CHALMERS
UNIVERSITY OF TECHNOLOGY

Interfacial Mass Transfer in Syngas Fermentation – A Single Bubble Study

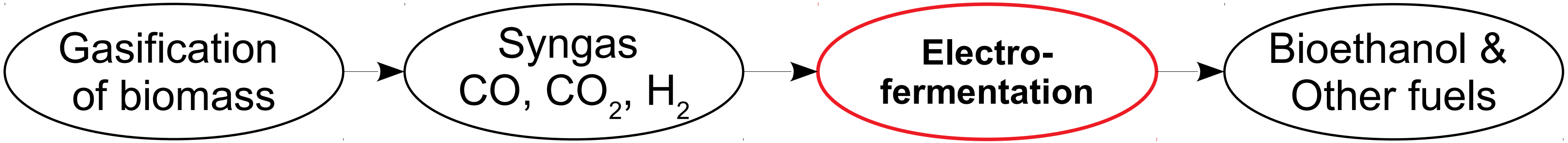
Mohsen Karimi & Henrik Ström

Nov - 2019

Problem Description:

Developing a theoretical model for mass transfer at the gas-liquid interface.

Why?

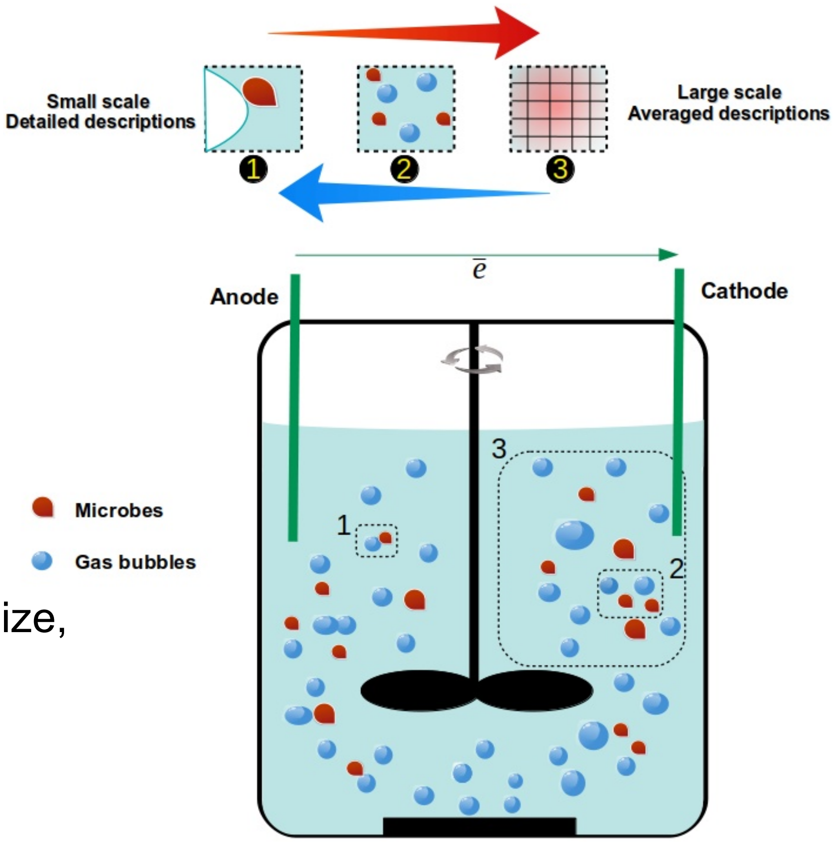


What's syngas electro-fermentation?

Converting syngas (H_2, CO, CO_2) into fuels using microorganisms augmented with electrical field to improve selectivity of target products and increase carbon efficiency.

Modeling challenges:

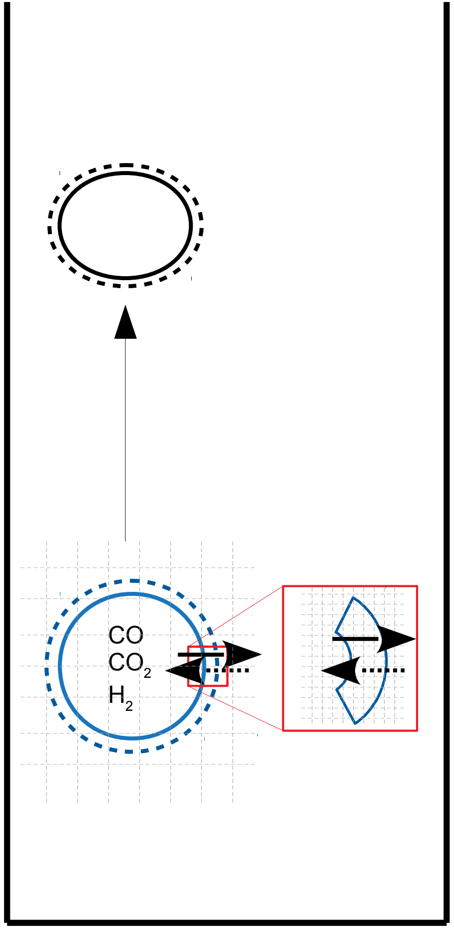
- Wide disparity of time and length scales,
- Transient changes of dispersed phase including size, shape, etc,
- Discontinuity of field variables at the interface,
- Non-Newtonian liquid phase,
- High Sc numbers.



Solution strategy:

Detailed simulation of mass transfer from single bubble into liquid:

- Rise of a single gas bubble
- Diffusion of species



Rise of a single gas bubble:

- Evaluating the solver for predicting the terminal rise velocity

- Validating with experiments for different ranges of:

$$760 \leq \rho \ [kg/m^3] \leq 1000$$
$$0.5 \leq \mu \ [mPa\,s] \leq 9.3$$
$$15.9 \leq \sigma \ [mN/m] \leq 72.8$$

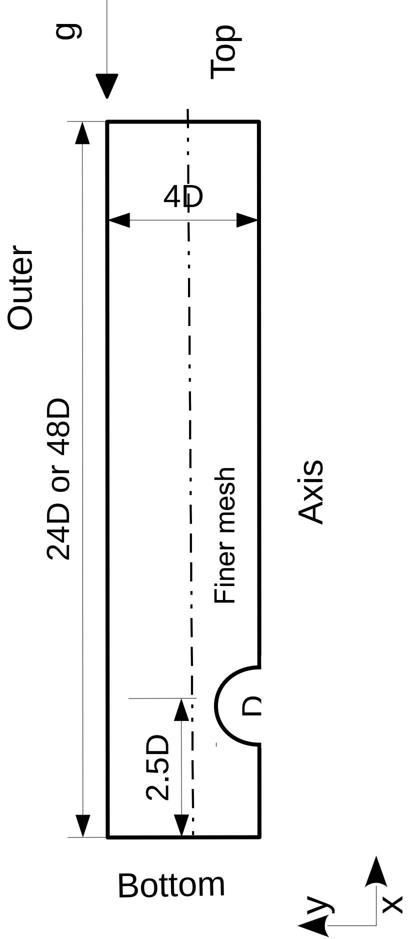
Rise of a single gas bubble | Case setup

Solver: **`interFoam`**

- Geometry: 2D Wedge
- Mesh:

$$8\ cells/D \rightarrow 1.25\ D < y \leq 4\ D$$
$$32\ cells/D \rightarrow 0 \leq y \leq 1.25\ D$$
$$64\ cells/D \rightarrow 0 \leq y \leq 1.25\ D$$
$$128\ cells/D \rightarrow 0 \leq y \leq 1.25\ D$$

- Boundary conditions
  - Axis of symmetry
  - Slip for the outer wall
- Post-processing: rise velocity based on center of mass displacement (i.e., **`functionObject`**)

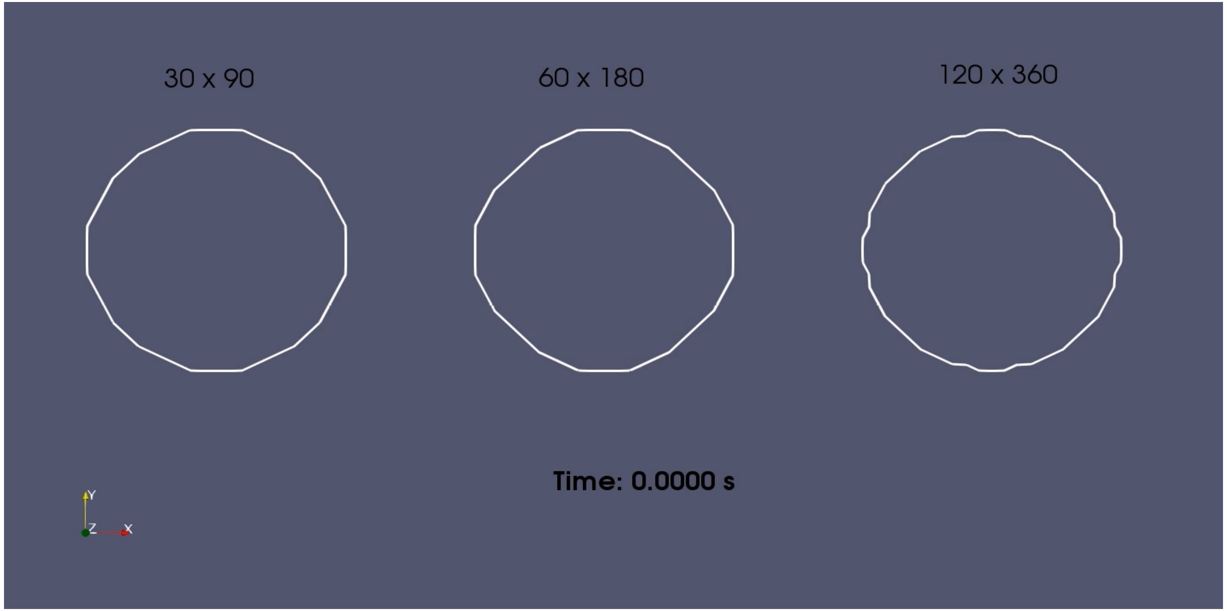


Rise of a single gas bubble | Case setup | Common problem

- Parasitic currents:
  - stationary bubble,
  - density ratio = 1,
  - no buoyancy,
    and thus

$$\Delta p = \sigma \kappa$$

- Remarks:
  - Mesh requirements
  - Time step & CFL recommendations
  - Inertia dominant flow



link2

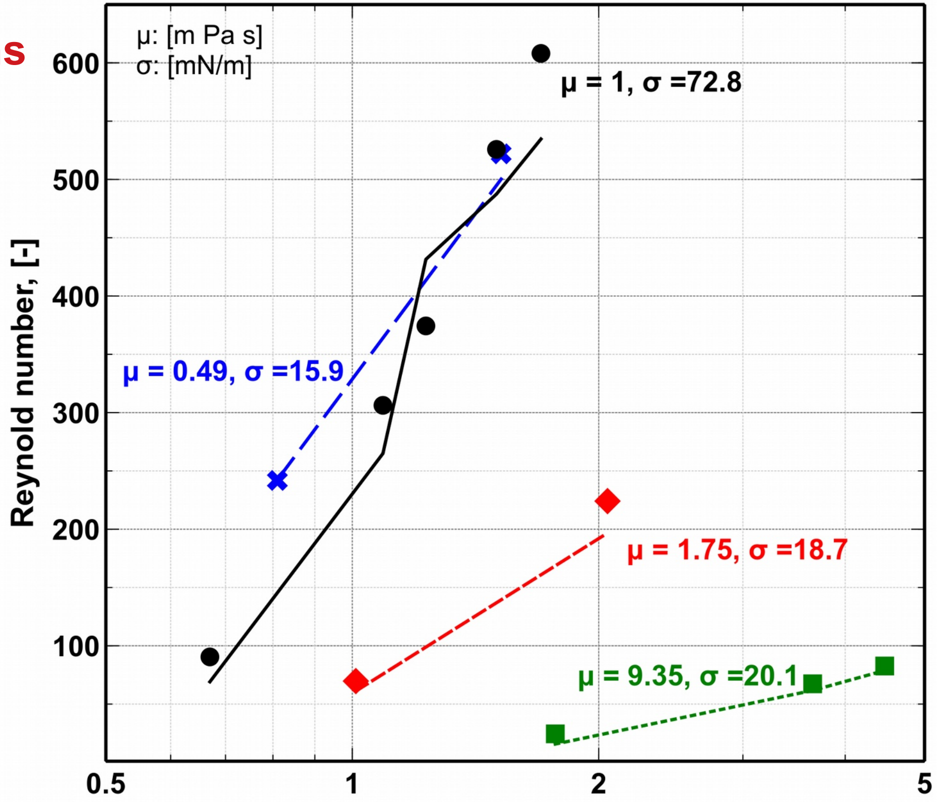
Rise of a single gas bubble | Validations

- Test cases

Liquid	$d, [mm]$	$\rho, [kg/m^3]$	$\mu, [mPa\,s]$	$\sigma, [mN/m]$
Water	0.67	1000	1.0	72.8
	1.09			
	1.23			
	1.5			
	1.7			
DMST00	0.81	761	0.49	15.9
	1.52			
DMST02	1.01	873	1.75	18.7
	2.05			
DMST11	1.77	935	9.35	20.1
	3.65			
	4.47			

	Min	Max
Diameter	0.67	4.47
Density	761	1000
Viscosity	0.49	9.35
Surface tension	15.9	72.8

Rise of a single gas bubble | Validations



Symbols: Experiments by Zenit et al. (2008)
Lines: Simulations

Remarks:

- Worst case: High Re, low viscosity
- Best cases: Low Re, high viscosity
- It is not perfect agreement, but for the target application it is acceptable.

Diffusion of species

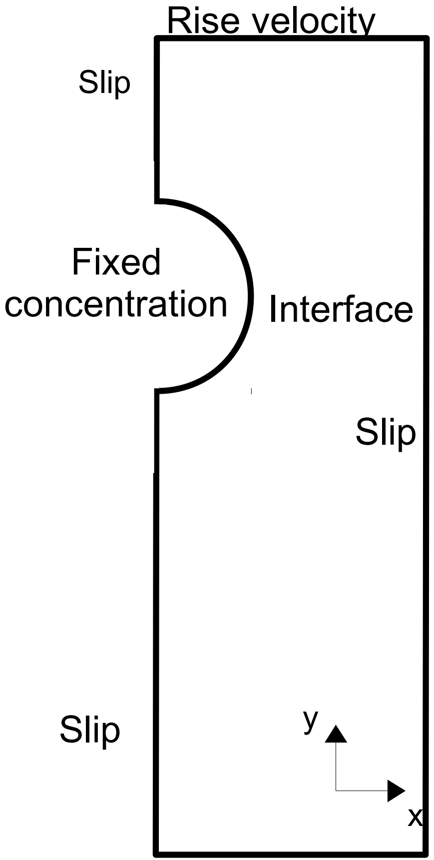
Resolve concentration profile:

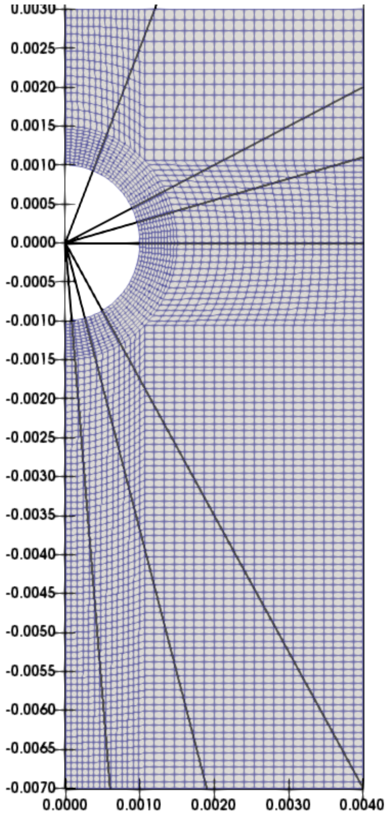
- Concentration & velocity on different polar angles,
- Force at the interface
- Flux at the outlet
- $L1$, $L2$, and L_inf norms for concentration, velocity and force

Is there a scaling factor between the thickness of concentration boundary layer and dimensionless numbers?

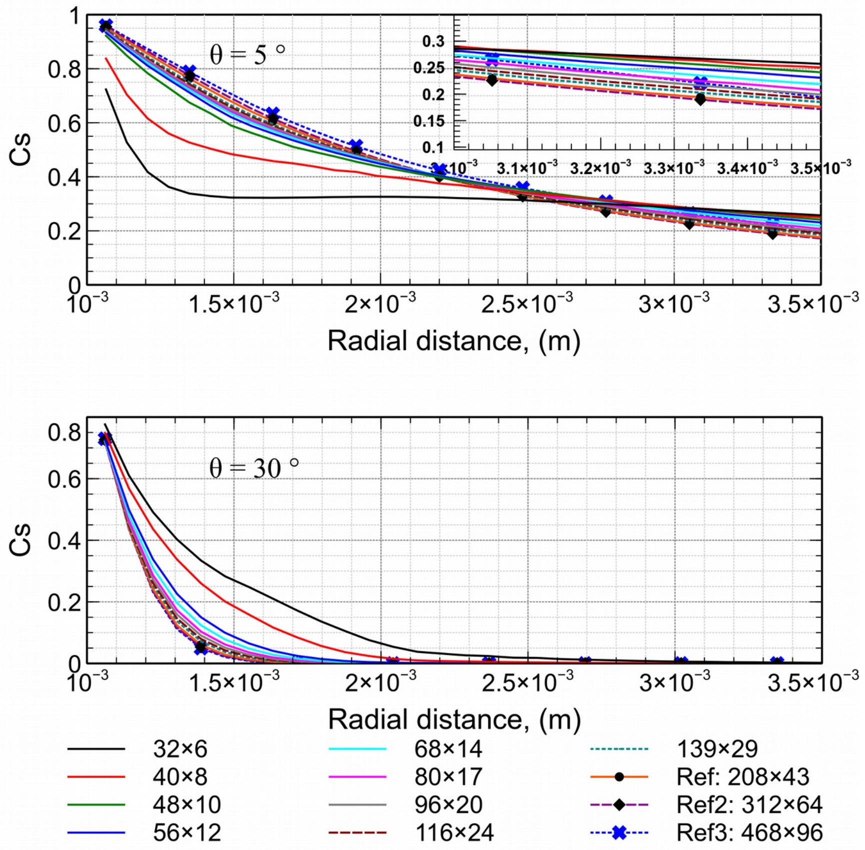
Diffusion of species | Case setup

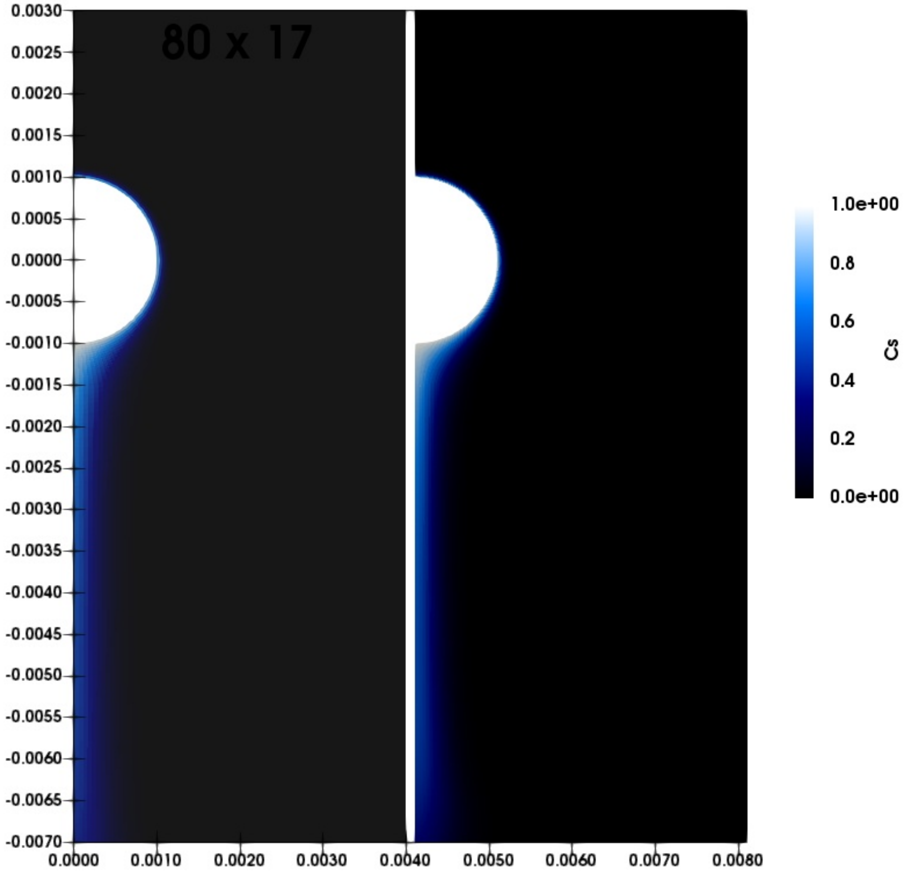
Case	Elements around interface	Total cells	Cells / d
Base	40 x 8	1,120	32
Watermelon	32 x 6	640	24
Kiwi	48 x 10	1,632	40
Apple	56 x 12	2,296	48
Plum	68 x 14	3,298	56
Grape	80 x 17	4,640	68
Strawberry	96 x 20	6,624	80
Mango	116 x 24	9,570	96
Cherry	139 x 29	12,530	116
ref	208 x 43	27,664	172
ref2	312 x 64	62,088	256
ref3	468 x 96	139,698	385





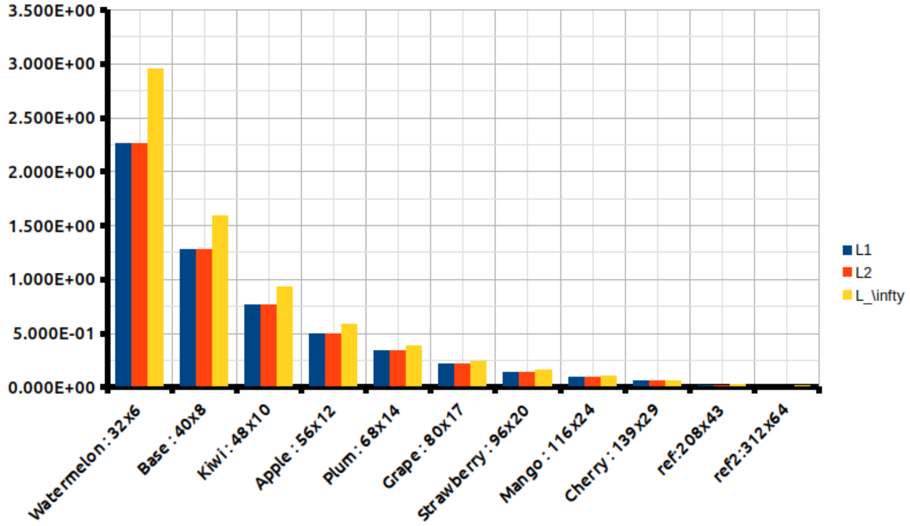
Diffusion of species | Concentration profiles



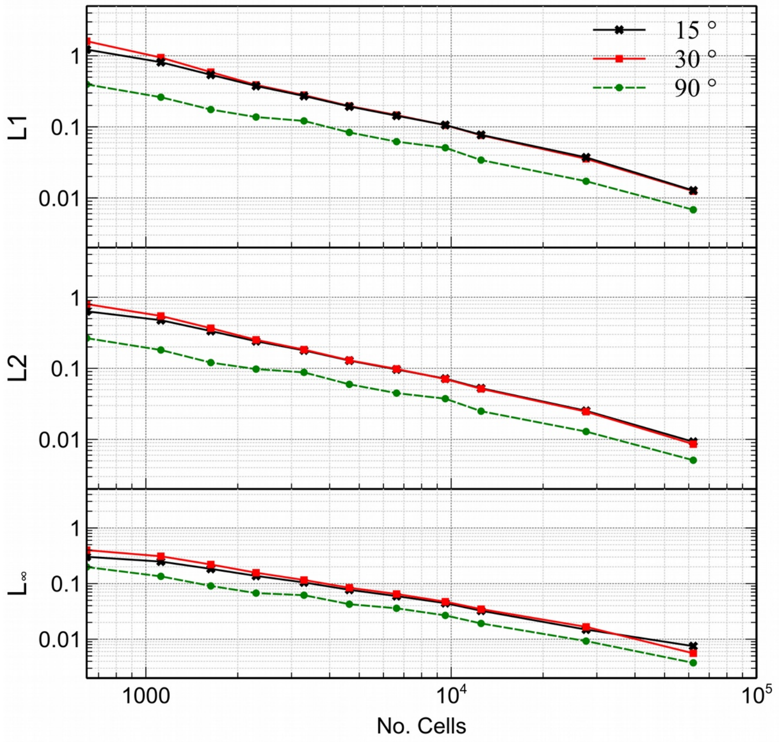


Diffusion of species | Norms

Force at the interface

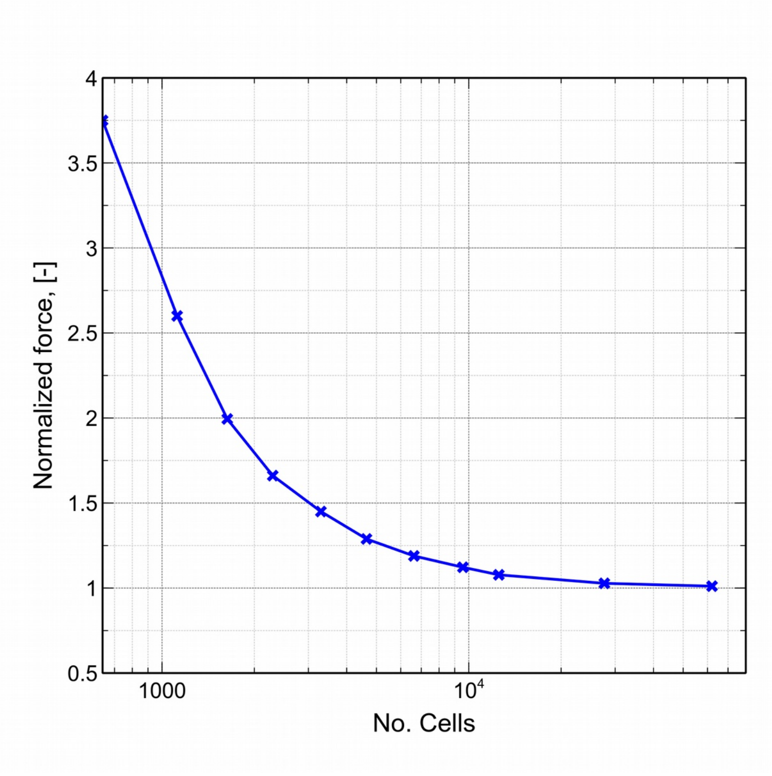


Concentration profile

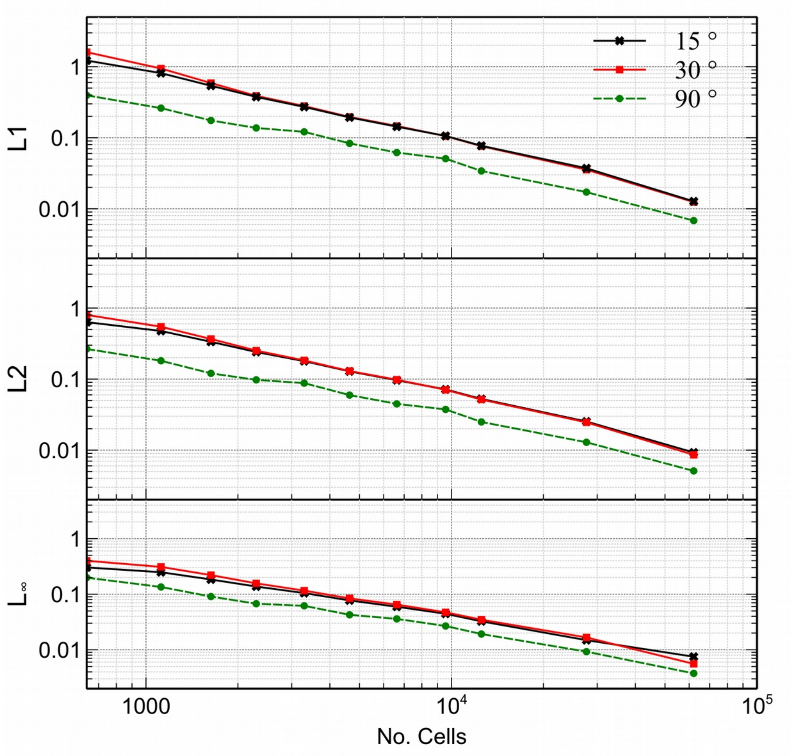


Diffusion of species | Norms

Force at the interface



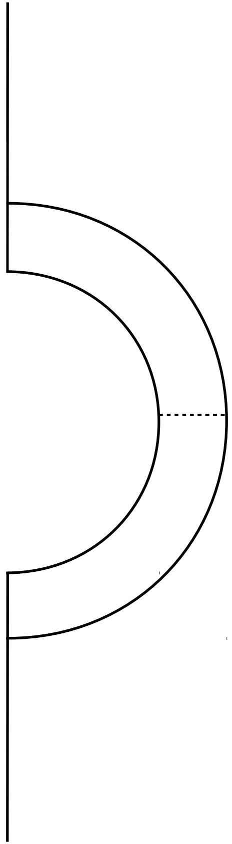
Concentration profile



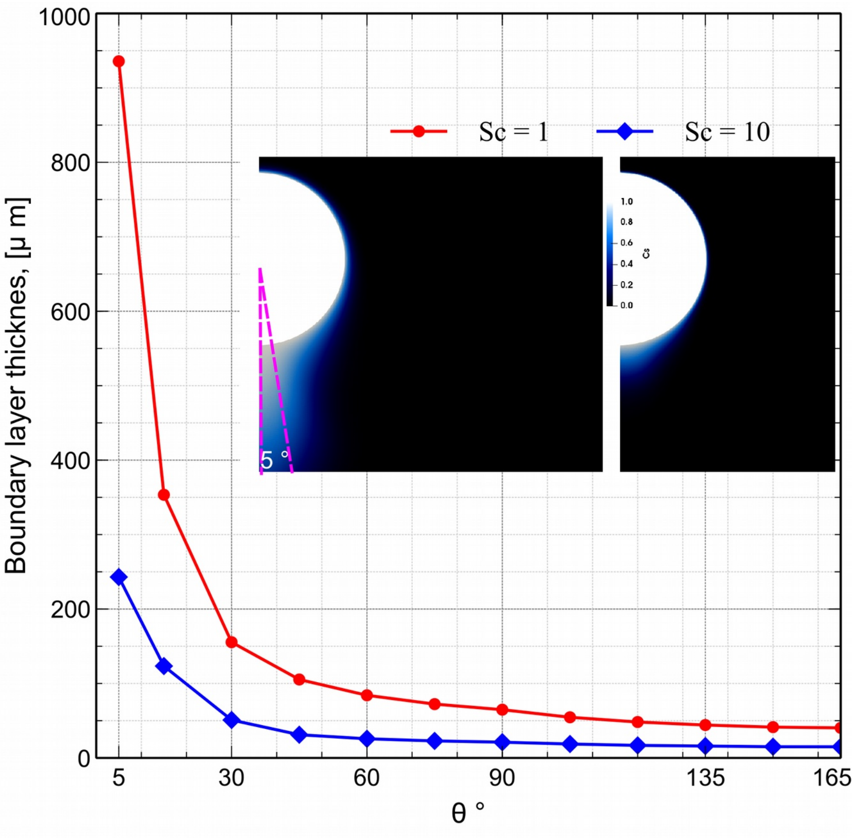
Diffusion of species | Boundary layer thickness & scaling

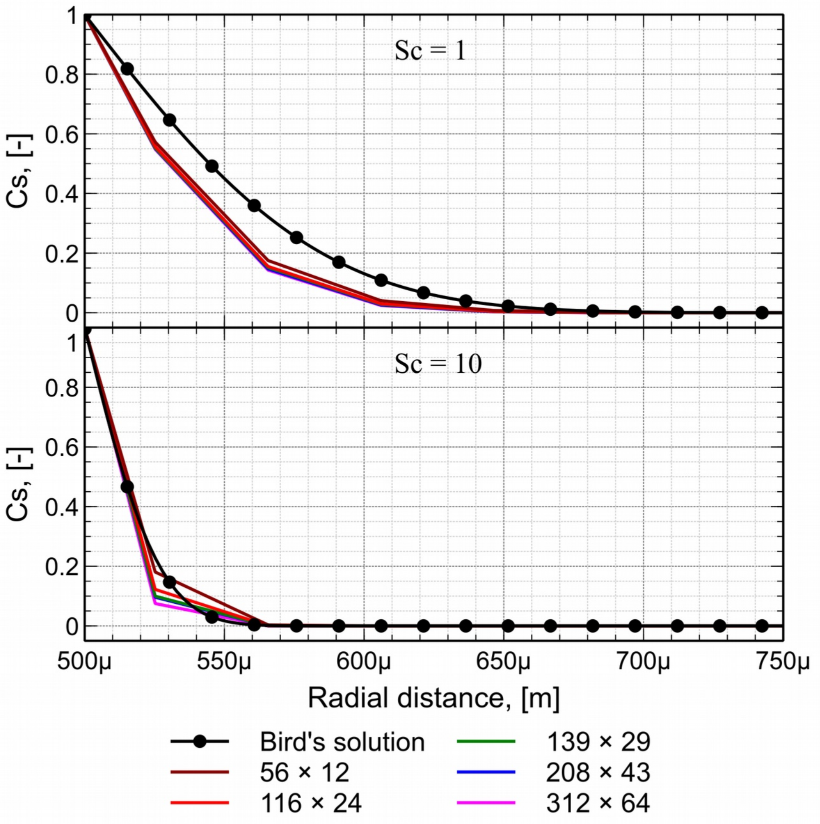
- A sub-grid model for:
  - Species diffusion around the bubble
  - Boundary layer thickness
  - High Sc numbers

- Case setup:
  - Single bubble in rectilinear regime with axis of symmetry.
  - Sc = 1 to 150.
  - Looking at the equator’s mass boundary layer thickness.
  - Assumption: $\delta \propto 1/\sqrt{Sc}$



Comparing concentration profile with Bird’s analytical solution for Fick’s second law

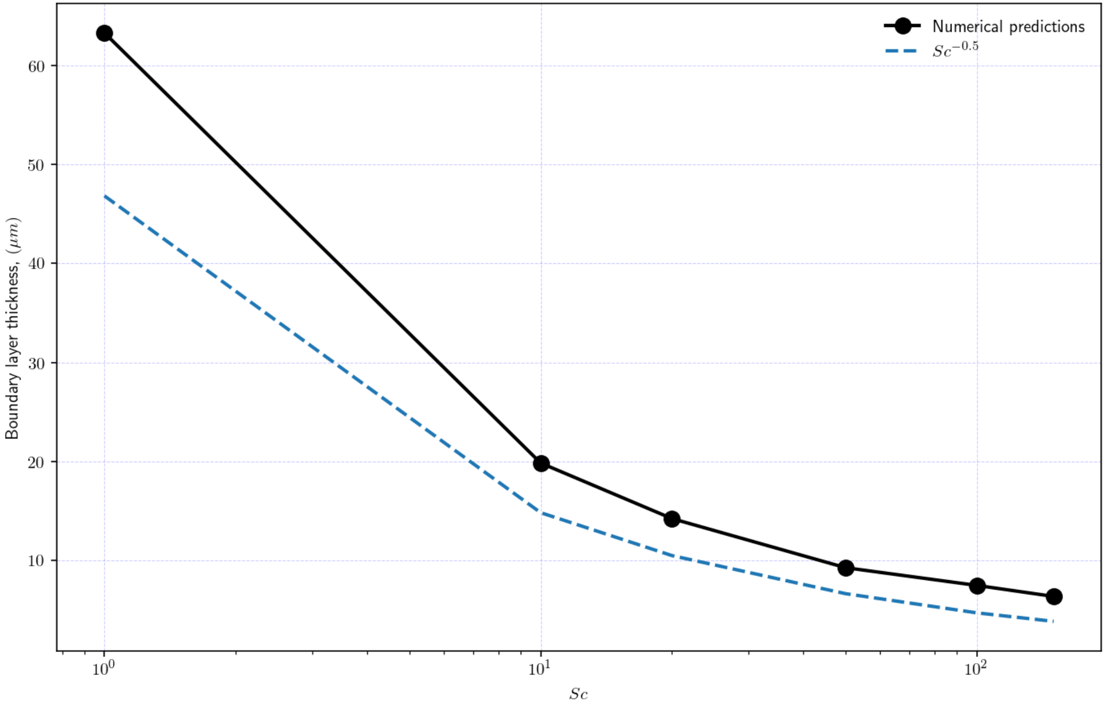




Diffusion of species | Boundary layer thickness & scaling

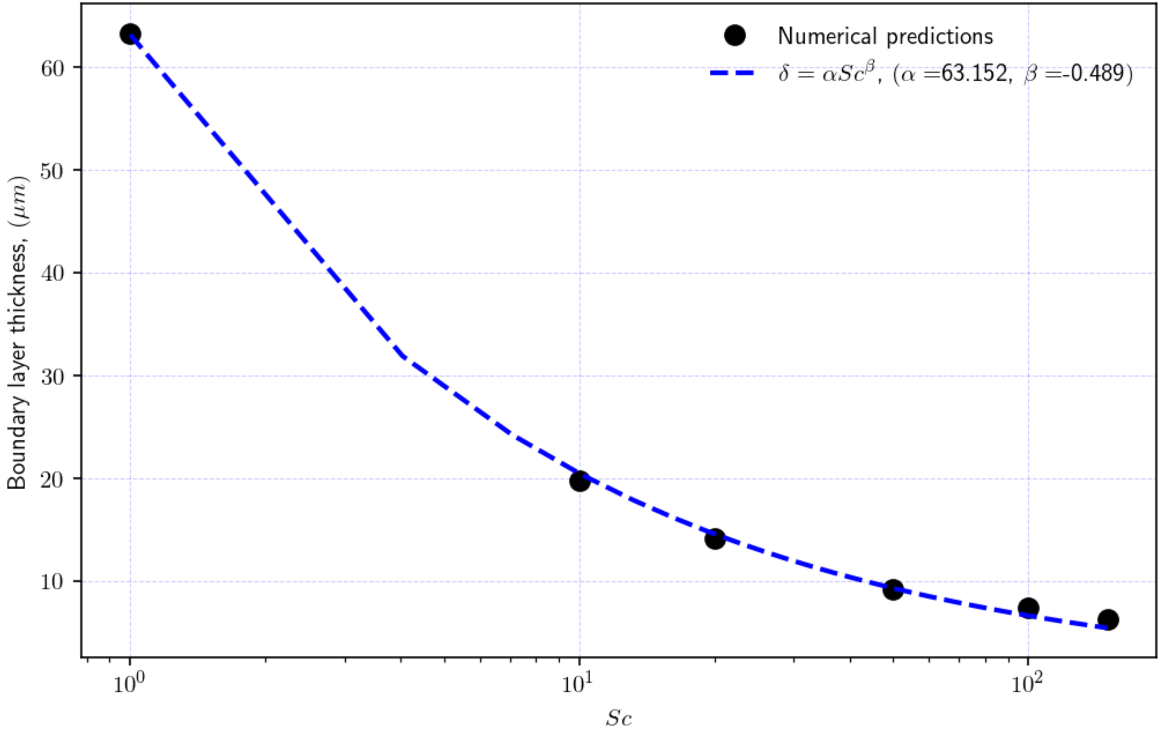
$$\delta \propto 1/\sqrt{Sc} \quad ?$$

$$\delta = \frac{d}{2}\sqrt{\frac{\pi}{ReSc}}$$

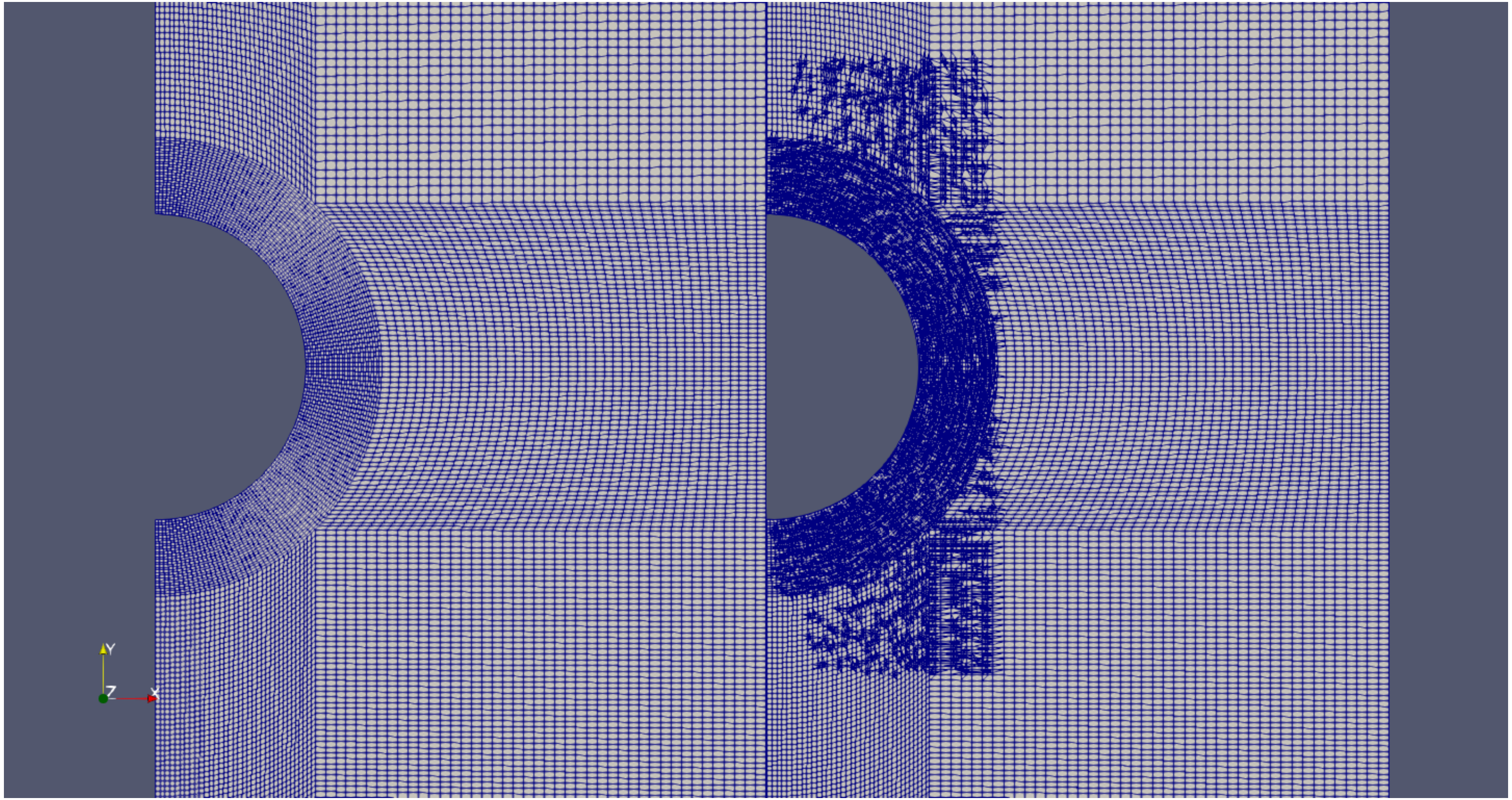


Diffusion of species | Boundary layer thickness & scaling

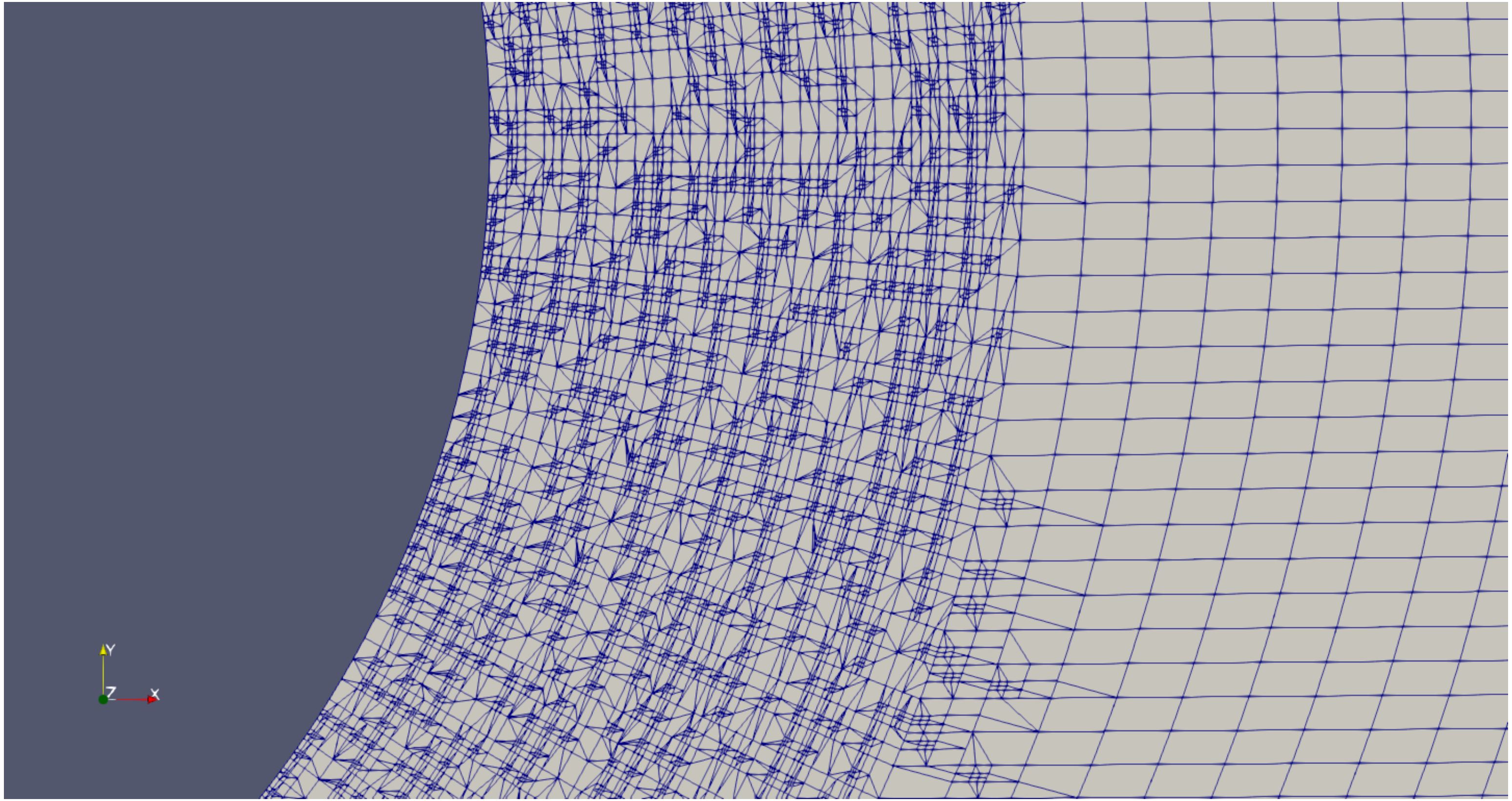
$\delta \propto \alpha Sc^{\beta}$?



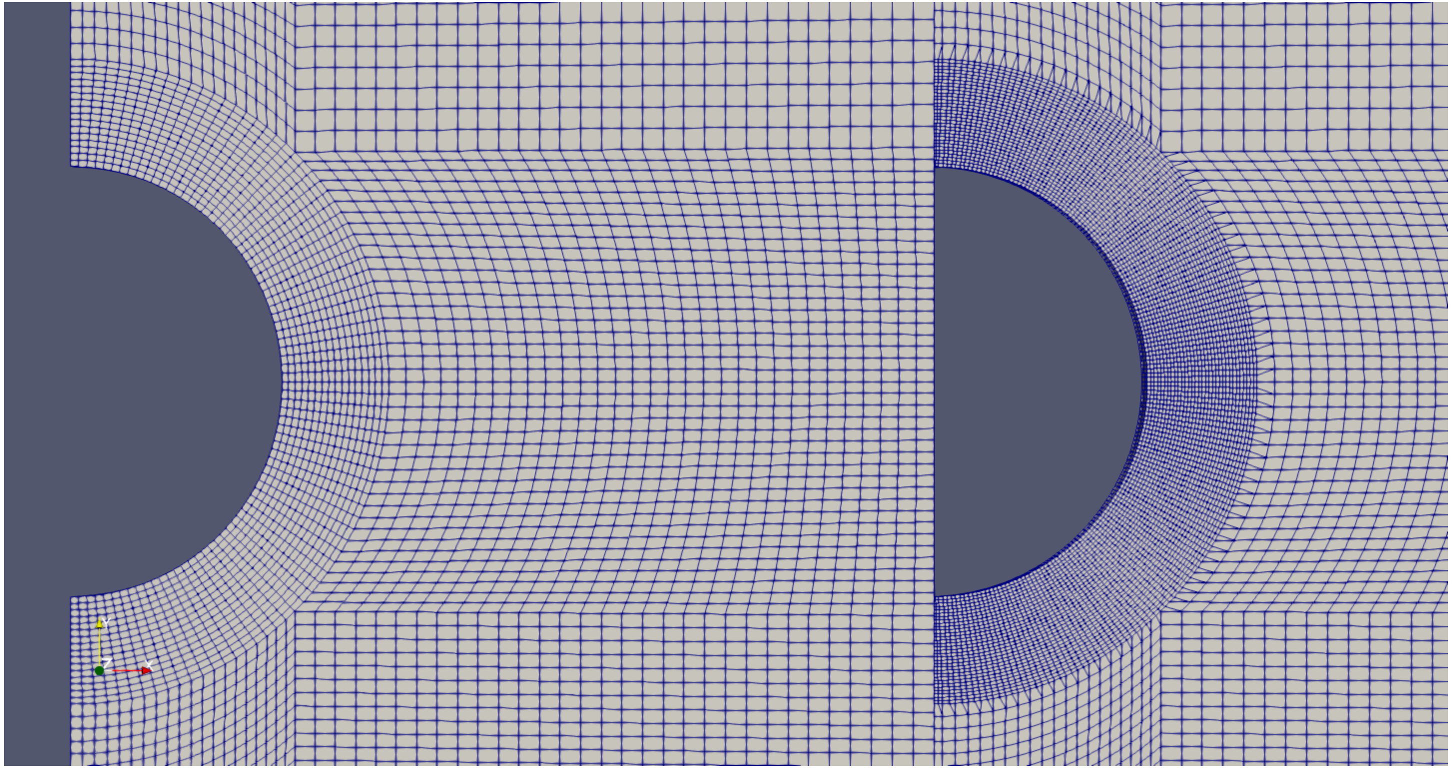
Diffusion of species | Boundary layer thickness & local refinement



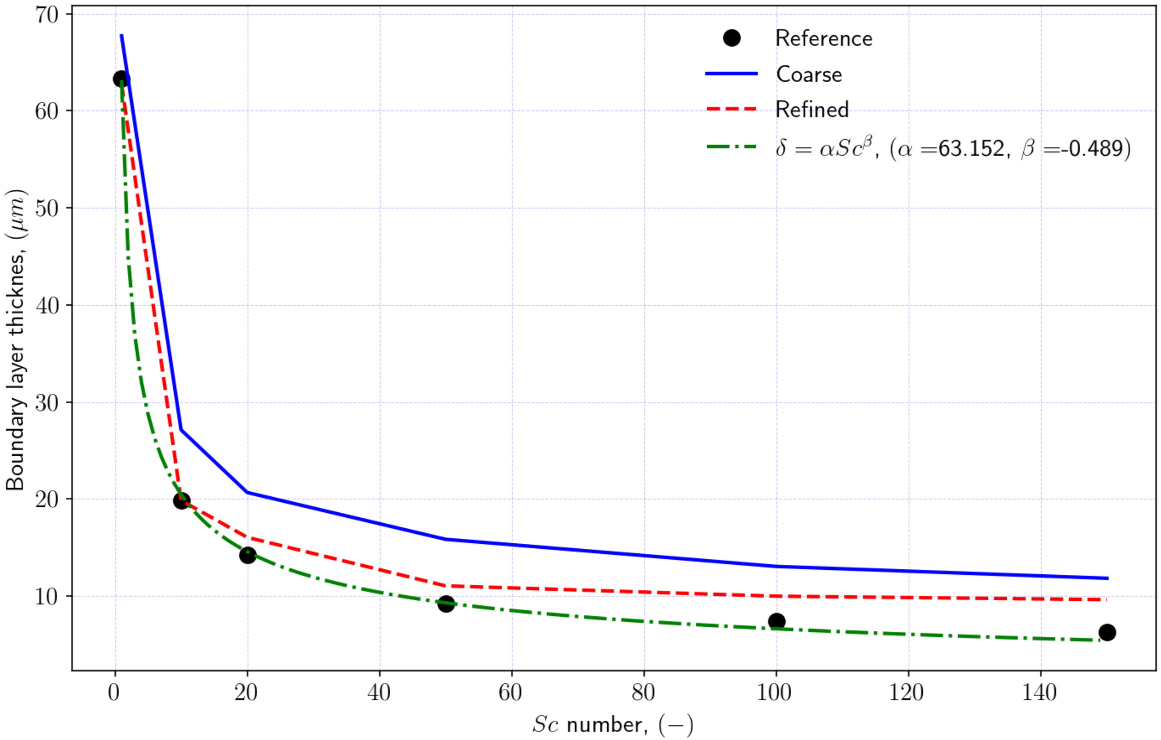
Diffusion of species | Boundary layer thickness & local refinement



Diffusion of species | Boundary layer thickness & local refinement



Diffusion of species | Boundary layer thickness & local refinement



Concluding remarks:

- Preliminary results are presented for formulating a model of mass transfer at gas-liquid interface.
- Model's components, rise velocity and species diffusion, are determined.
- Validations of rise velocities with experimental data are performed.
- Mesh requirements for species diffusion are evaluated using various quantities (norms, force at the interface).
- A sub-grid model for concentration profile is investigated.
- A scaling factor for the thickness of mass boundary layer is tested.
- The sub-grid model should be implemented within OpenFOAM.

CHALMERS
UNIVERSITY OF TECHNOLOGY