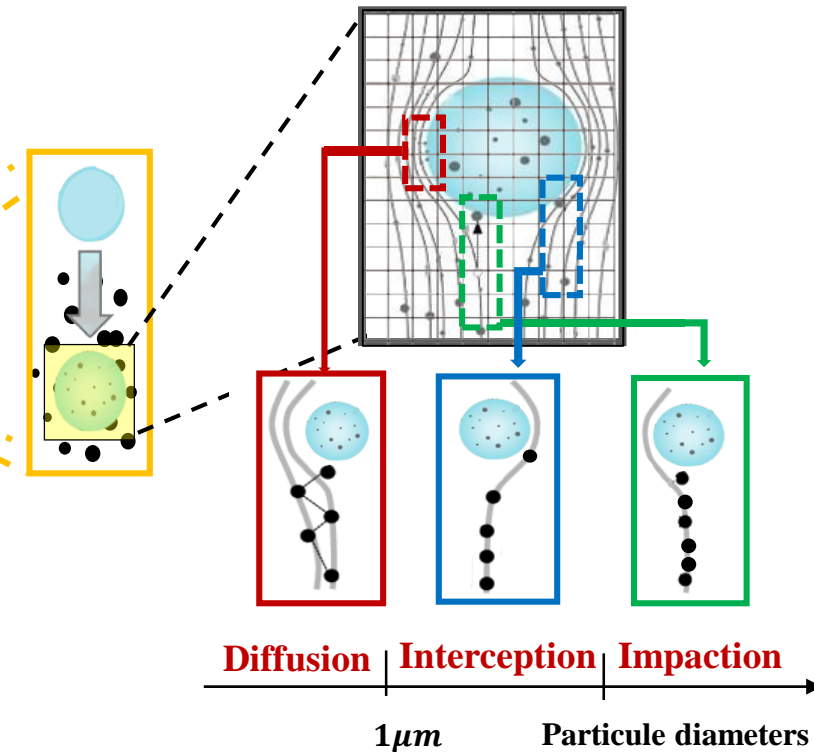
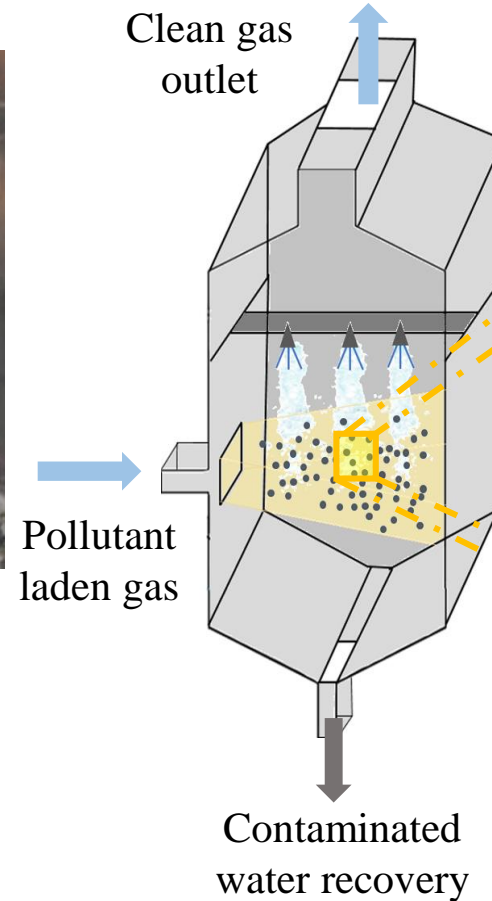
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Introduction

- **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

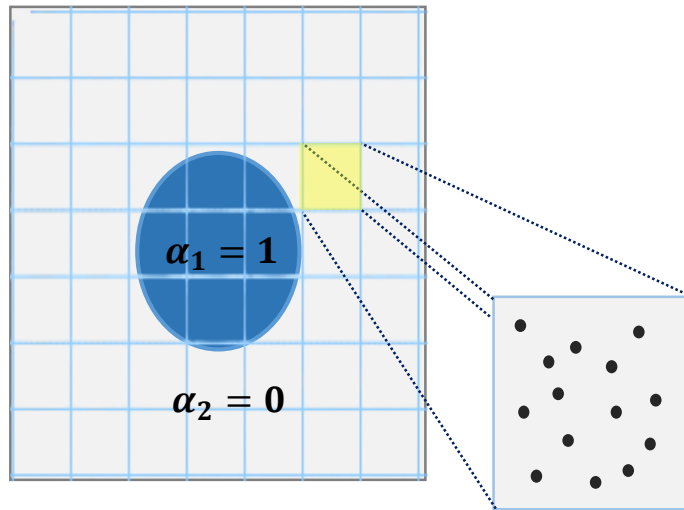
- Single field formulation involving a specific source-term
- Ghost-Fluid Method (GFM)
- Directional Cut-Cell method (D-CCM)

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

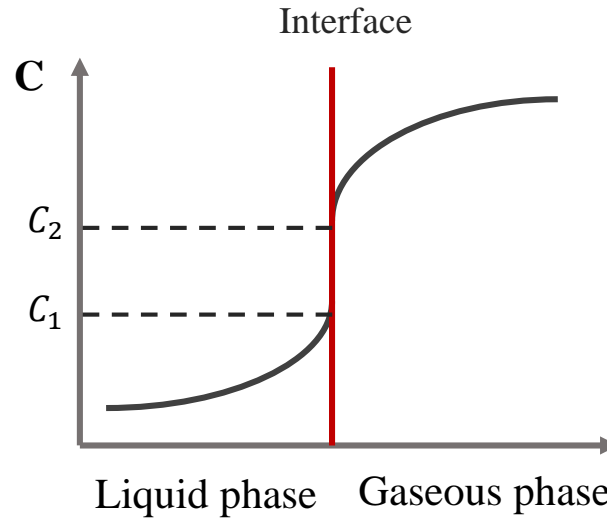
- One-dimensional steady diffusion
- Three-dimensional steady diffusion
- Three-dimensional unsteady diffusion

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

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

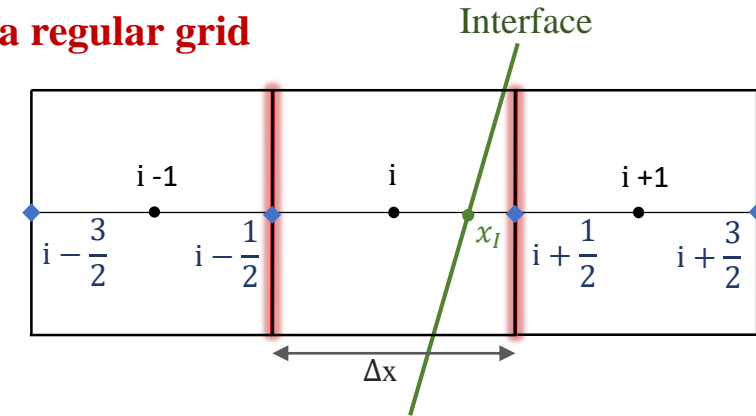
$$\beta = \frac{\beta_1 \beta_2}{\beta_2(1 - \alpha) + \beta_1 \alpha}$$

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** $\frac{d}{dx} \left(\beta \frac{dc}{dx} \right) = \frac{\partial c}{\partial t}$

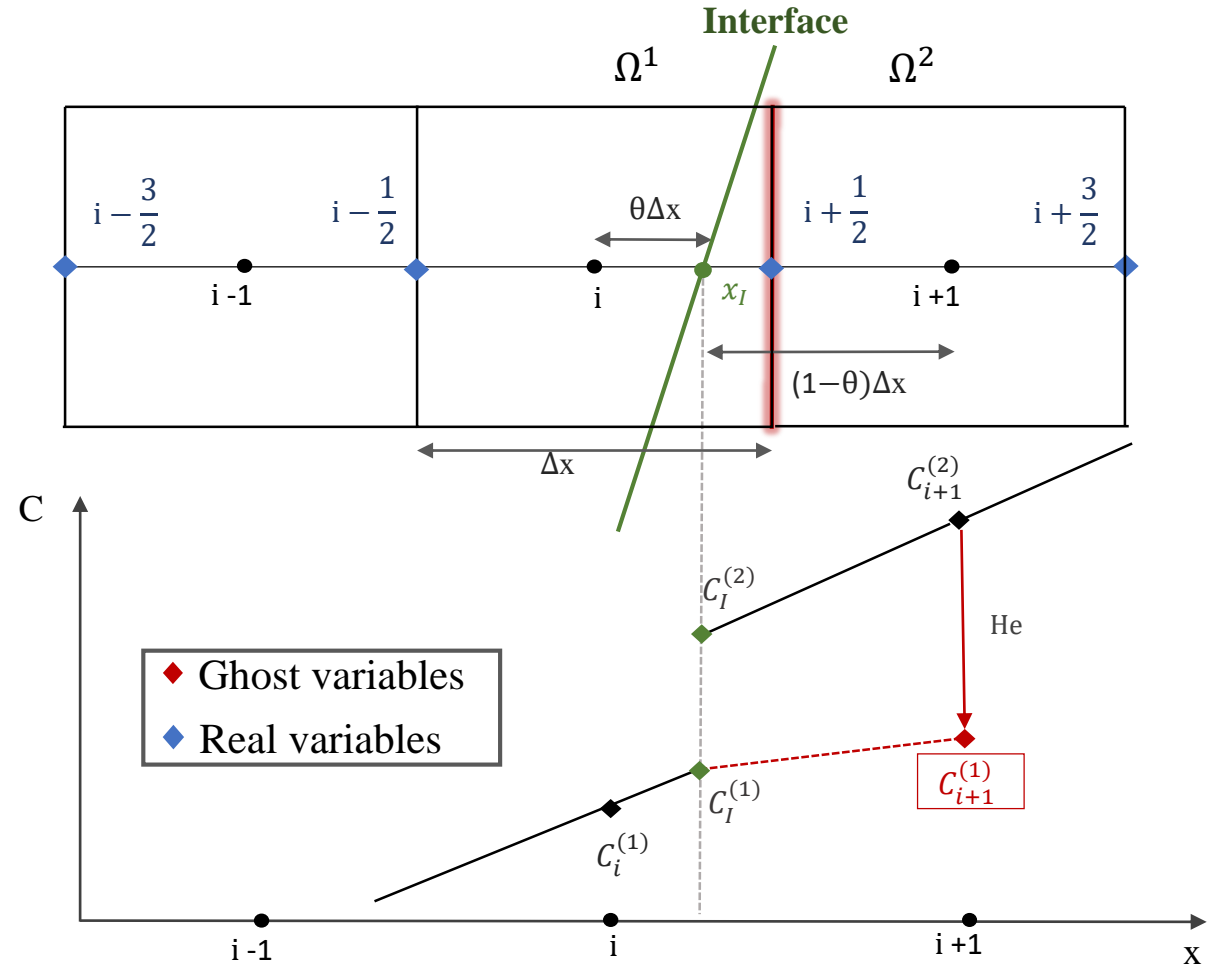
Numerical scheme

- 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)=liquid, (2)= gas

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

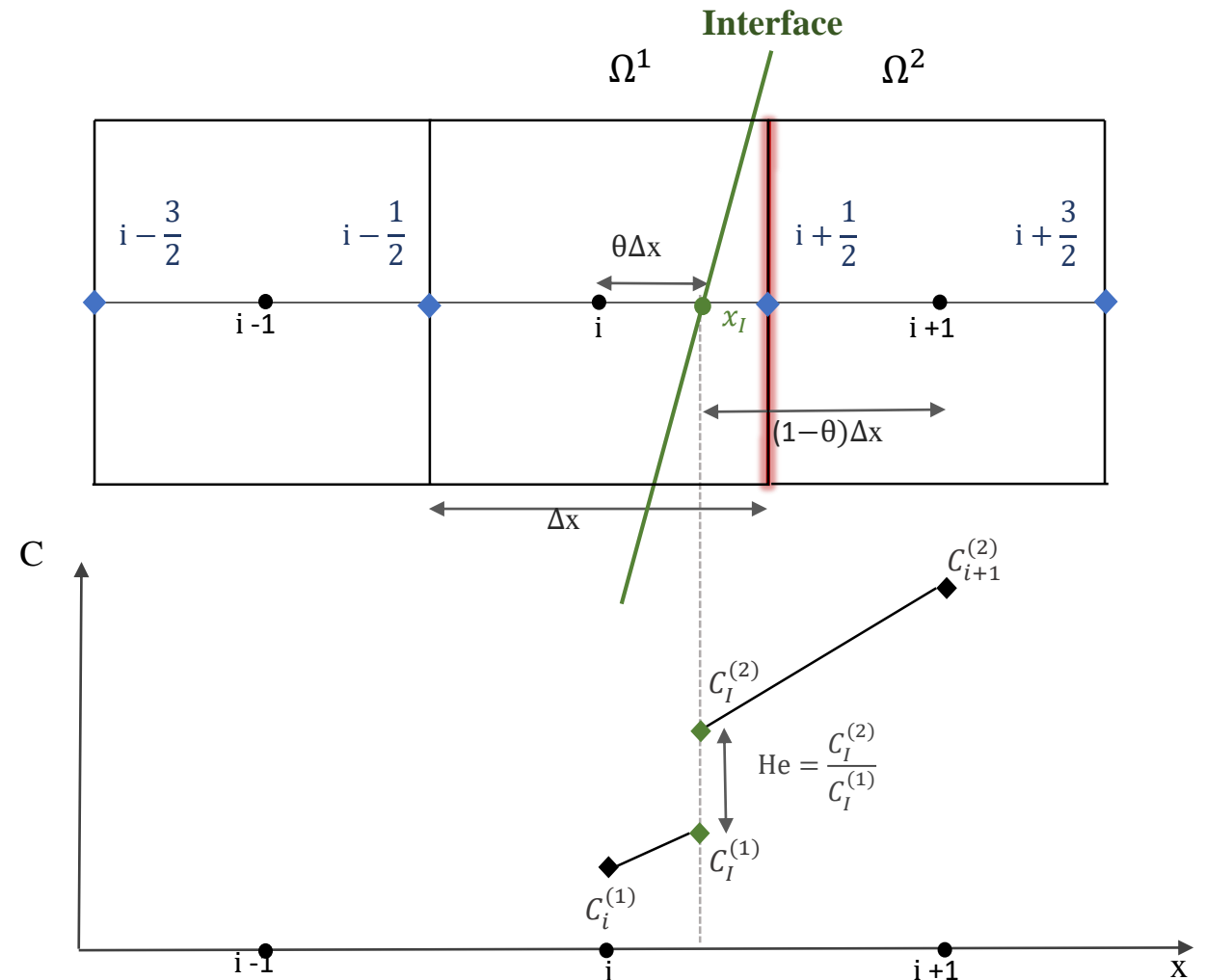
Numerical scheme

- Flux balance in the cell centred at i

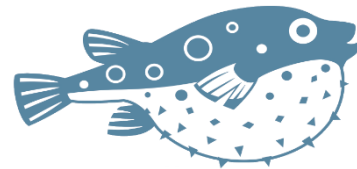
$$\int_{x_{i-1/2}}^{x_{i+1/2}} \frac{d}{dx} \left(\beta \frac{dc}{dx} \right) dx = \hat{\beta} \frac{c_{i+1}^{(2)} - c_i^{(1)}}{\Delta x} - \beta_1 \frac{c_i^{(1)} - c_{i-1}^{(1)}}{\Delta x}$$

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

Finite volume discretization on a regular grid



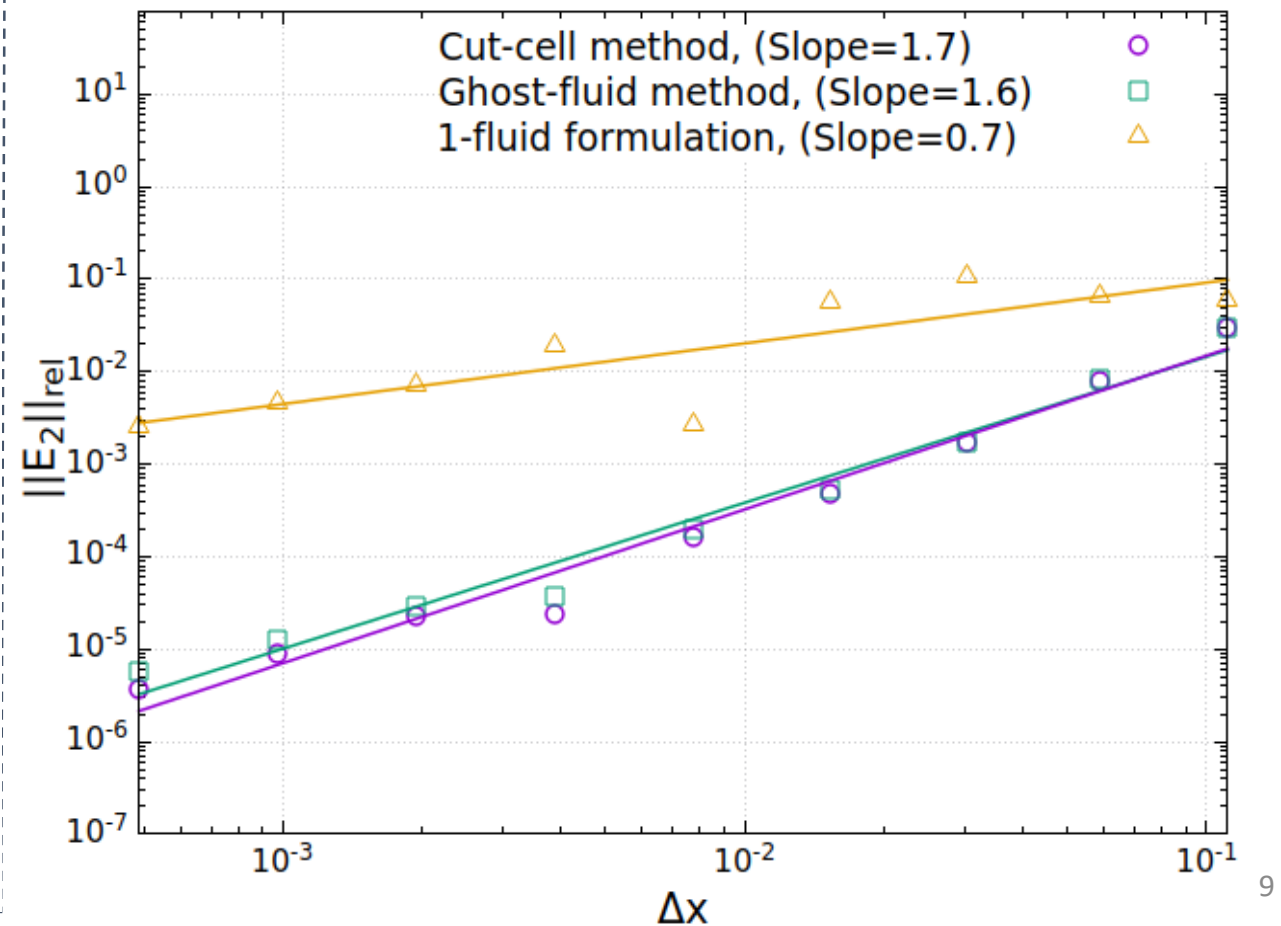
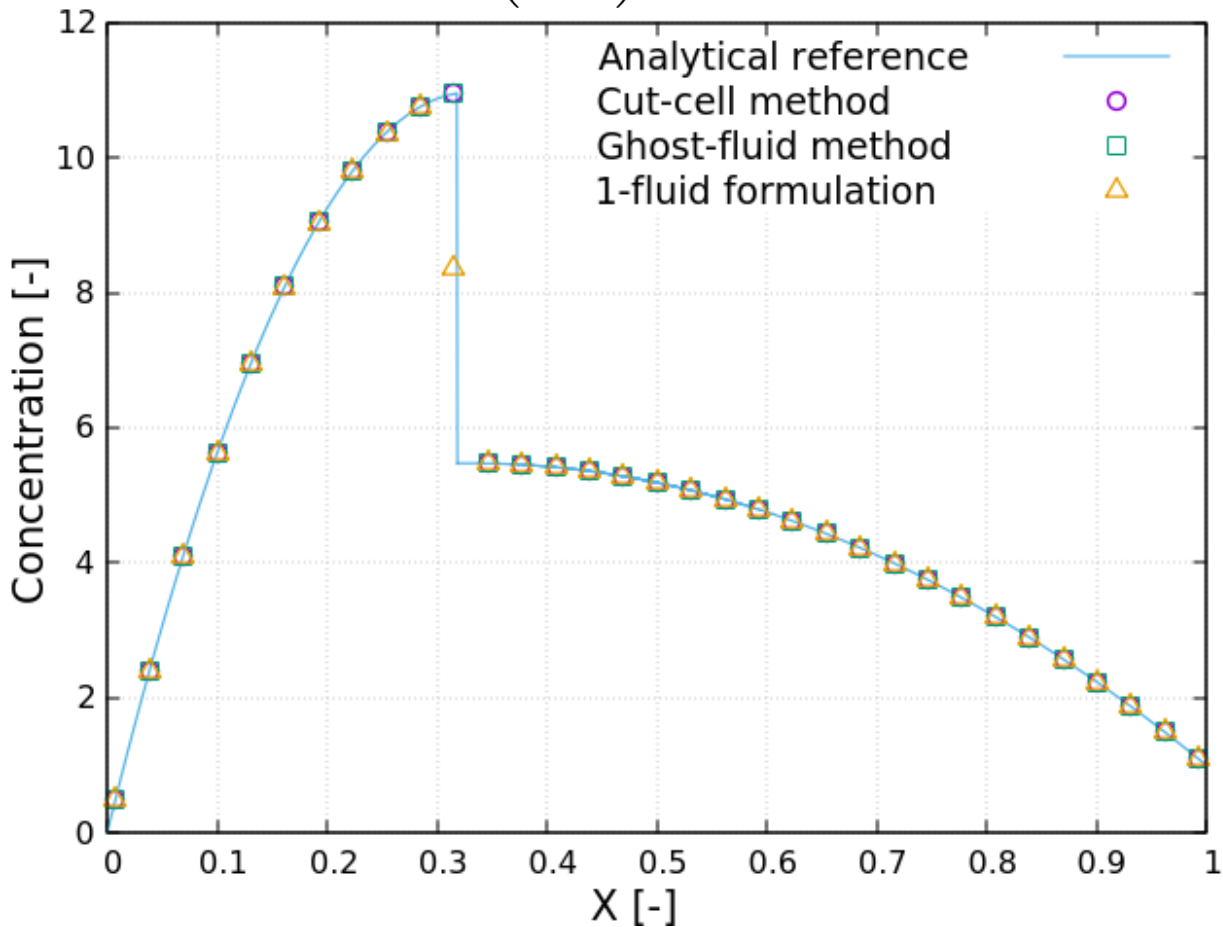
Results and discussion



Test cases: Steady 1D diffusion across a flat interface

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

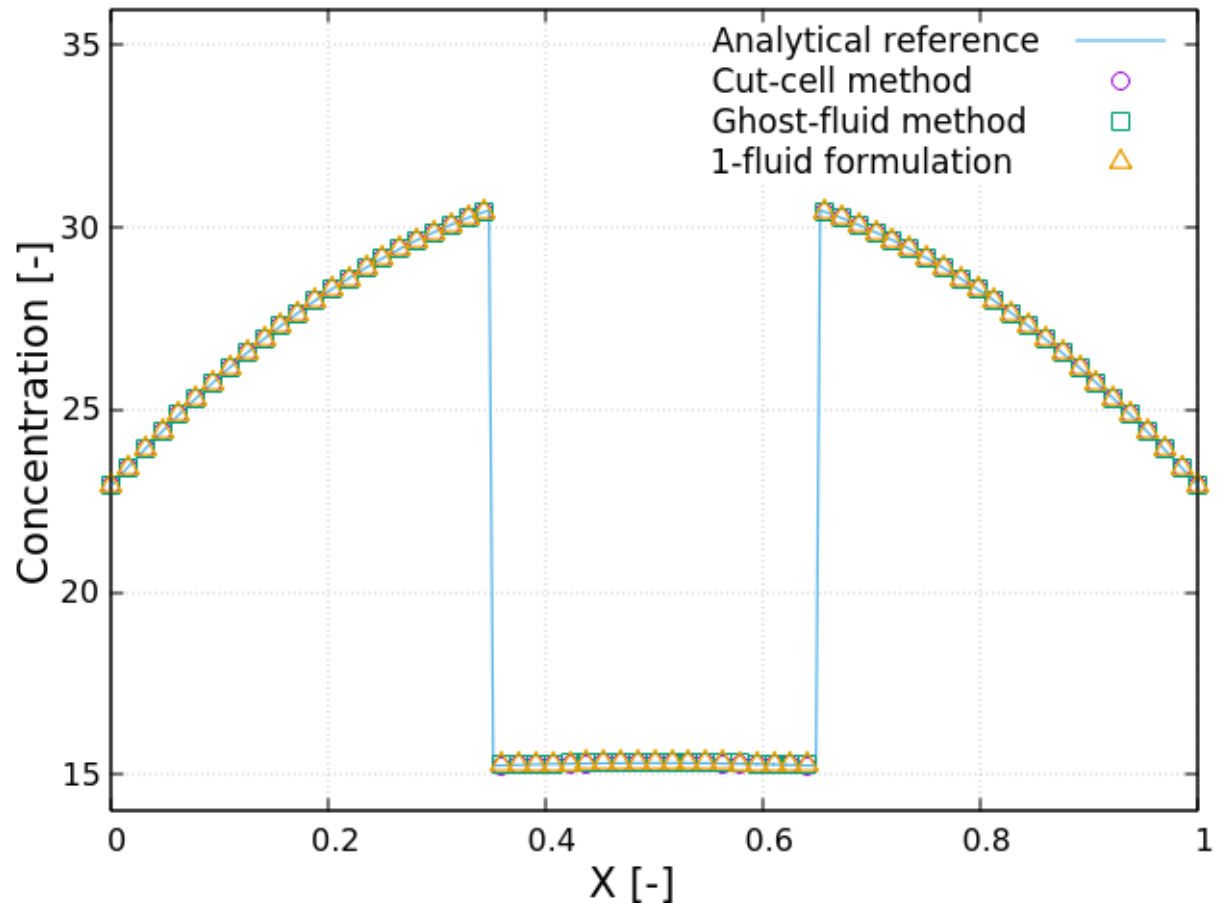
$$\frac{d}{dx} \left(\beta \frac{dc}{dx} \right) + \omega = 0$$



Test cases: Steady 3D diffusion across a spherical interface

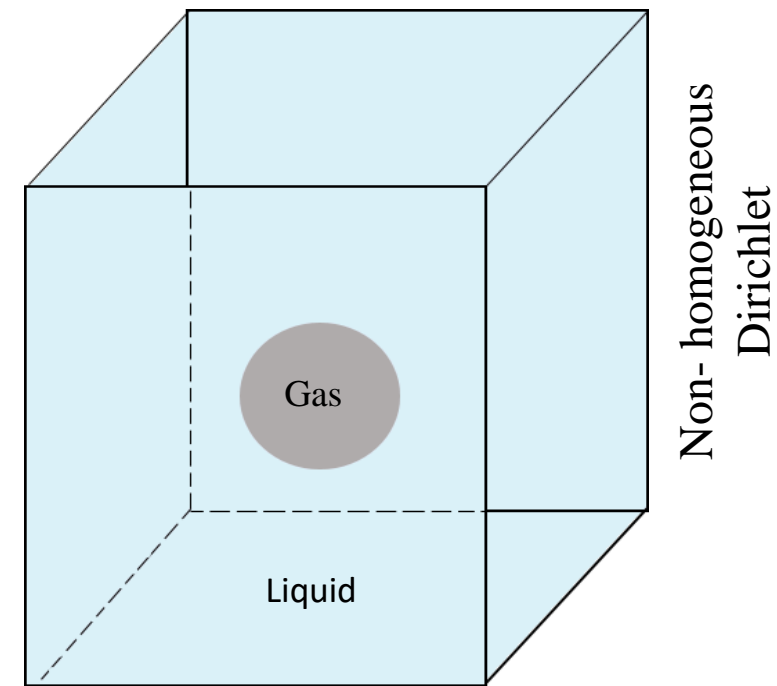
- Numerical model**

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



- Physical and geometrical parameters**

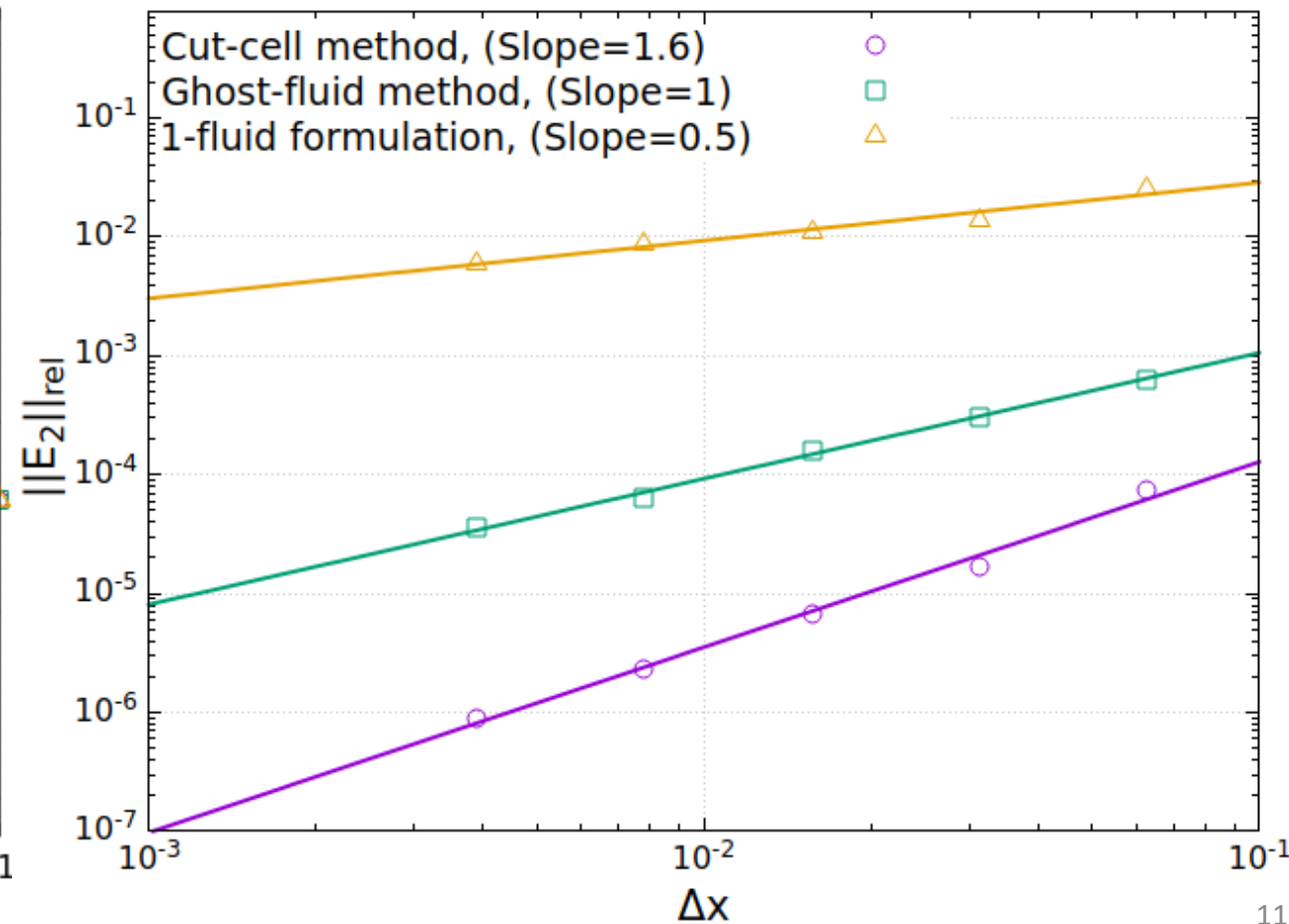
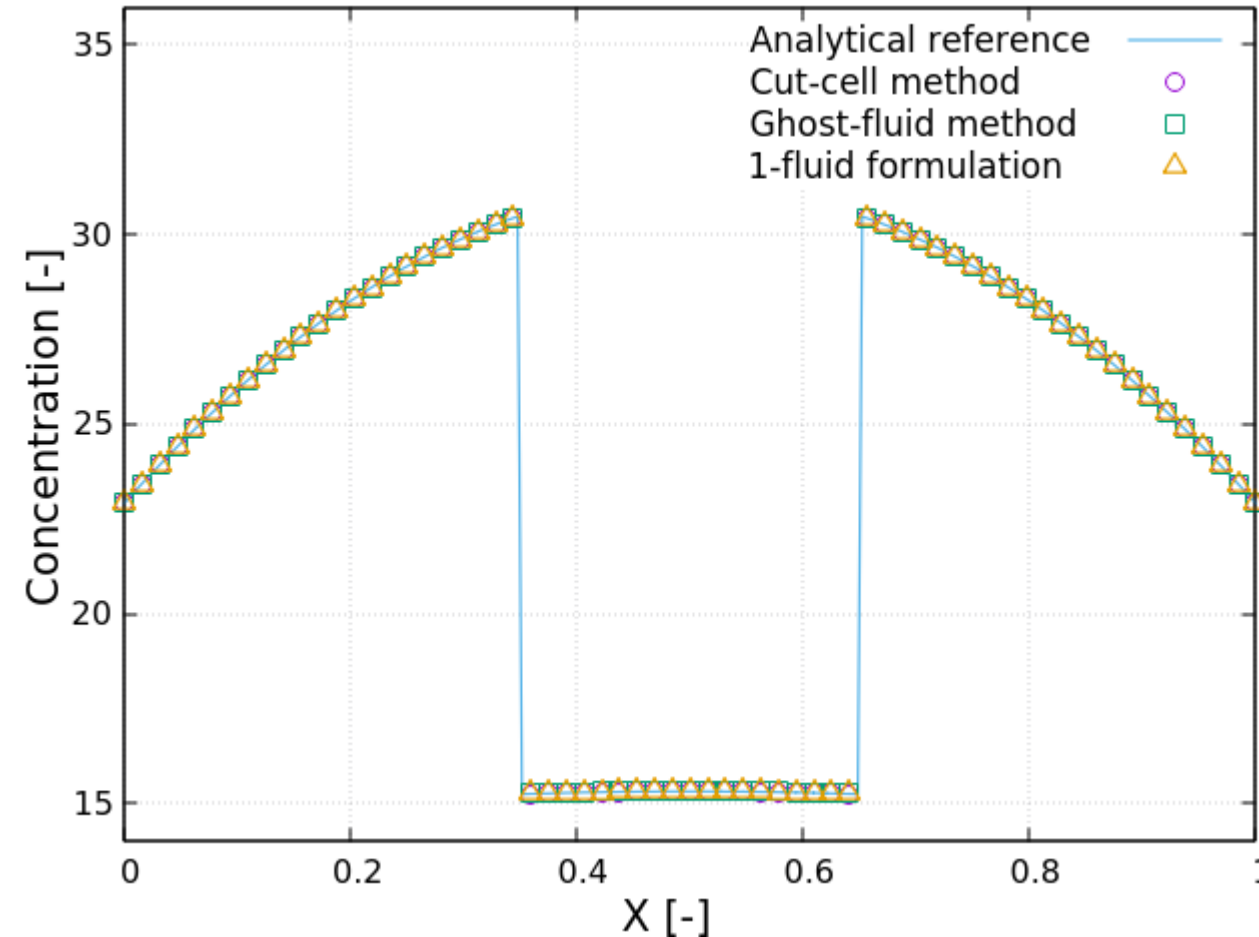
- ✓ $He = C_l^1 / C_l^2 = 0,5$
- ✓ $\beta_2 / \beta_1 = 10$
- ✓ $d_0 / L = 0,3$
- ✓ $\omega = 200$
- ✓ BC : Non-homogeneous Dirichlet



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

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

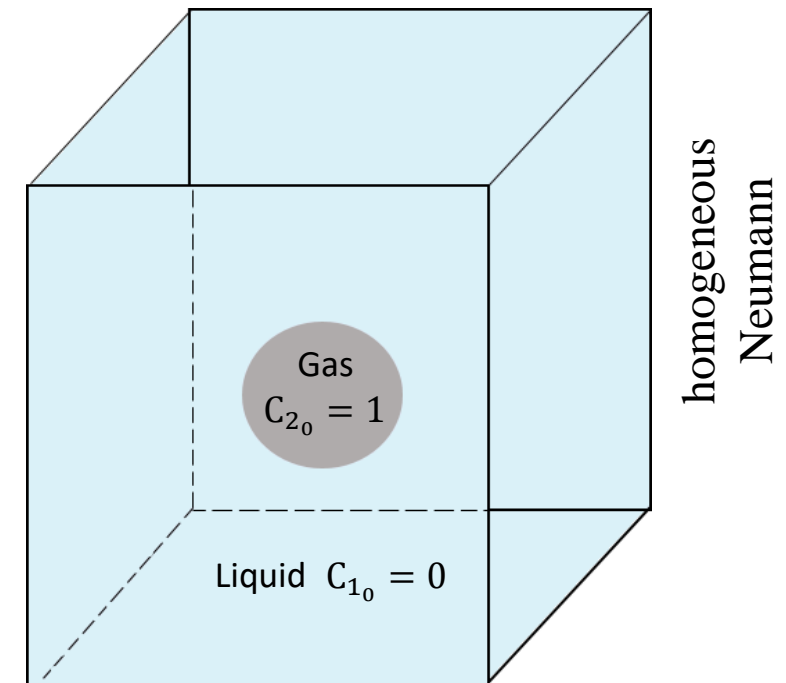
- Analytical reference (spherical symmetry solution [4])

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

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

- Physical and geometrical parameters

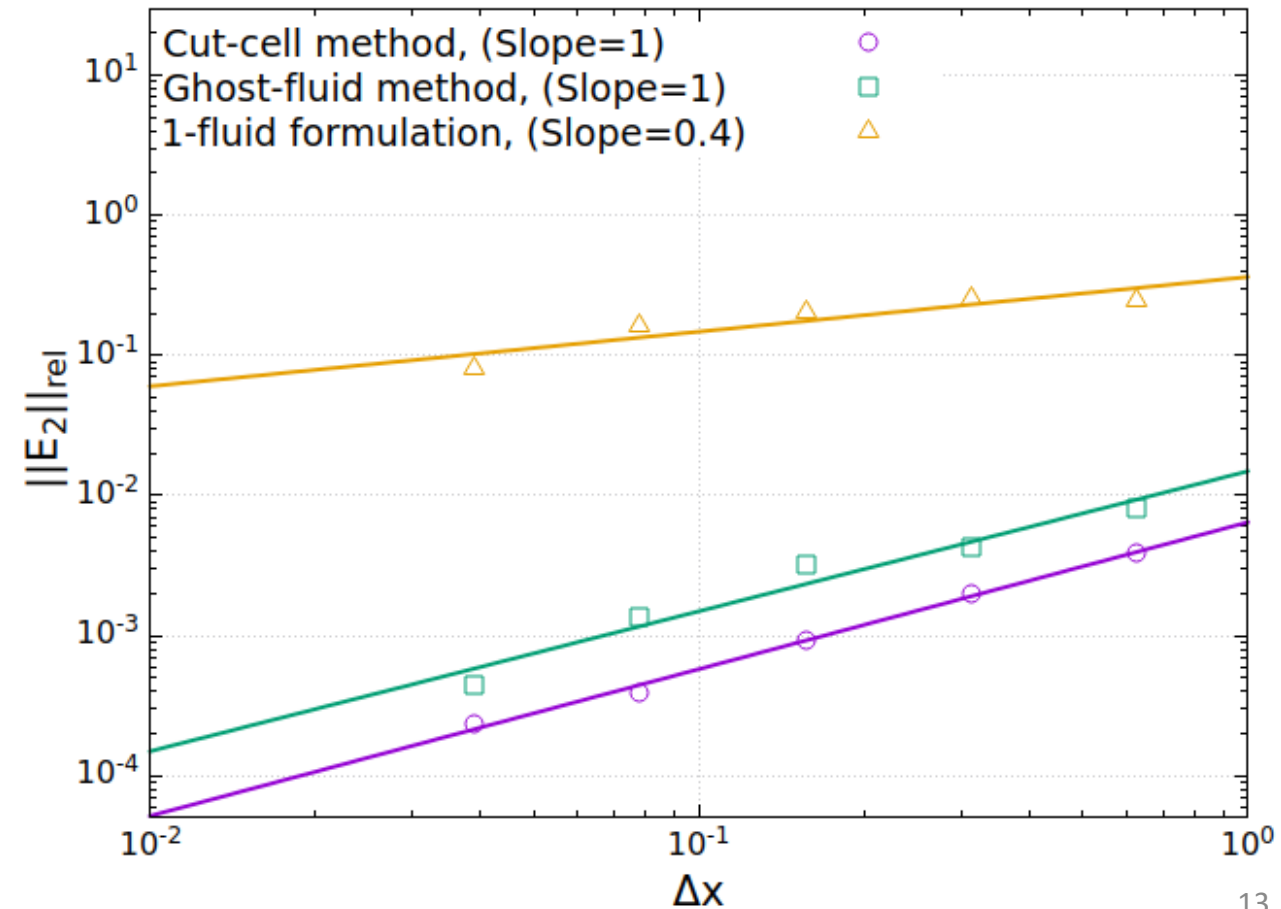
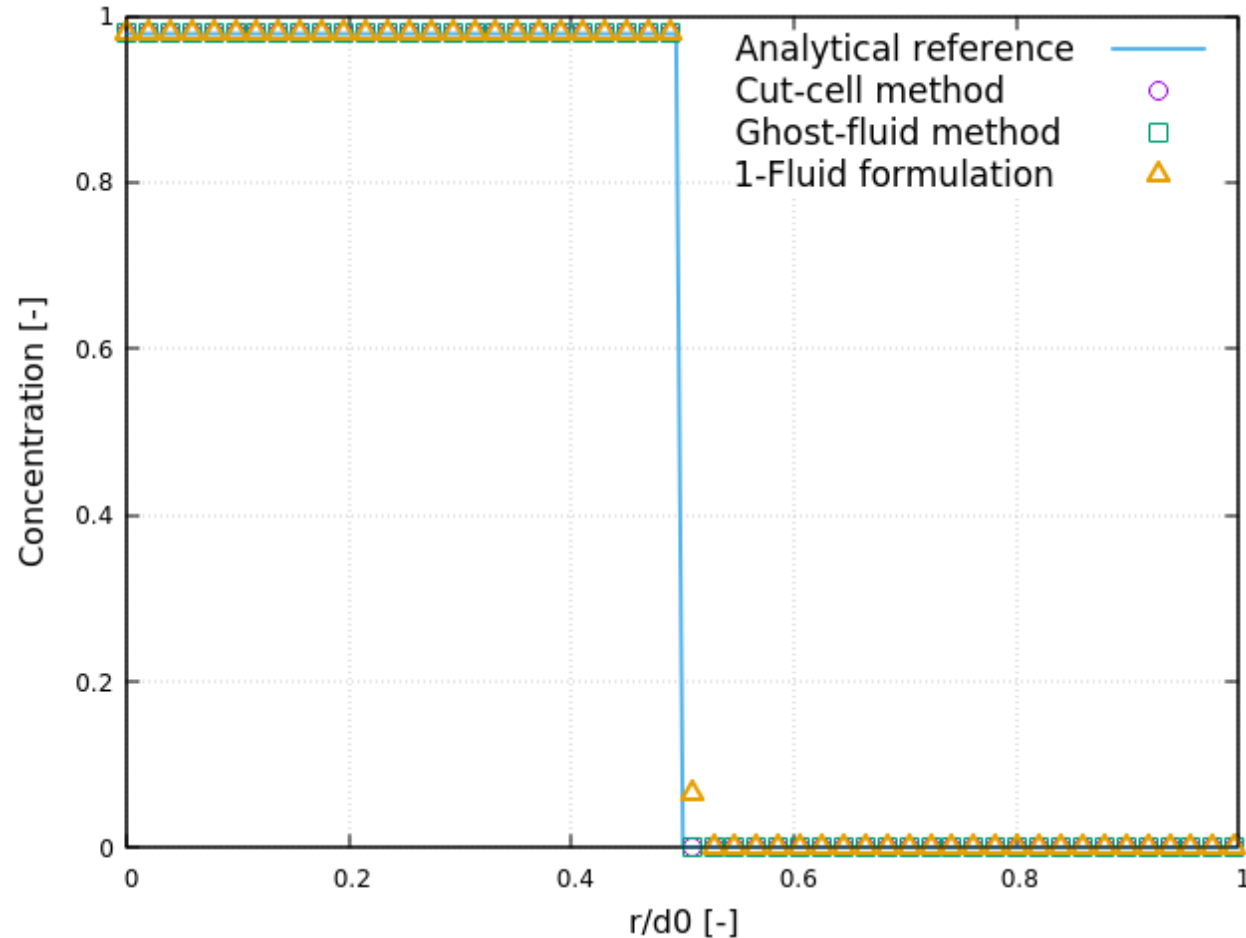
- ✓ $He = C_I^1 / C_I^2 = 10^{-3}$
- ✓ $\beta_2 / \beta_1 = 10$
- ✓ $d_0 / L = 0,2$
- ✓ BC : Homogeneous Neumann



Test cases: Unsteady 3D diffusion across a spherical interface

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

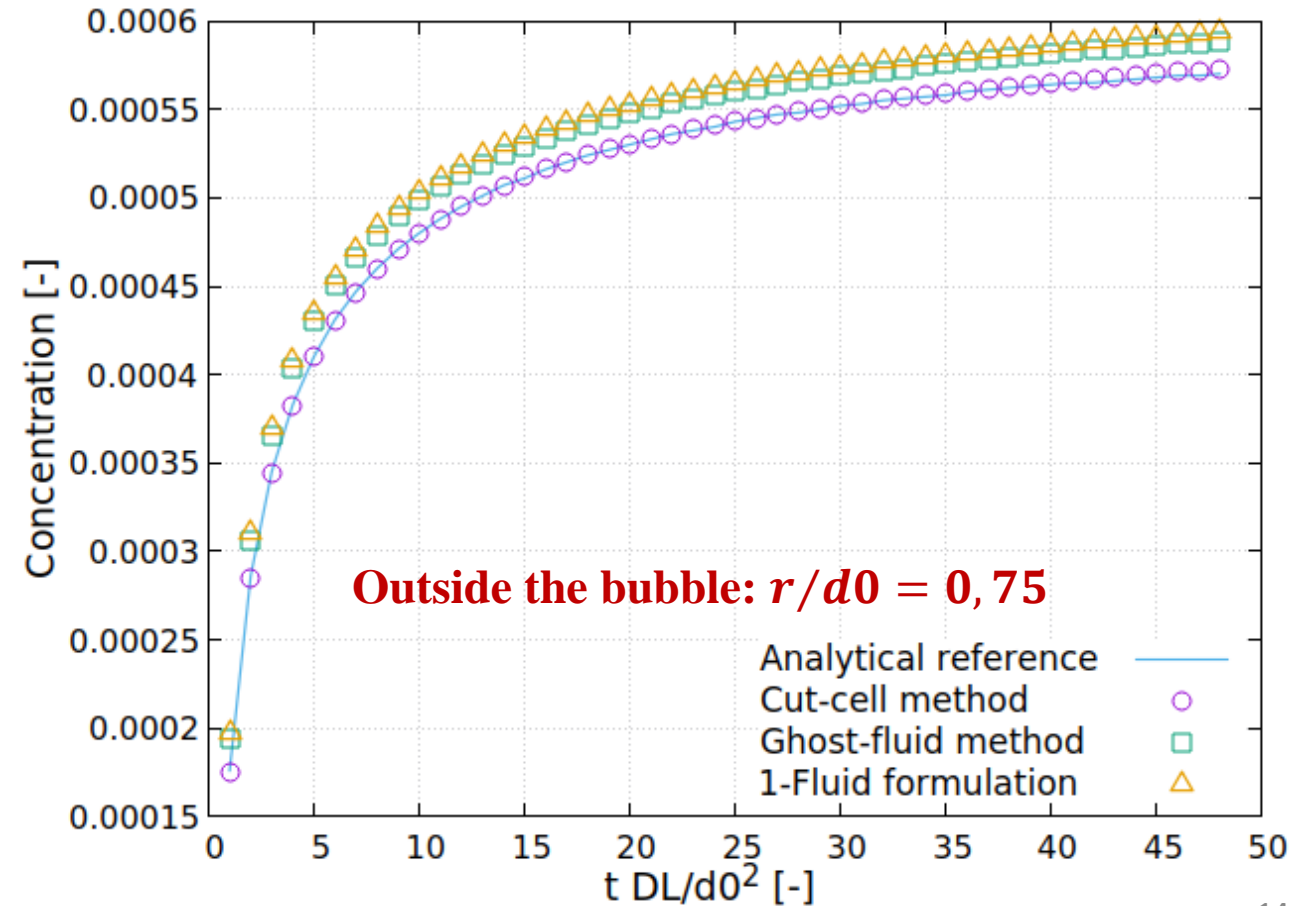
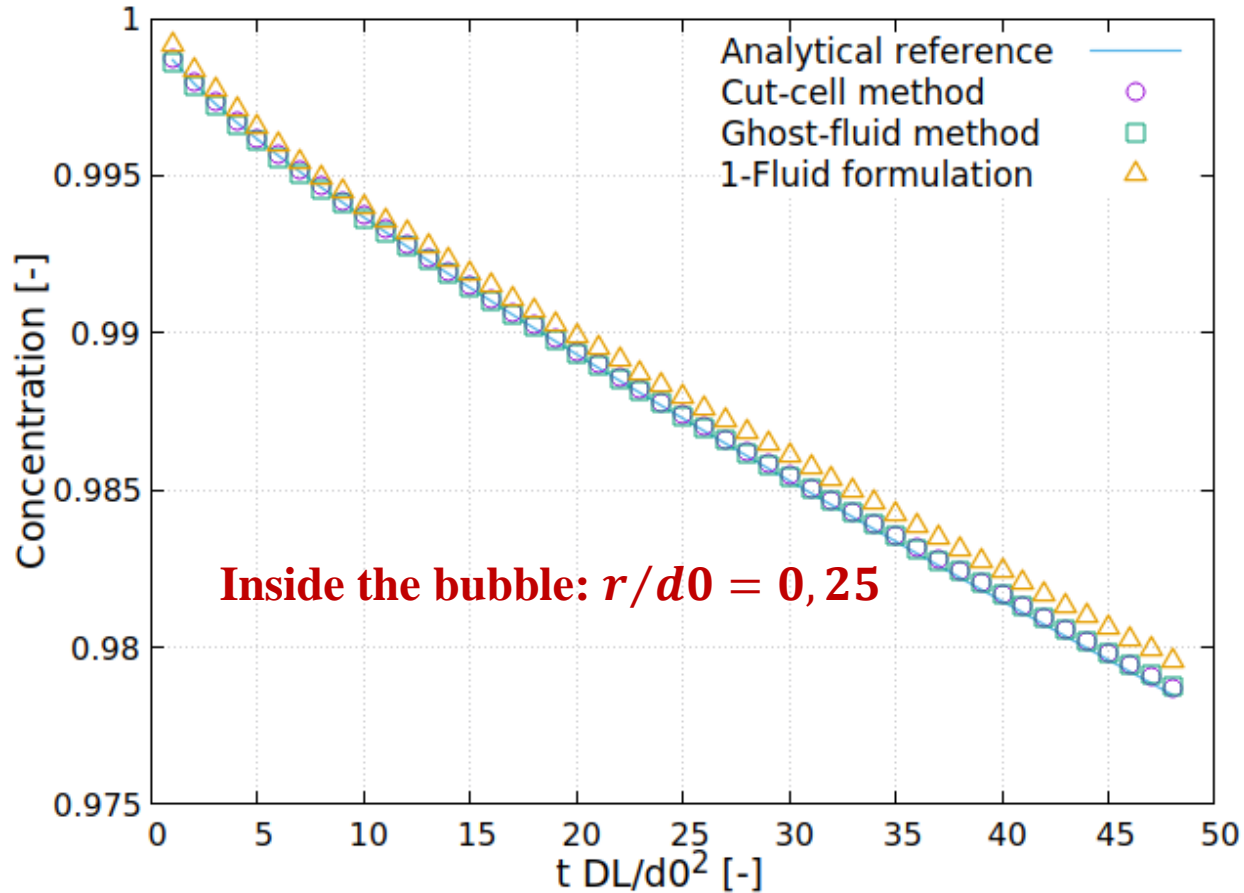
Physical problem parameters: $He = 0,001$; $\beta_1/\beta_2 = 10$; $d_0/L = 0,2$



Test cases: Unsteady 3D diffusion across a spherical interface

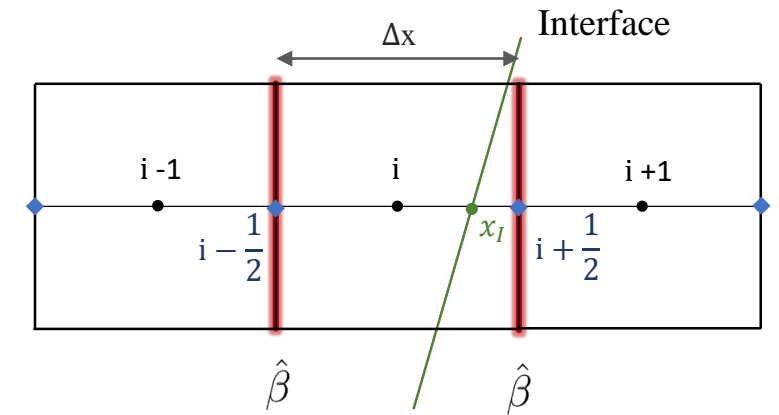
Temporal evolution at a two fixed positions

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