



Towards two-sided subgrid-scale modeling of mass transfer at fluid interfaces

Highlights from our preprint

A two-sided subgrid-scale model for mass transfer across fluid interfaces

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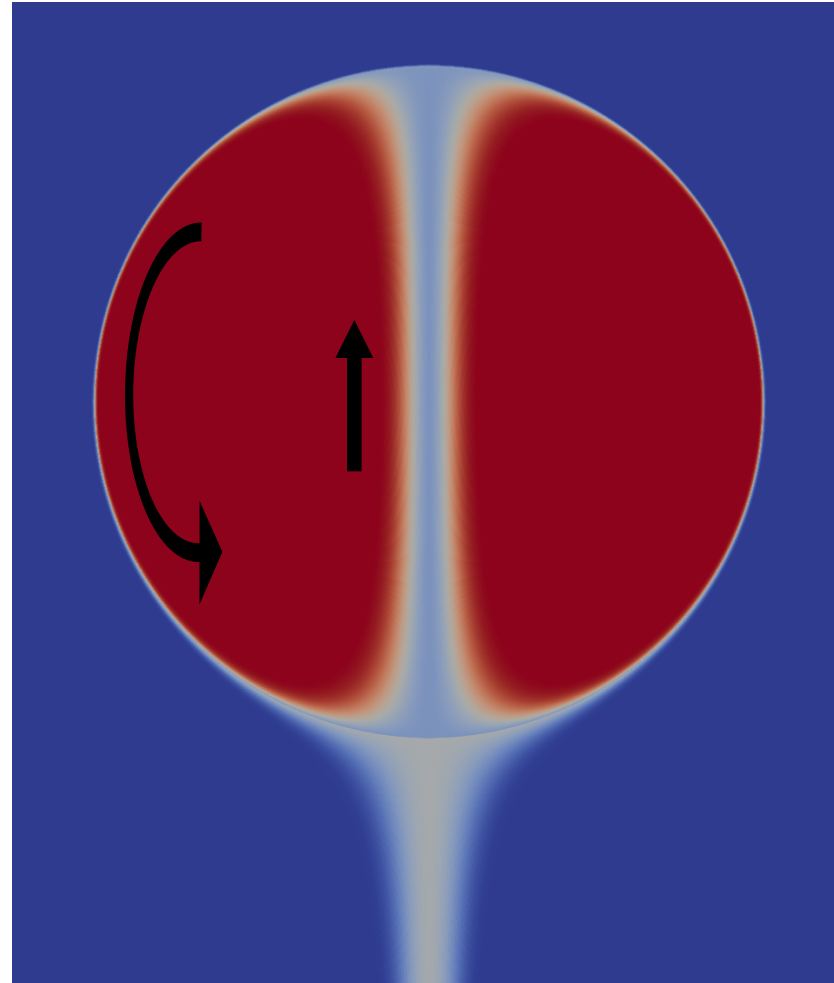
² Faculty of Mechanical Engineering and Naval Architecture, FSB Zagreb



This presentation

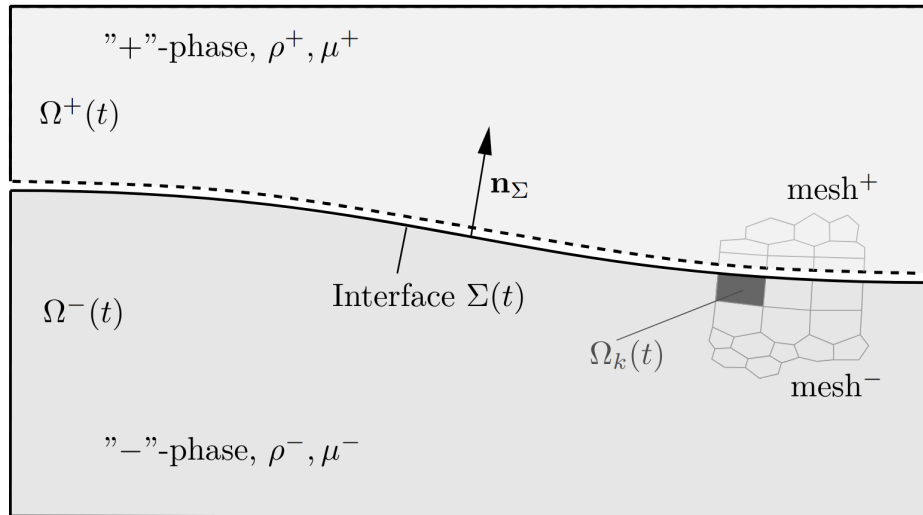


Motivation



(preliminary
reference result)

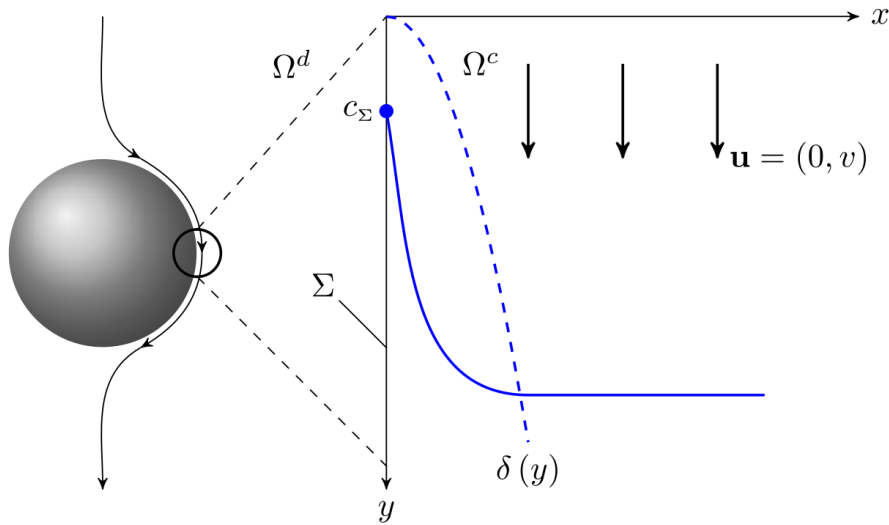
Mathematical model



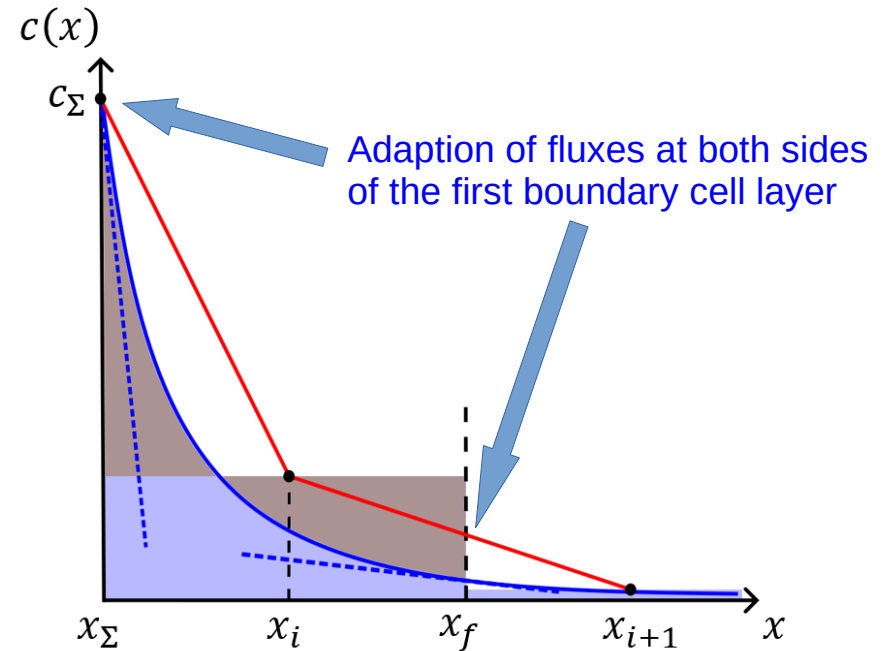
Setting

- Dilute species as passive scalar
- No mass sources or sinks
- Mass-less interface
- Henry-jump at the interface
- Unstructured Finite Volume ALE Interface Tracking
 - Sharp interface represented by coinciding two surface meshes

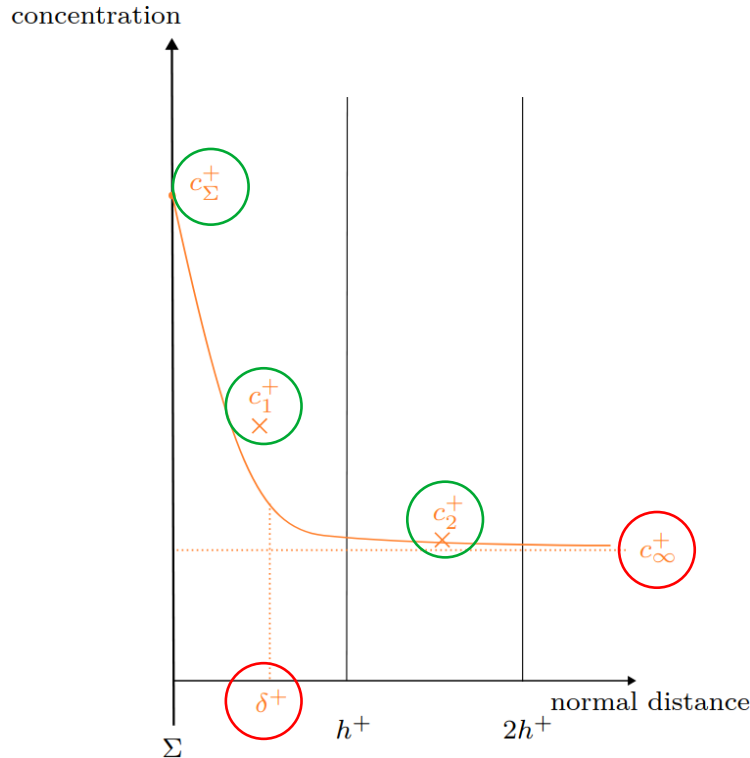
What is subgrid-scale modeling?



$$c(x, y) = c_{\Sigma} + (c_{\infty} - c_{\Sigma}) \cdot \operatorname{erf}(x/\delta) \quad \text{with } \delta(y) = \sqrt{4Dy/\nu}$$



The concentration inside a bubble changes: an extension to SGS modeling



- Far-field concentration is unknown.
- Far-field concentration can be time- and space-dependent.
- Use values in the first two cells to determine concentration profile

$$c_\Sigma h + \delta \cdot (c_\infty - c_\Sigma) E(h/\delta) = c_1 h$$

$$2c_\Sigma h + \delta \cdot (c_\infty - c_\Sigma) E(2h/\delta) = (c_1 + c_2) h$$

$$\text{with } E(x) = x \cdot \text{erf}(x) + e^{-x^2} - 1/\sqrt{\pi}$$



Is two-sided modeling just $2 * \text{one-sided modeling?}$

```
62  class twoSidedSubGridScaleModel
75  | // Pointer to SGS model on side 1
    | 27 refs
76  | autoPtr<baseSubGridScaleModel> sgs1Ptr_;
77  |
78  | // Pointer to SGS model on side 2
    | 26 refs
79  | autoPtr<baseSubGridScaleModel> sgs2Ptr_;
80  |
```

Yes*



*but

$$c_{\Sigma}^{+} + (c_{\infty}^{+} - c_{\Sigma}^{+})E(y^{+}) = c_1^{+}$$

$$c_{\Sigma}^{+} + (c_{\infty}^{+} - c_{\Sigma}^{+})E(2y^{+}) = (c_1^{+} + c_2^{+})/2$$

$$c_{\Sigma}^{-} + (c_{\infty}^{-} - c_{\Sigma}^{-})E(y^{-}) = c_1^{-}$$

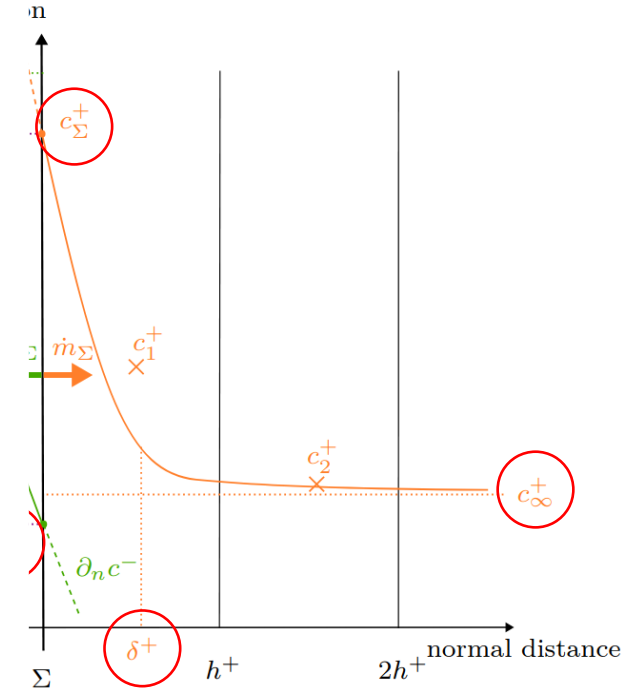
$$c_{\Sigma}^{-} + (c_{\infty}^{-} - c_{\Sigma}^{-})E(2y^{-}) = (c_1^{-} + c_2^{-})/2$$

$$c_{\Sigma}^{+} = c_{\Sigma}^{-} / H$$

$$D^{+} \frac{c_{\Sigma}^{+} - c_{\infty}^{+}}{\delta^{+}} = D^{-} \frac{c_{\Sigma}^{-} - c_{\infty}^{-}}{\delta^{-}}$$

with

$$y^{\pm} = \frac{h^{\pm}}{\delta^{\pm}} \text{ and } E(x) = \text{erf}(x) + \frac{e^{-x^2} - 1}{x\sqrt{\pi}}$$



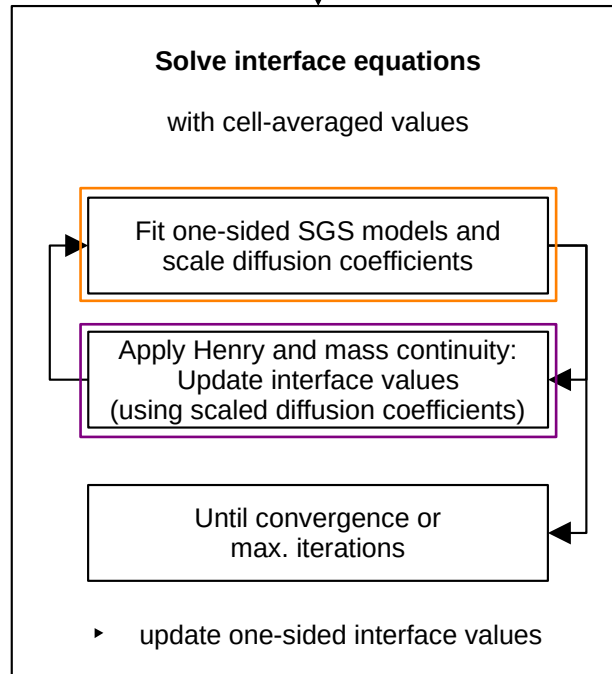
We solve the equation system iteratively

- Iterate over
 - Bulk equation system

$$\begin{aligned}
 c_{\Sigma}^+ + (c_{\infty}^+ - c_{\Sigma}^+)E(y^+) &= c_1^+ \\
 c_{\Sigma}^+ + (c_{\infty}^+ - c_{\Sigma}^+)E(2y^+) &= (c_1^+ + c_2^+)/2 \\
 c_{\Sigma}^- + (c_{\infty}^- - c_{\Sigma}^-)E(y^-) &= c_1^- \\
 c_{\Sigma}^- + (c_{\infty}^- - c_{\Sigma}^-)E(2y^-) &= (c_1^- + c_2^-)/2
 \end{aligned}$$

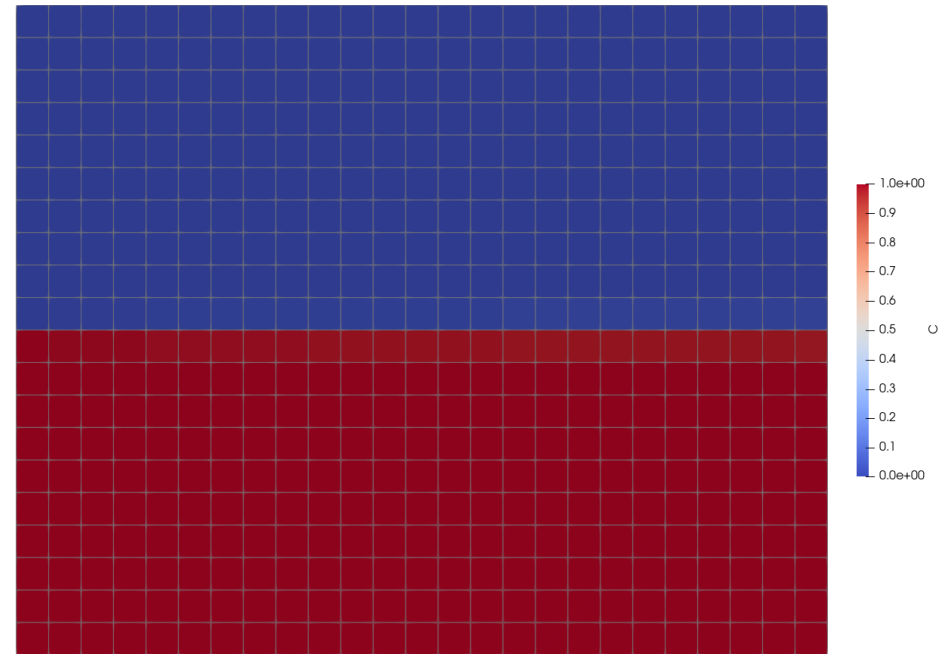
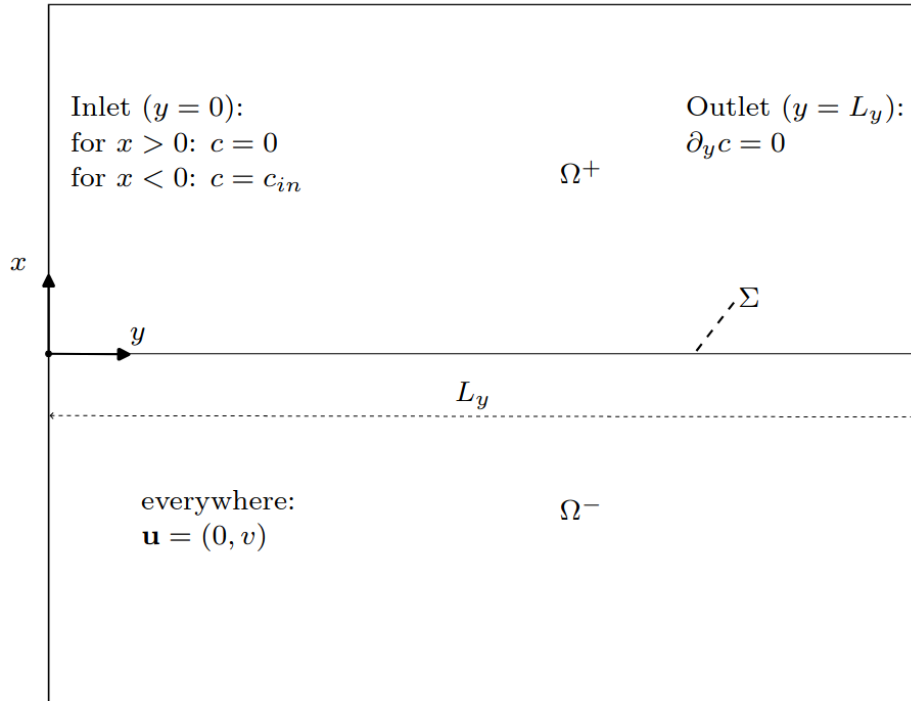
$$\begin{aligned}
 c_{\Sigma}^+ &= c_{\Sigma}^- / H \\
 D^+ \frac{c_{\Sigma}^+ - c_{\infty}^+}{\delta^+} &= D^- \frac{c_{\Sigma}^- - c_{\infty}^-}{\delta^-}
 \end{aligned}$$

interface
conditions

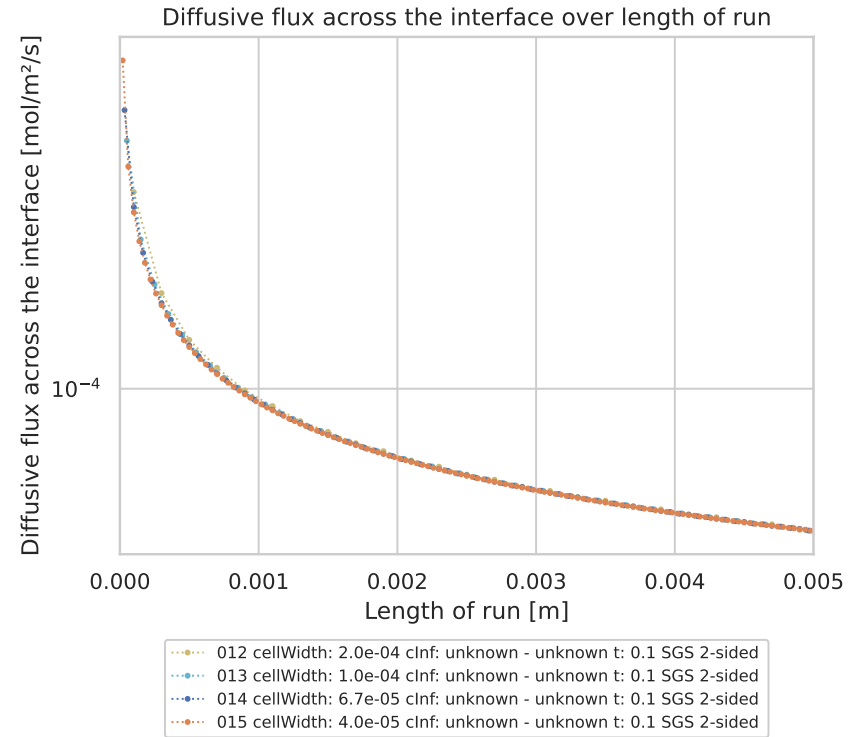
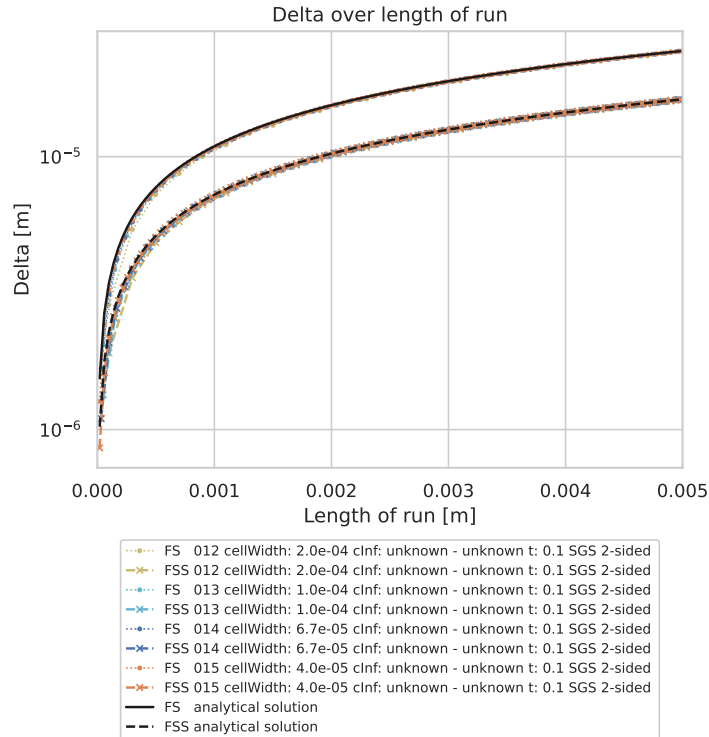


- Iterate over
 - 2 one-sided SGS models
 - Mass flux continuity & Henry-Jump
- converged, when interfacial value is found
- Interfacial values are used as Dirichlet-Dirichlet boundary conditions!

Mass transfer in parallel flow along planar interface



Mass transfer in parallel flow along planar interface

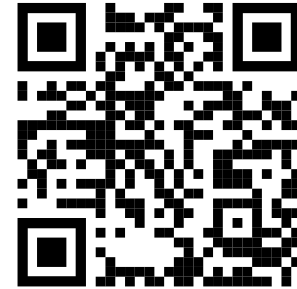


Wrap-up

- We improved SGS modeling:
 - extended for unknown far-field concentrations
 - (improvements reported in our preprint)
- We model two-sided subgrid-scale mass transfer:
 - Very thin boundary layers on both sides
 - One subgrid-scale model for each side
 - Iterations to find the right Dirichlet-Dirichlet boundary conditions
- Publicly available:
in the OpenFOAM Arbitrary Lagrangian/Eulerian Interface Tracking (ALE-IT) framework *twoPhaseInterTrackFoam*

Further reading

- This presentation
DOI: 10.48328/tudatalib-1755
- Preprint
M. Schwarzmeier, T. Marić, Ž. Tuković, and D. Bothe. A two-sided subgrid-scale model for mass transfer across fluid interfaces. Preprint, May 2025
- Code repository:
<https://gitlab.com/interface-tracking/>
- Published papers
 - twoPhaseInterTrackFoam (ALE Interface Tracking with surfactants and subgrid-scale model)
 - M. Schwarzmeier, S. Raju, Ž. Tuković, M. Fricke, D. Bothe, and T. Marić. twoPhaseInterTrackFoam: an OpenFOAM module for Arbitrary Lagrangian/Eulerian Interface Tracking with Surfactants and Subgrid-Scale Modeling. *Computer Physics Communications*, 308:109460, Mar. 2025. doi:10.1016/j.cpc.2024.109460.
 - ALE Interface Tracking
 - Tuković, Ž. & Jasak, H. A moving mesh finite volume interface tracking method for surface tension dominated interfacial fluid flow. *Computers & Fluids* 55, 70–84 (2012).
 - Subgrid-scale model
 - Pesci, C., Weiner, A., Marschall, H. & Bothe, D. Computational analysis of single rising bubbles influenced by soluble surfactant. *J. Fluid Mech.* 856, 709–763 (2018).
 - Weiner, A. & Bothe, D. Advanced subgrid-scale modeling for convection-dominated species transport at fluid interfaces with application to mass transfer from rising bubbles. *Journal of Computational Physics* 347, 261–289 (2017).



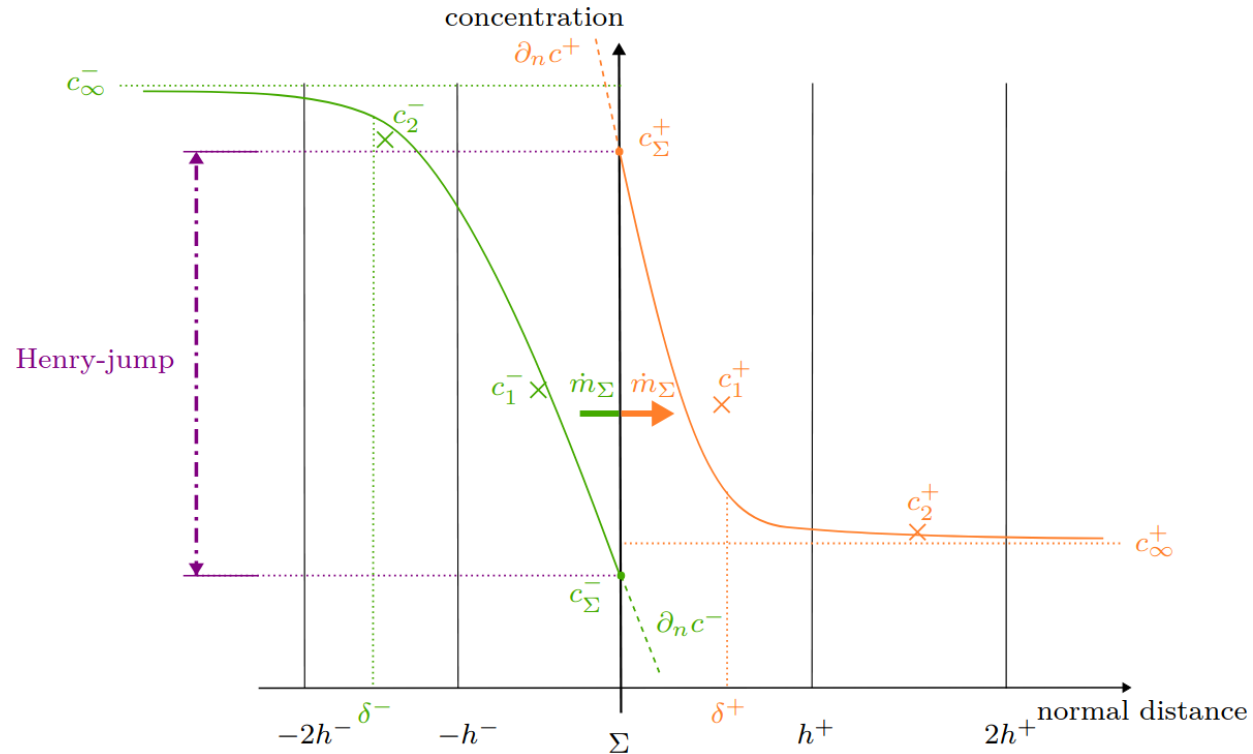
This presentation



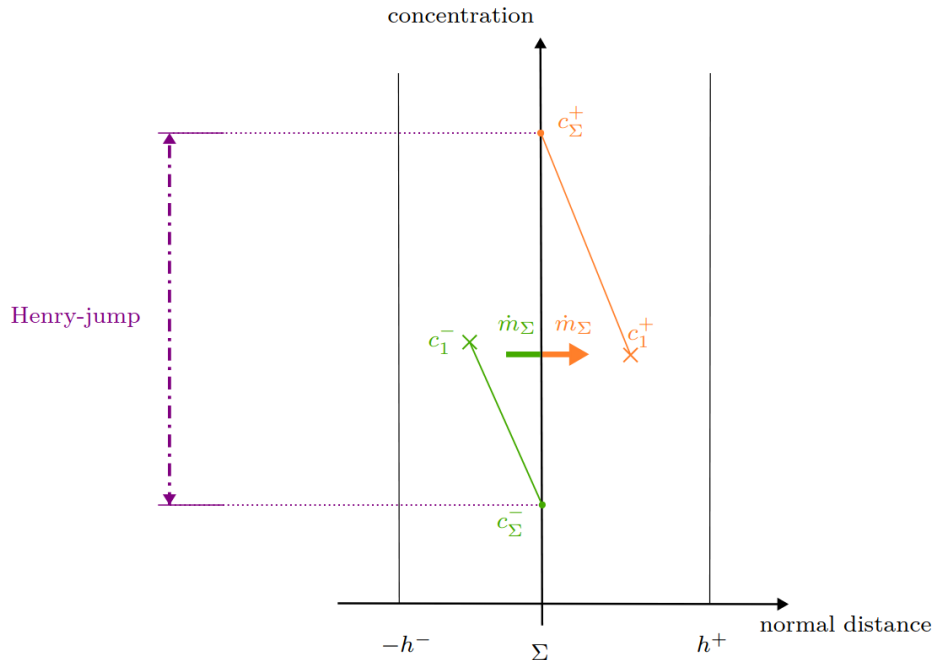
Code repository

Appendix

Two-sided subgrid-scale mass transfer



Mass transfer without SGS modeling



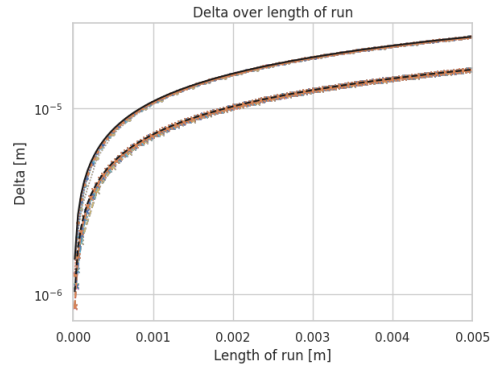
$$D^+ \frac{c_1^+ - c_\Sigma^+}{h^+/2} = D^- \frac{c_\Sigma^- - c_1^-}{h^-/2}$$

transforms to

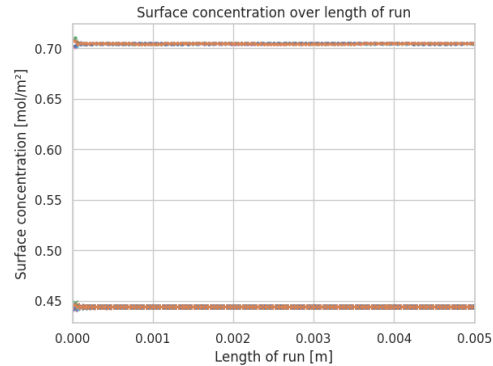
$$c_\Sigma^- = H c_\Sigma^+$$

$$c_\Sigma^+ = \frac{\alpha c_1^- + c_1^+}{\alpha/H + 1} \quad \text{with} \quad \alpha = \frac{D^- h^+}{D^+ h^-}$$

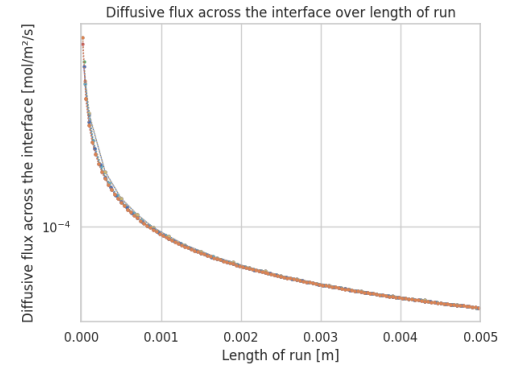
Mass transfer in parallel flow along planar interface



- FS 000 cellWidth: 2.0e-04 cinf: prescribed - prescribed t: 0.1 SGS 2-sided
- FSS 000 cellWidth: 2.0e-04 cinf: prescribed - prescribed t: 0.1 SGS 2-sided
- FS 001 cellWidth: 1.0e-04 cinf: prescribed - prescribed t: 0.1 SGS 2-sided
- FSS 001 cellWidth: 1.0e-04 cinf: prescribed - prescribed t: 0.1 SGS 2-sided
- FS 002 cellWidth: 6.7e-05 cinf: prescribed - prescribed t: 0.1 SGS 2-sided
- FSS 002 cellWidth: 6.7e-05 cinf: prescribed - prescribed t: 0.1 SGS 2-sided
- FS 003 cellWidth: 4.0e-05 cinf: prescribed - prescribed t: 0.1 SGS 2-sided
- FSS 003 cellWidth: 4.0e-05 cinf: prescribed - prescribed t: 0.1 SGS 2-sided
- FS 008 cellWidth: 2.0e-04 cinf: prescribed - unknown t: 0.1 SGS 2-sided
- FSS 008 cellWidth: 2.0e-04 cinf: prescribed - unknown t: 0.1 SGS 2-sided
- FS 009 cellWidth: 1.0e-04 cinf: prescribed - unknown t: 0.1 SGS 2-sided
- FSS 009 cellWidth: 1.0e-04 cinf: prescribed - unknown t: 0.1 SGS 2-sided
- FS 010 cellWidth: 6.7e-05 cinf: prescribed - unknown t: 0.1 SGS 2-sided
- FSS 010 cellWidth: 6.7e-05 cinf: prescribed - unknown t: 0.1 SGS 2-sided
- FS 011 cellWidth: 4.0e-05 cinf: prescribed - unknown t: 0.1 SGS 2-sided
- FSS 011 cellWidth: 4.0e-05 cinf: prescribed - unknown t: 0.1 SGS 2-sided
- FS 012 cellWidth: 2.0e-04 cinf: unknown - unknown t: 0.1 SGS 2-sided
- FSS 012 cellWidth: 2.0e-04 cinf: unknown - unknown t: 0.1 SGS 2-sided
- FS 013 cellWidth: 1.0e-04 cinf: unknown - unknown t: 0.1 SGS 2-sided
- FSS 013 cellWidth: 1.0e-04 cinf: unknown - unknown t: 0.1 SGS 2-sided
- FS 014 cellWidth: 6.7e-05 cinf: unknown - unknown t: 0.1 SGS 2-sided
- FSS 014 cellWidth: 6.7e-05 cinf: unknown - unknown t: 0.1 SGS 2-sided
- FS 015 cellWidth: 4.0e-05 cinf: unknown - unknown t: 0.1 SGS 2-sided
- FSS 015 cellWidth: 4.0e-05 cinf: unknown - unknown t: 0.1 SGS 2-sided
- FS analytical solution
- FSS analytical solution



- FS 000 cellWidth: 2.0e-04 cinf: prescribed - prescribed t: 0.1 SGS 2-sided
- FSS 000 cellWidth: 2.0e-04 cinf: prescribed - prescribed t: 0.1 SGS 2-sided
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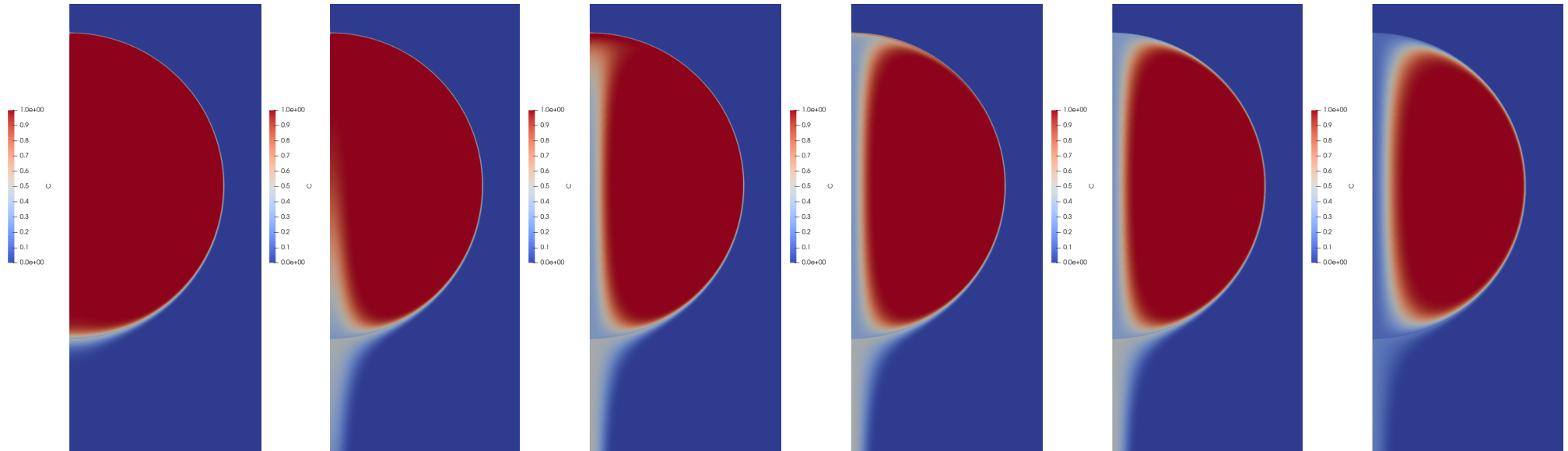


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- 015 cellWidth: 4.0e-05 cinf: unknown - unknown t: 0.1 SGS 2-sided

FS/FSS: +/- side

Motivation

(preliminary reference results (without SGS))



$t = \{0.01, 0.02, 0.03, 0.04, 0.05, 0.2\} \text{ s}$



Motivation (preliminary results)

