POLITECNICO DI MILANO
CFD for Nuclear Engineering

Single Phase Case
BALI-2

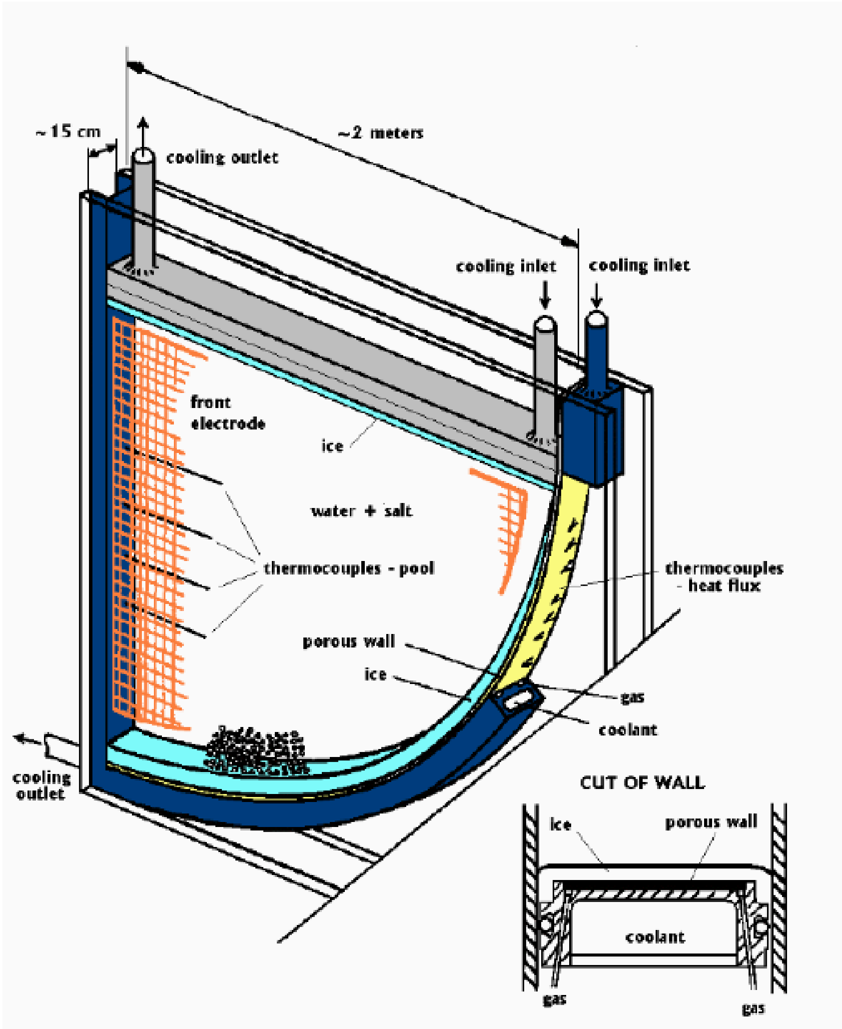
Introduction

Facility, purpose, goals

Objective: Validate simulation results with experimental data and compare results with literature benchmarks.

Our case study:

- 2m depth
- 15kW of grid power
- Ra = 2.36e16
- Pr = 6.5
- No top cooling



The BALI-2 facility is a

- 2D, quarter-cylinder used to simulate and study single-phase flow under Rayleigh numbers ~ 10^{17}.
- Investigates thermo-hydraulic phenomena such as in-vessel melt retention (IVMR).
- Operates with water to achieve thermal properties comparable to **oxidic corium**
- Internally heated using a grid of heaters.

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Preprocessing

Experimental data & Heat Transfer

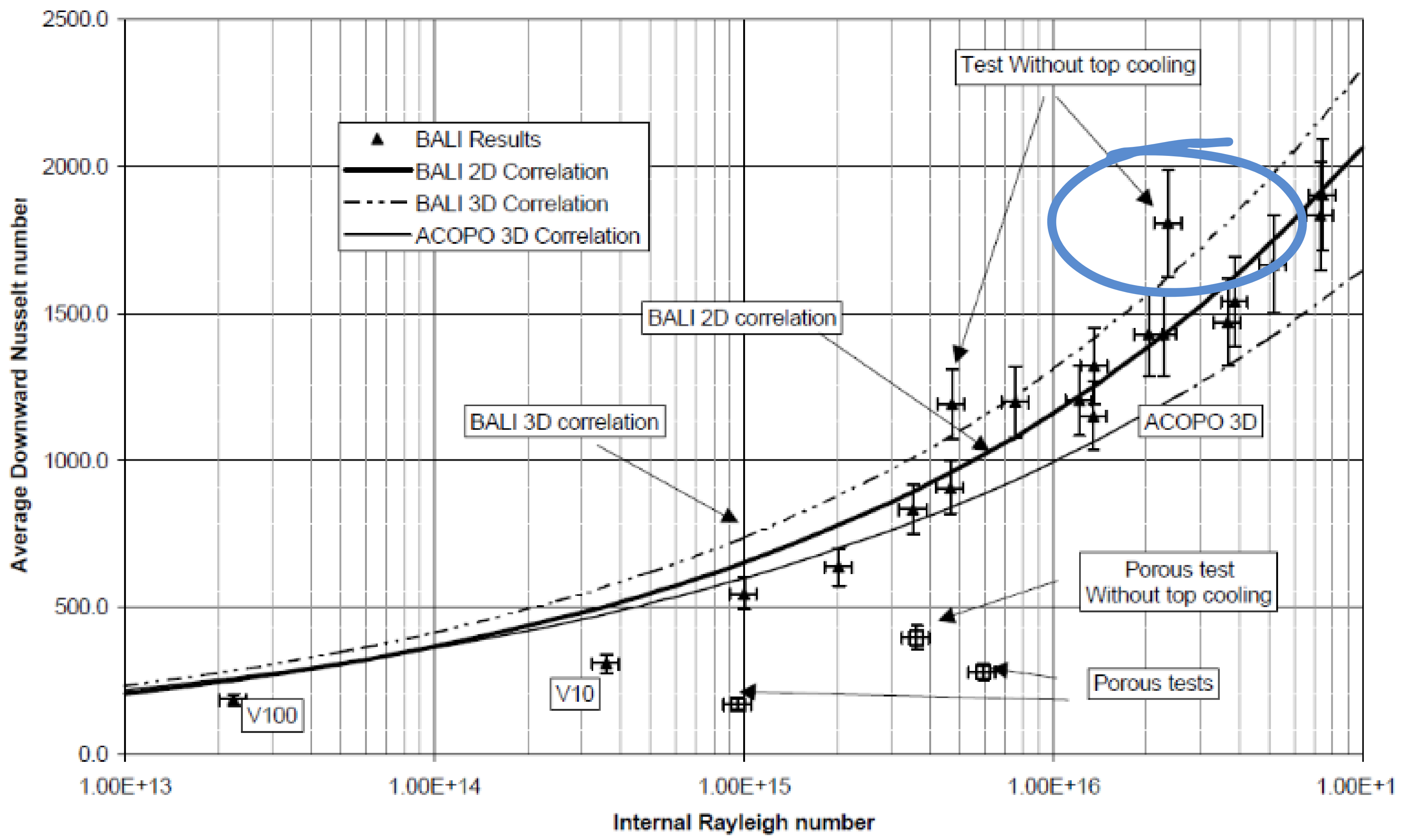
Bulk temperature was computed analytically with the given Nusselt number correlation.

From the given literature we see that our particular case is the furthest away from the correlation

$$Q = \alpha A \Delta T$$

$$\Delta T = \langle T \rangle - T_{\text{ice wall}}$$

<T> = 98C = 370K



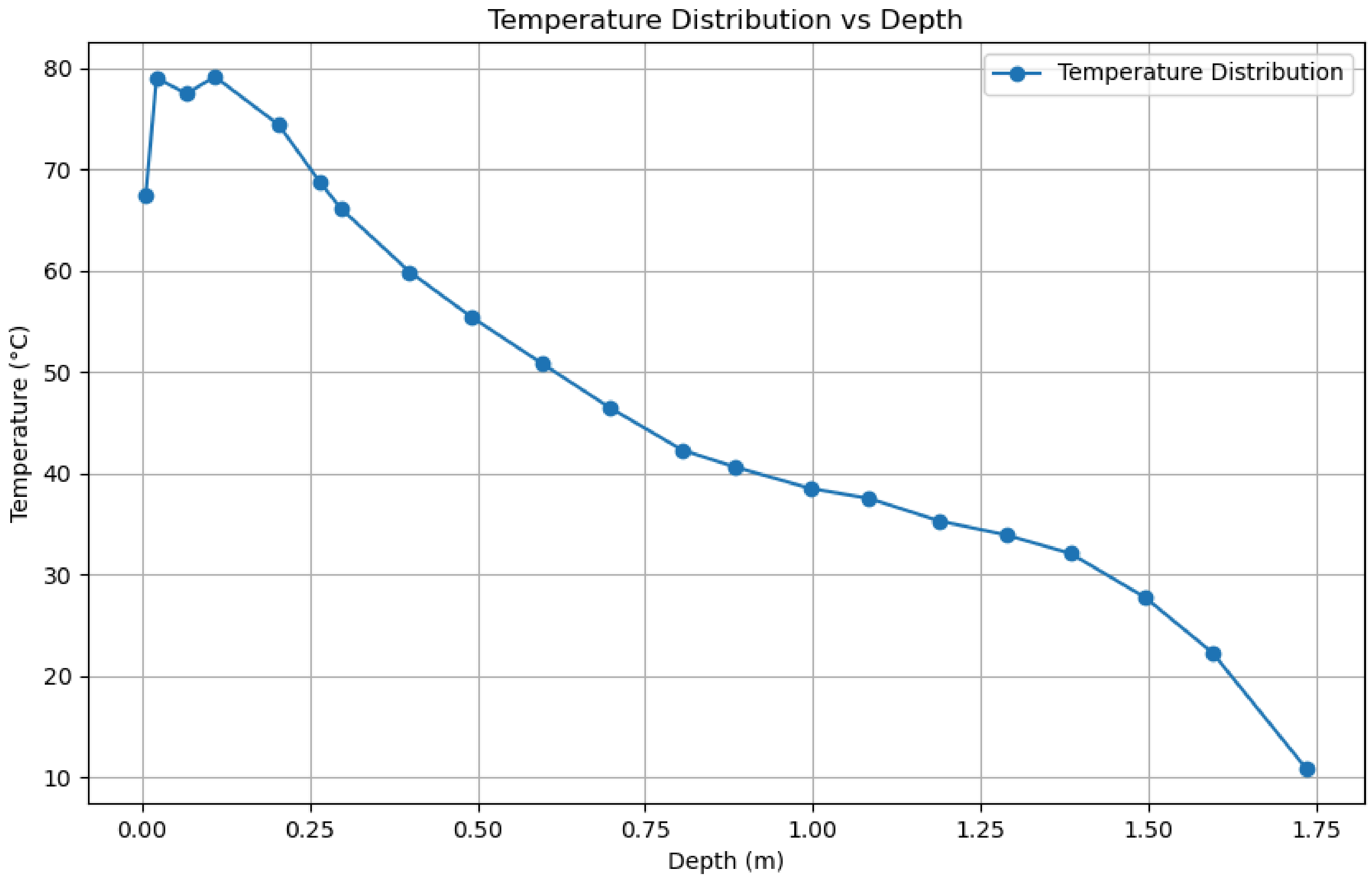
We immediately noticed that the temperature is really high which could be a concern for the fluid proprieties.

Preprocessing

Experimental data & Heat Transfer

From given experimental data we computed the average temperature along the straight vertical wall to use as a reference

We used it as a convergence monitor



Average T = 50C = 323K

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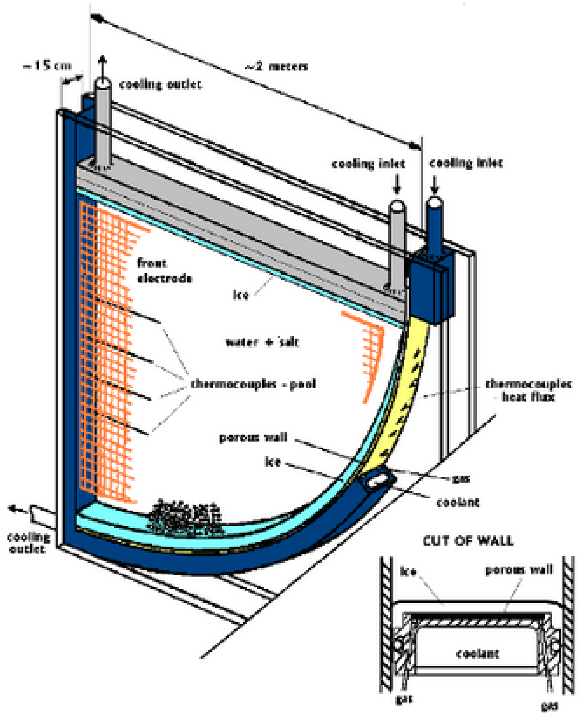
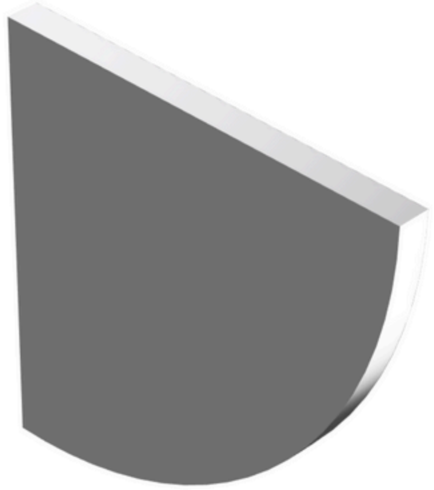
Meshing

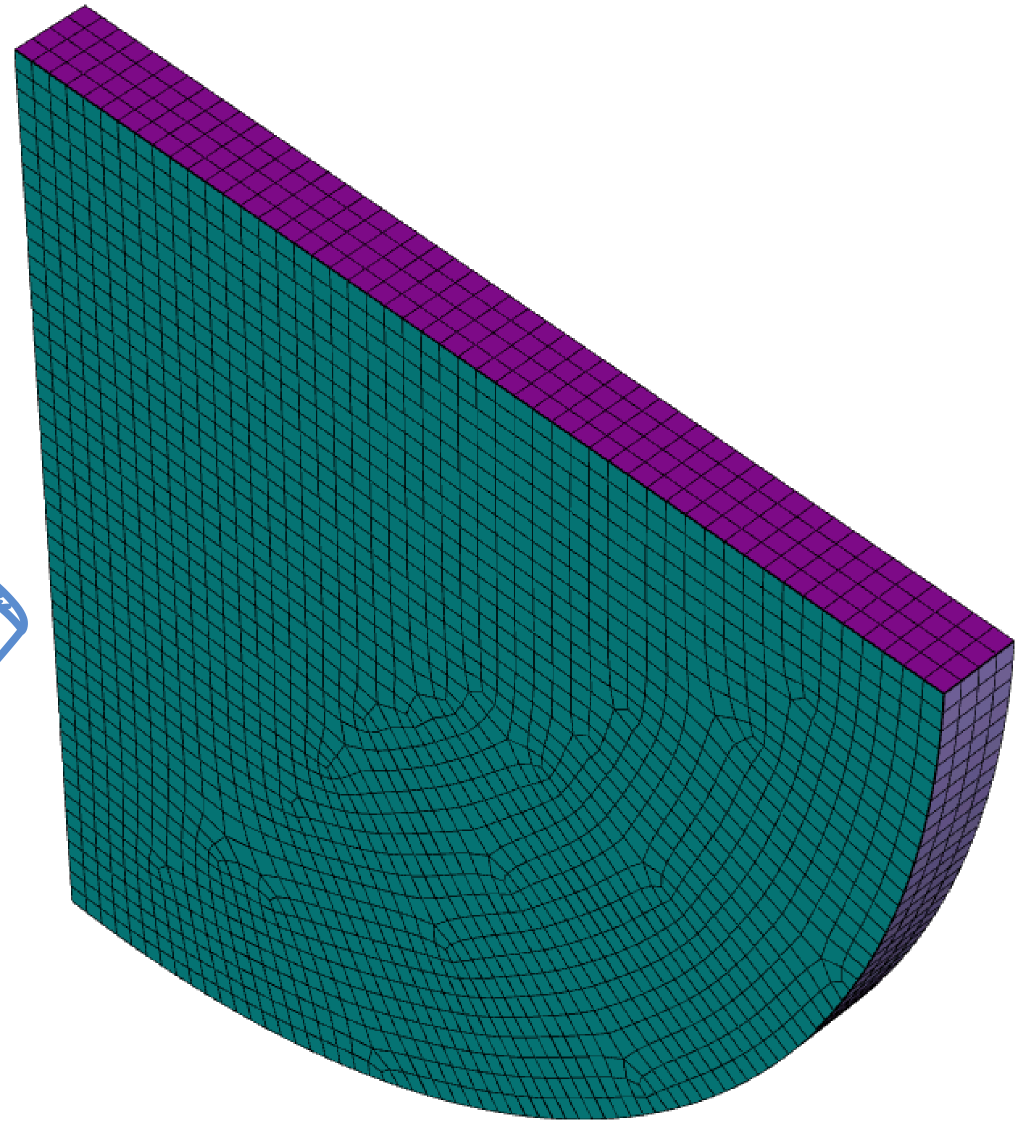
From Real Geometry to Mesh

Due to the thin geometry we where constrained on how we could define the boundary layer.

We had to compromise between a fine boundary layer and a light overall mesh for computation time optimization





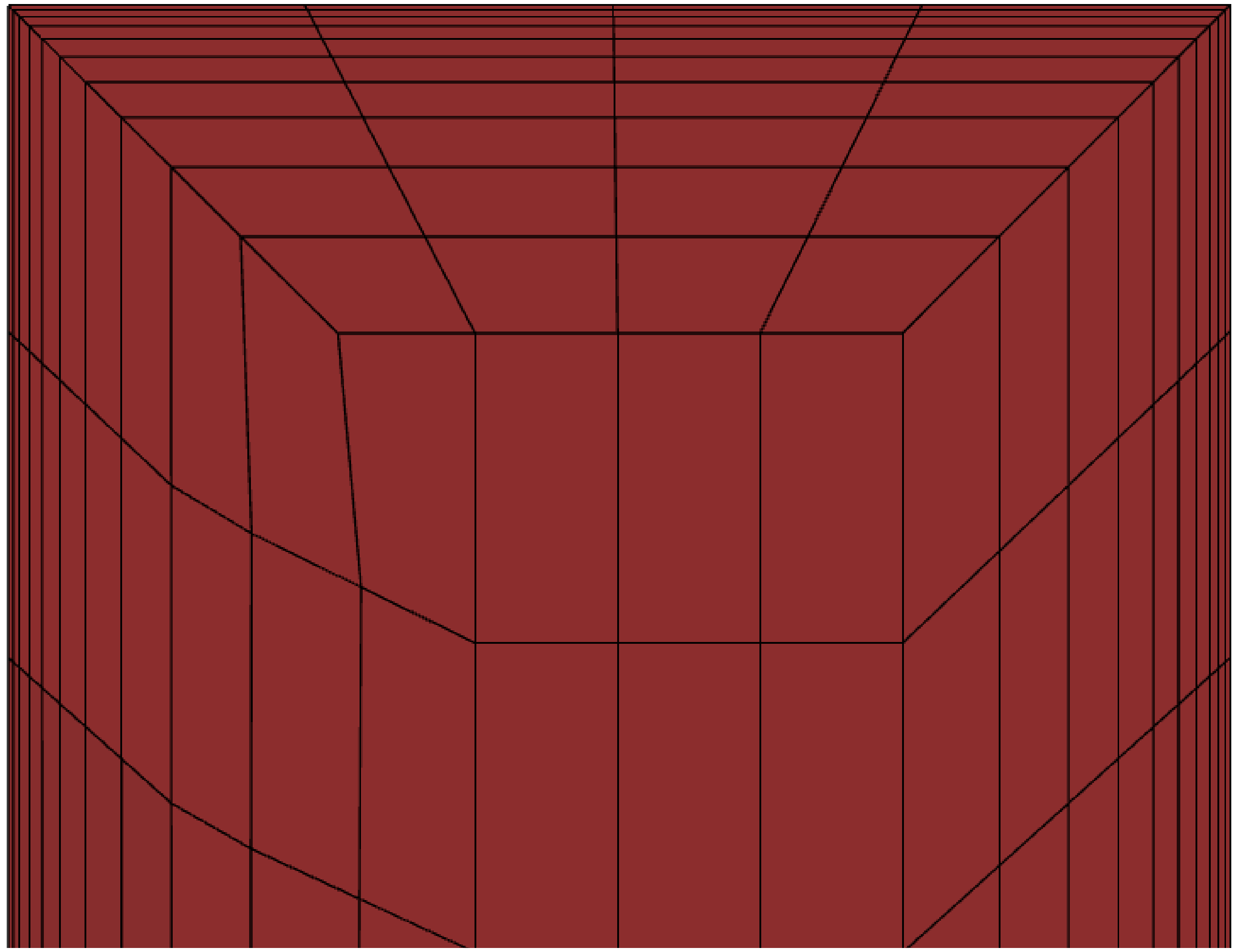


	AR	Orthogonality	Swekness
min	2.23	0.565	4.8e-5
avg	29.20	0.815	0.333
max	161.15	0.999	0.619

Meshing

Boundary Layer

Uniform boundary of 10 Layers with a growth rate of 1.4 and a first height of 1mm

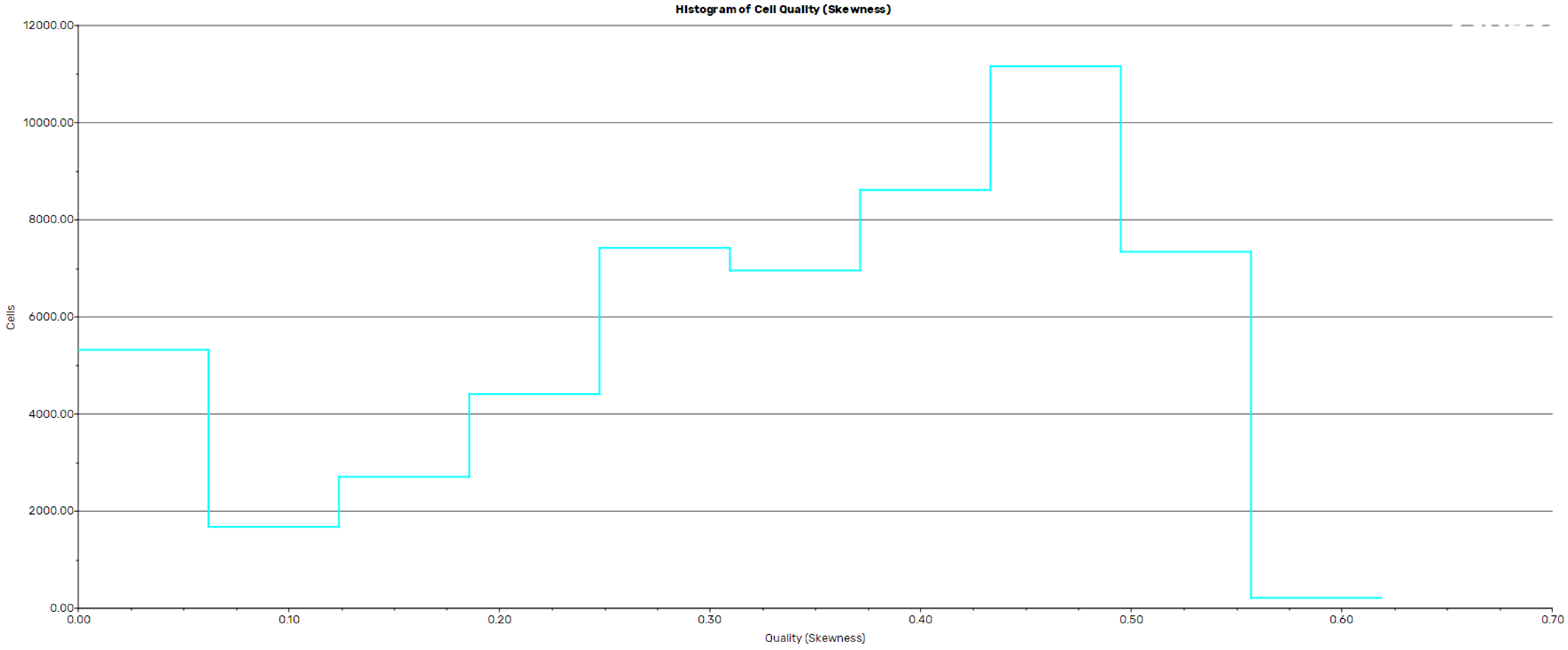


A section across the XZ plane

The boundary layer was supposed to be relatively thin, as the highest velocity was expected along the wall subjected to cooling.

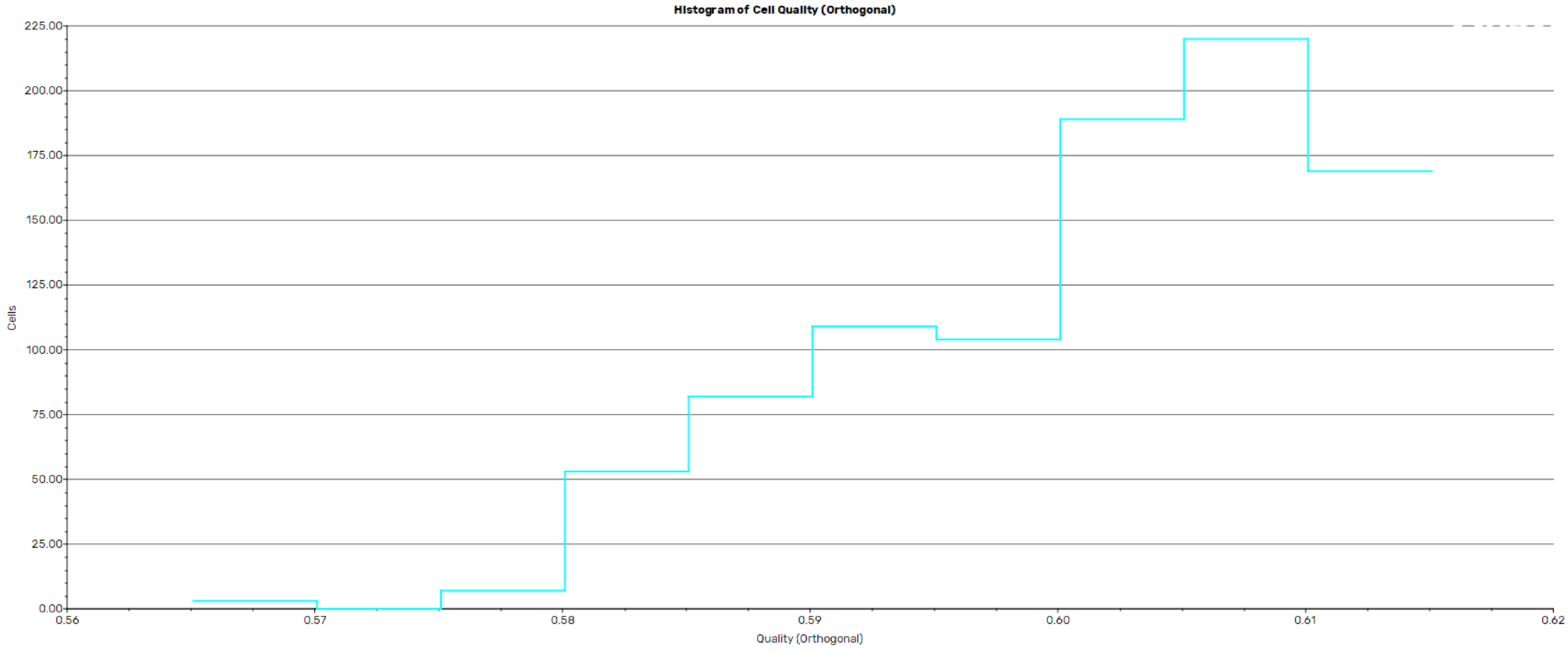
Meshing

Mesh stats - Skweness



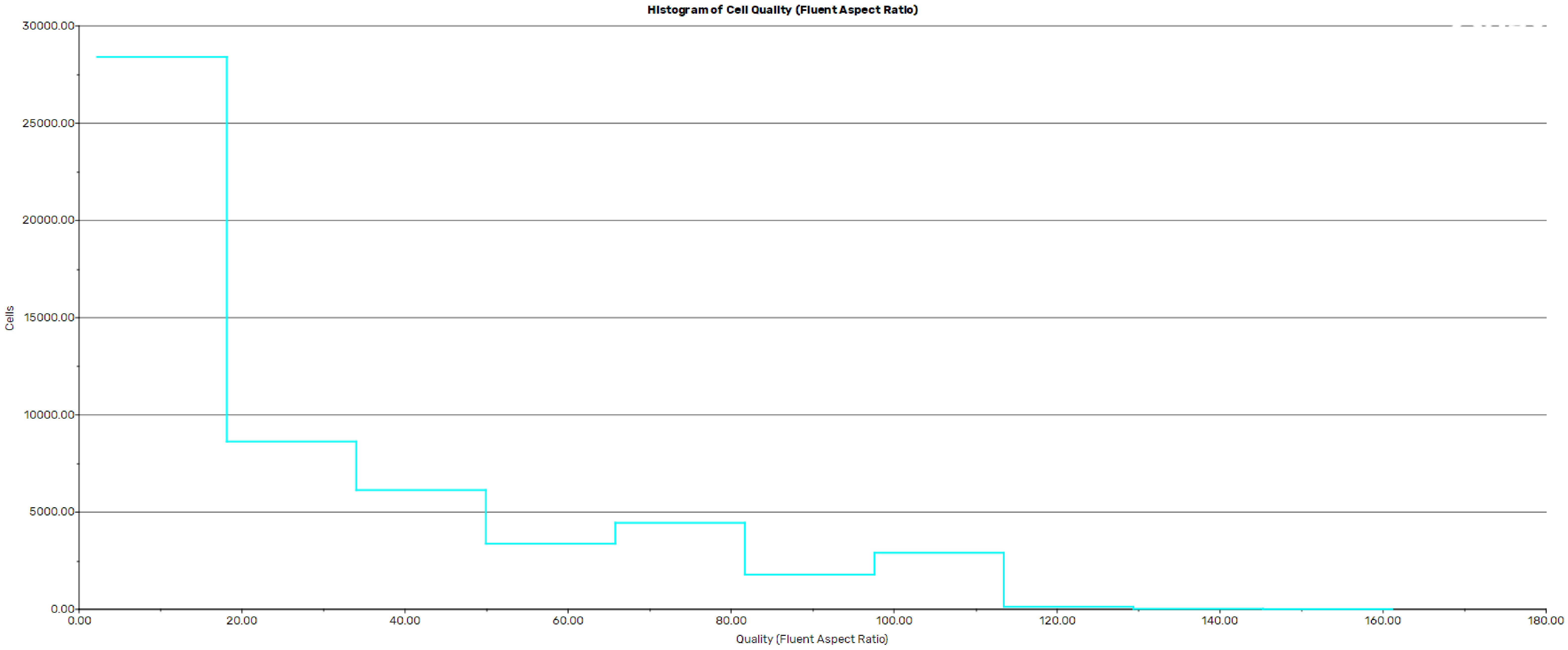
Meshing

Mesh stats - Orthogonality



Meshing

Mesh stats - Aspect Ratio



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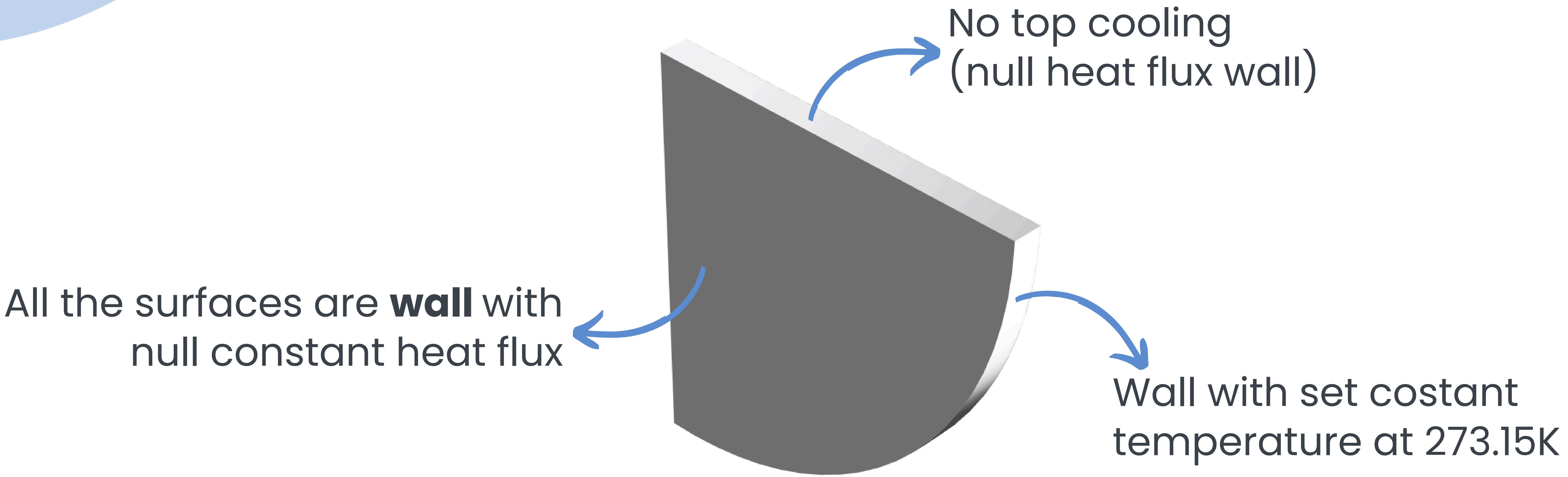
Modelling & Simulation

Boundary Conditions



Modelling & Simulation

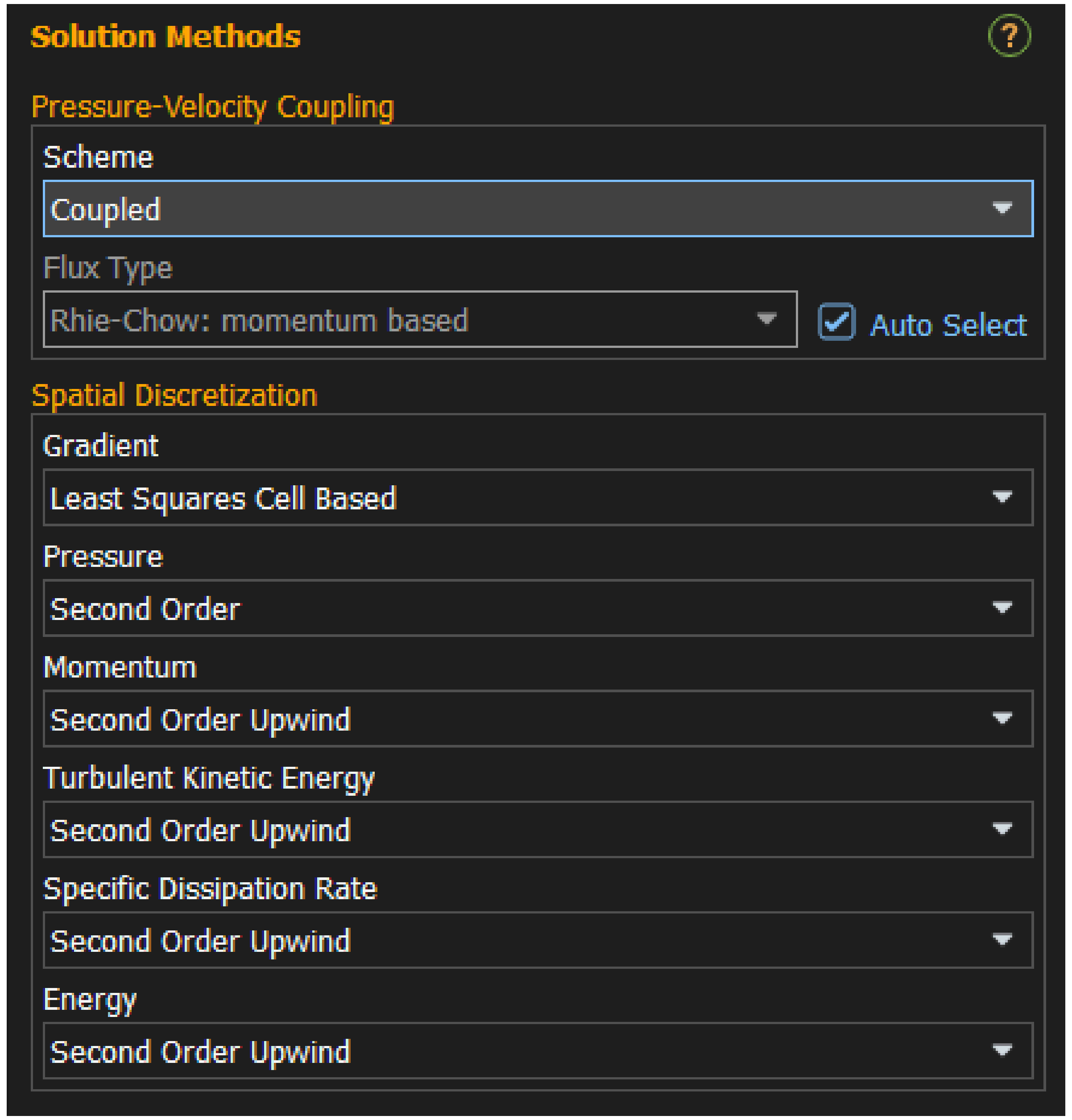
Discretization Methods

The first 100 iterations were performed with very low relaxation factors to prevent the simulation from immediately overwriting the initial conditions.

The simulation began with most methods set to first-order accuracy for the initial 1000 iterations.

Subsequently, it was switched to **second-order** accuracy for over 10,000 iterations.

When the simulation appeared not to improve anymore, we transitioned to a **coupled** discretization scheme, which ultimately facilitated convergence.



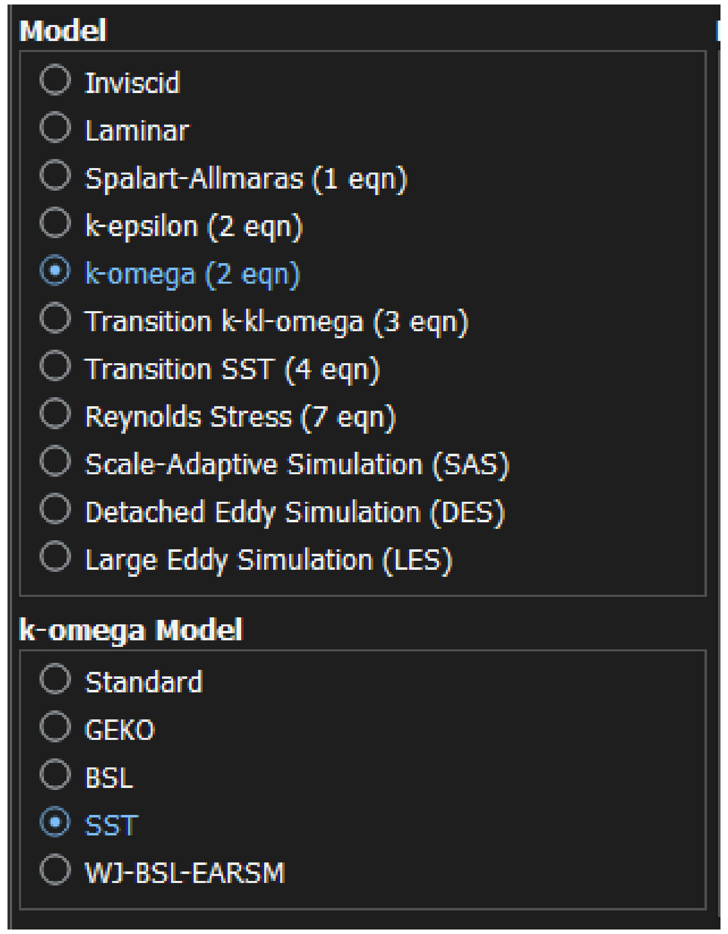
Modelling & Simulation

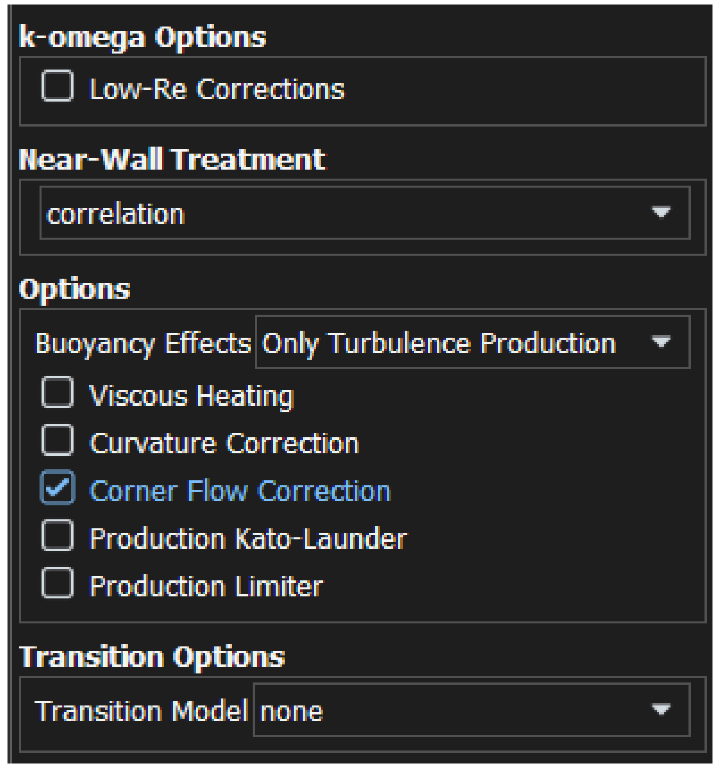
Turbulence Models

We selected the k-omega SST model with quadratic closure.

The k-epsilon realizable model was avoided because, despite improving the Boussinesq hypothesis with quadratic terms, it would require a Low-Re correction and additional boundary layer mesh refinement.

The laminar model was excluded due to the high Rayleigh number.





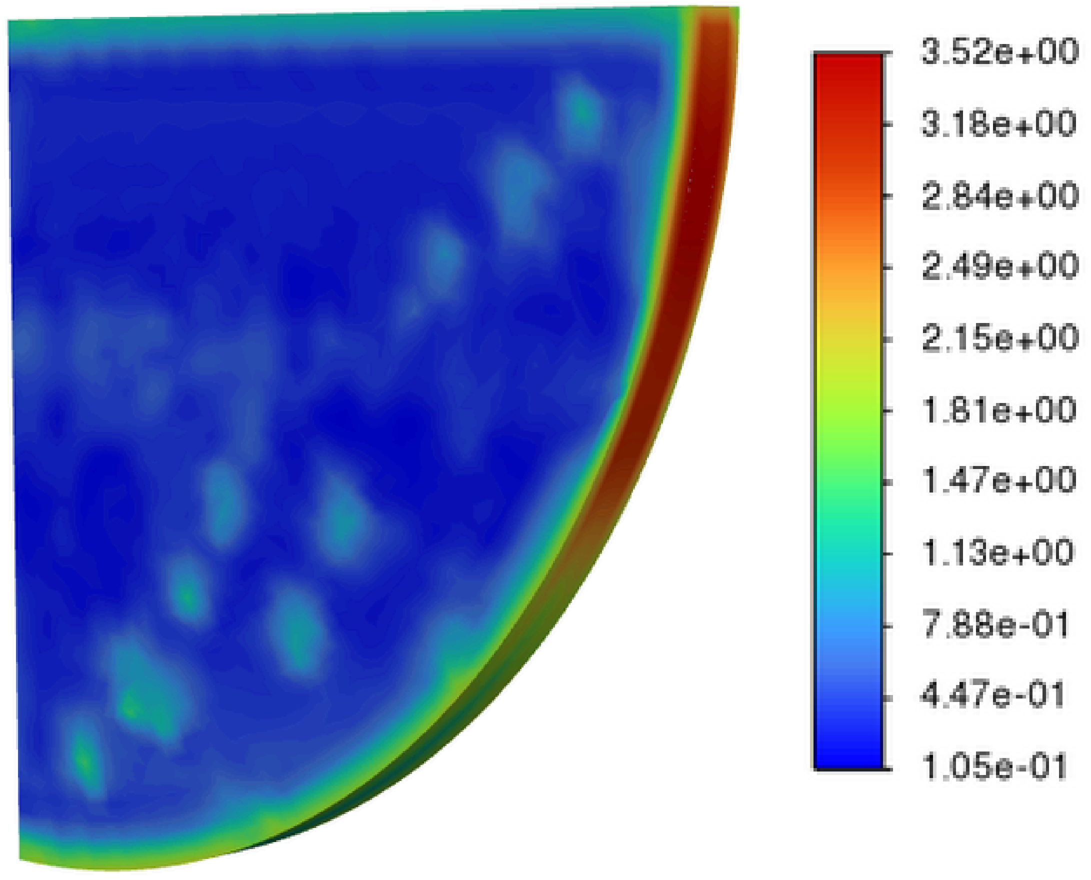
We selected the quadratic closure (*corner flow correction*) to the SST model due to the irregular and thin geometry of the edges which are expected to cause strong anisotropies. This ruled out the use of standard turbulence models which rely on the isotropic Boussinesq hypothesis.

Modelling & Simulation

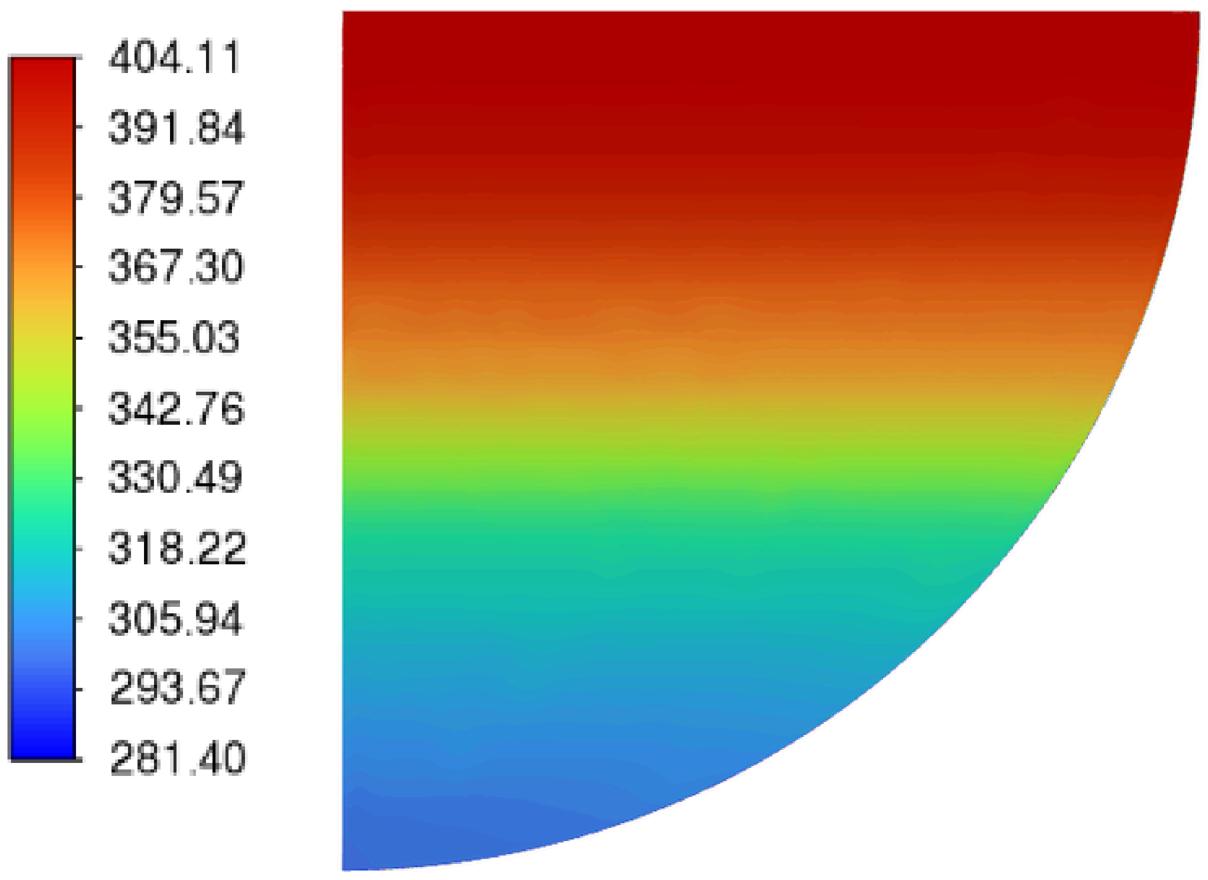
Simulation Results

To monitor the behavior of the solution we set up the following monitors:

- Average bulk temperature & Average temperature along the vertical line
- Rayleigh number



y+ at the wall was satisfactory as it was mostly below 1

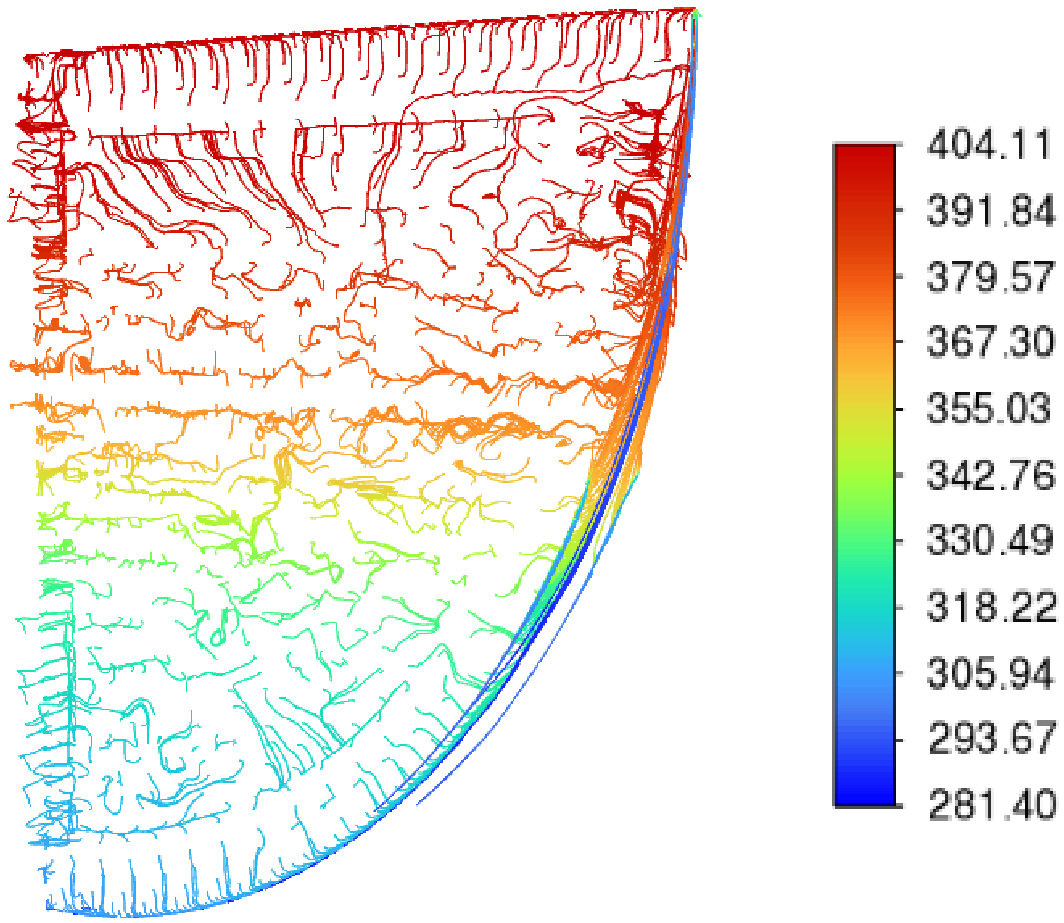


The temperature gradient [K] on the midplane

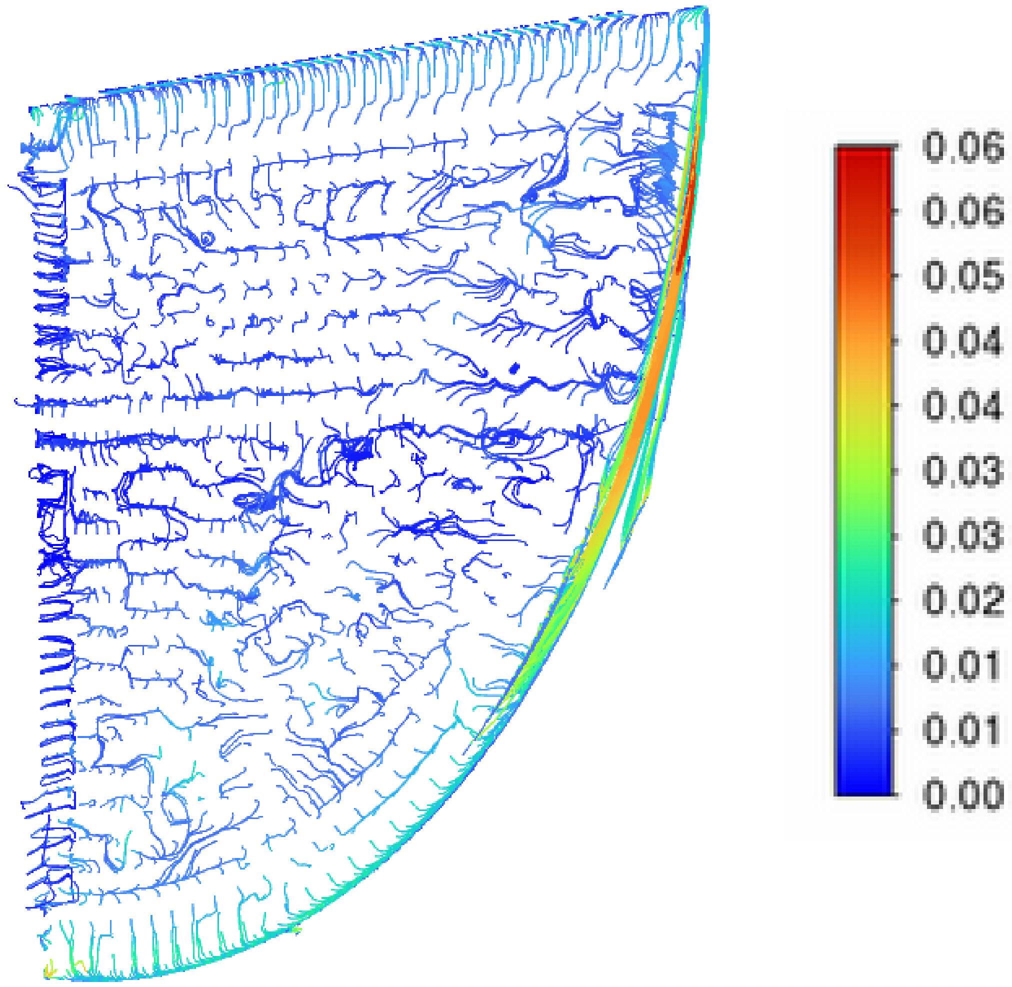
Modelling & Simulation

Simulation Results

The pathlines highlight the anisotropy of the flow



Pathlines colored by temperature [K]



Pathlines colored by velocity magnitude [m/s]

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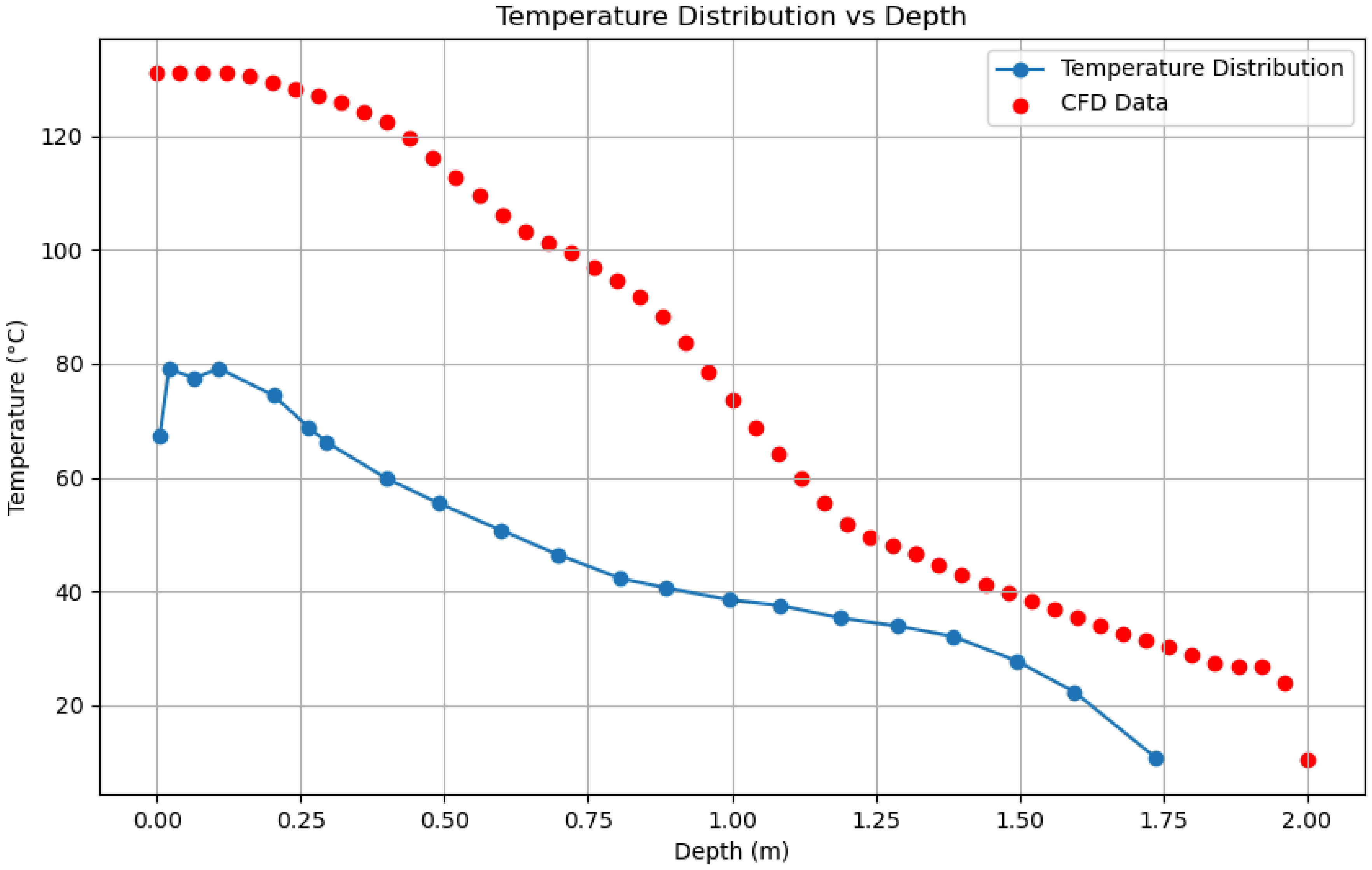
Postprocessing & Results

Simulation vs Experimental evidence

It is evident the the CFD results do not predict the real behaviour, this is caused by:

- Simple Gradient Hypothesis
- Modelling of Buoyancy driven flow near the wall
- Highly anisotropic flow
- Lack of top cooling
- High source power determines bulk temperature close to boiling condition



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Conclusions

Modelling Concern: Simple Gradient

Temperature transport equation

$$\rho \frac{\partial T}{\partial t} + \rho\, div(T\underline{\boldsymbol{u}}) = k\, div(grad\ T)$$

RANS Temperature transport equation

$$\frac{\partial \bar{T}}{\partial t} + div(\bar{T}\underline{\boldsymbol{U}}) = div\left(\frac{k}{\rho C_p} grad\ \bar{T} - \overline{\theta \boldsymbol{u}'}\right)$$

$$\Downarrow$$

$$\frac{\partial \bar{T}}{\partial t} + div(\bar{T}\underline{\boldsymbol{U}}) = div\left(\left(\alpha - \frac{\mu_t}{\sigma_t}\right) grad\ \bar{T}\right)$$

The Simple Gradient Hypothesis appears to **neglect anisotropies**, as it assumes that the temperature gradient fully dictates the heat transfer, without considering the independent movement of fluid at a given temperature.

It assumes a linear relationship between turbulent heat flux and the mean temperature gradient, simplifying turbulence effects on heat transfer without solving an additional equation.

However, in buoyancy-driven flows, this isotropic assumption breaks down, as heat transfer does not align with the model's underlying assumptions.

We can conclude that the hypothesis is not feasible for our case

Conclusions

Proposal for improvement

Temperature transport equation

$$\rho \frac{\partial T}{\partial t} + \rho\, div(T\underline{\mathbf{u}}) = k\, div(grad\ T)$$

RANS Temperature transport equation

$$\frac{\partial \bar{T}}{\partial t} + div(\bar{T}\underline{\boldsymbol{U}}) = div\left(\frac{k}{\rho C_p} grad\ \bar{T} - \overline{\theta \boldsymbol{u}'}\right)$$

$$\frac{\partial \bar{T}}{\partial t} + div(\bar{T}\underline{\boldsymbol{U}}) = div\left(\left(\alpha - \frac{\mu_t}{\sigma_t}\right) grad\ \bar{T}\right)$$

The turbulent heat flux in our domain exhibits significant directionality and anisotropy, particularly in the lower left corner, where accelerated fluid particles decelerate and are lifted due to the high-density difference. The Simple Gradient Hypothesis may not accurately capture these complex physics.

The transport of temperature due to turbulence is simplified by assuming it only depends on the gradient of the temperature.
A possible improvement would be to consider the influence of buoyancy in the transport of temperature, adding other transports terms to this.

In the literature this problem is handled by improving the definition of the turbulent Prandtl number with two-Equation heat flux models or by Algebraic Heat Flux models

Conclusions

Literature Survey

All the reviewed papers confirmed that the Simple Gradient Hypothesis is unsuitable for accurate simulations. The literature also highlighted that most CFD simulations failed to predict behavior accurately near the bottom region, which is the reason for the lack of data in that area.

“Thermal-Hydraulic Analysis for Inversely Stratified Molten Corium in Lower Vessel"

Masanori Fukasawa, Satoshi Hayakawa, Masaki Saito

Shows that Large Eddie Simulation models incorporating buoyancy anisotropy performed better than low-Reynolds-number approaches, accurately capturing stratified layers and anisotropic effects in heat transfer, crucial for analyzing inversely stratified configurations.

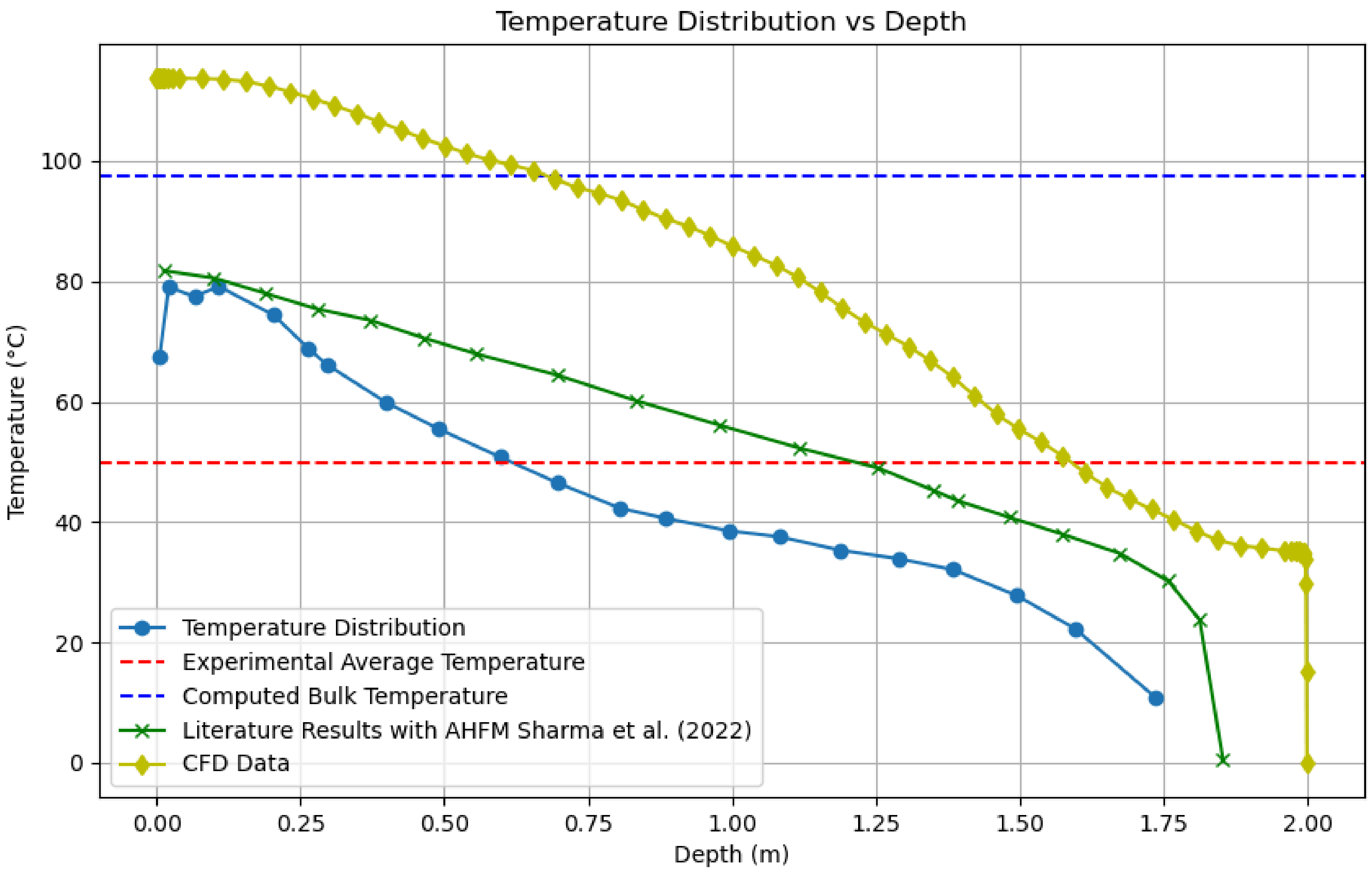
"Computational Simulation of Turbulent Natural Convection in a Corium Pool"

Camila B. Vieira, Bojan Ničeno, Jian Su

This study compared heat flux approaches, including a basic turbulence heat flux model, an advanced model considering directional gradients, and a detailed model incorporating buoyancy and mechanical effects.

Conclusions

Literature Survey



"Validation and Application of Numerical Modeling for In-Vessel Melt Retention in Corium Pools"

Avadhesh Kumar Sharma, Marco Pellegrini, Koji Okamoto, Masahiro Furuya, Shinya Mizokami

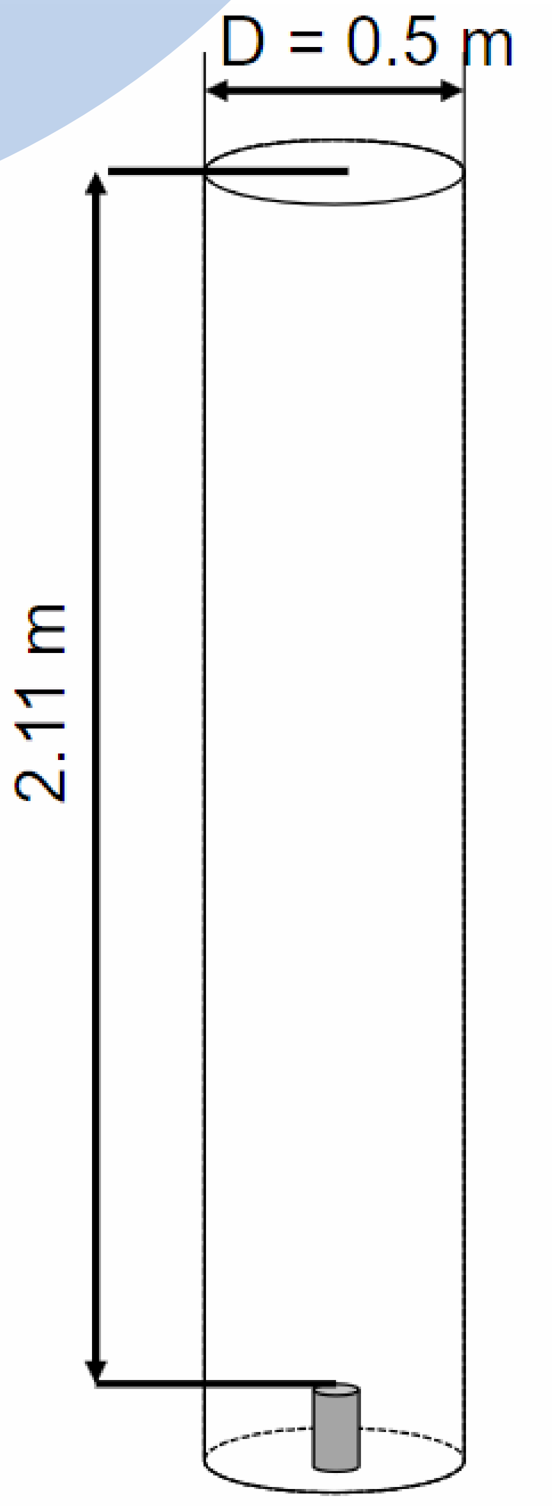
Validated turbulence models, including k-ε and a turbulence model enhancement for buoyancy-driven heat transfer (AHFM).

The validated models successfully predicted heat transfer in stratified and mixed flow regions, as shown by comparisons with BALI experiments

Multi Phase Case
BUBBLE COLUMN

Introduction

Facility, purpose, goals



The bubble column is designed to study decontamination processes in nuclear power plants during accidents with pool scrubbing.

The correct prediction of scrubbing decontamination depends on the correct prediction of the bubble dynamics which includes the bubble size distribution, the velocity and the volume fraction.

The facility allows for the observation of bubble size distribution, velocity, and volume fraction at various points in the column.

Our case study:

- 1000L/min

Objective: Validate simulation results with experimental data simulating the bubble column using the Eulerian-Eulerian approach to assess the physical behavior of the system.

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Preprocessing

Flow Regime Evaluation

We were assigned a volume flow rate of 1000L per minute from which we computed (given the geometry) the mass flow rate and the superficial gas velocity as well.

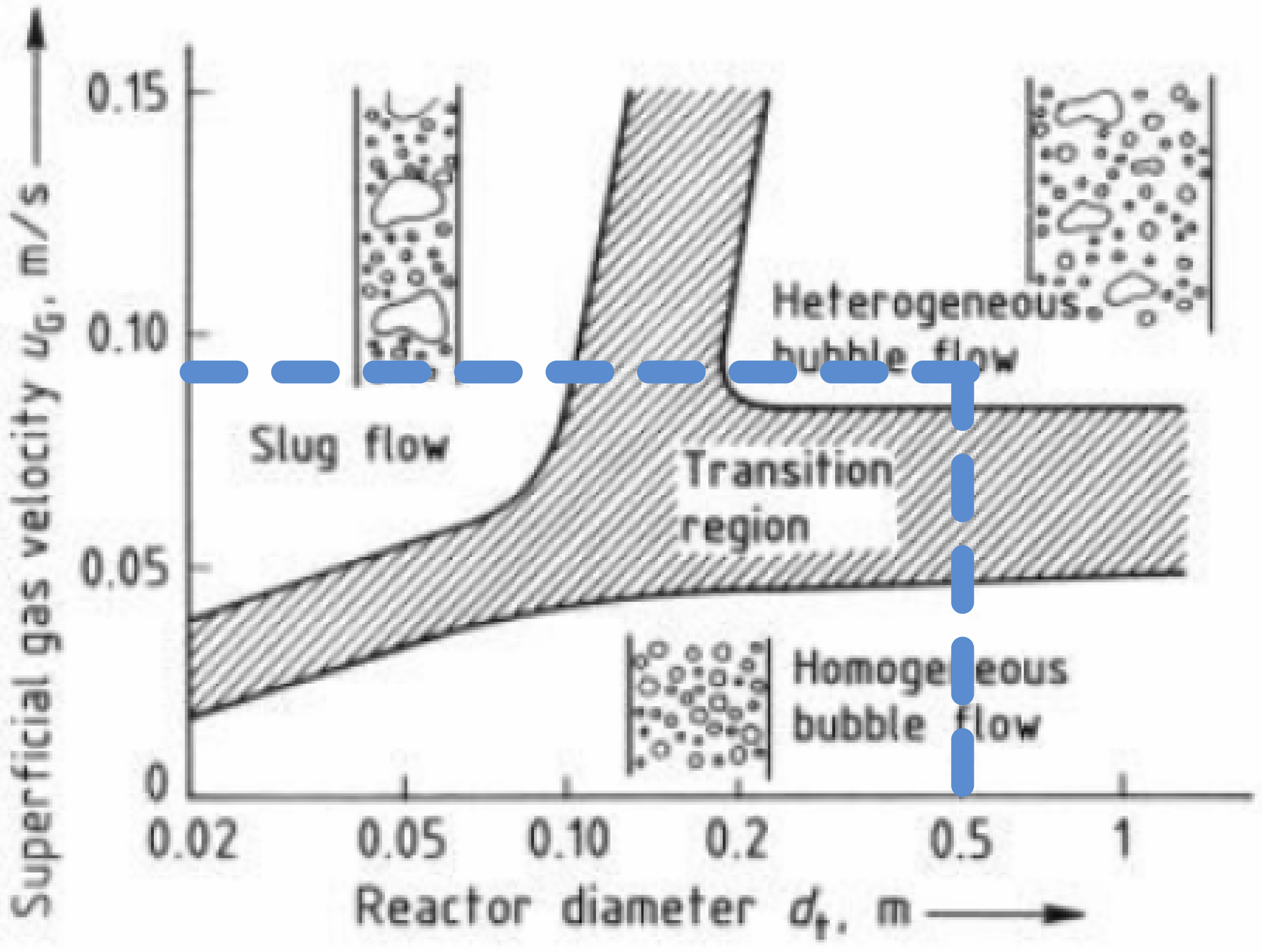
$Q = 0.0166\ m^3/s$ $\quad \dot{m} = 0.0204\ kg/s$ $\quad J_g = 0.0840\ m/s$

We evaluated the critical diameter of the column to understand the flow regime.

$$D^* = \frac{d_C}{\sqrt{\sigma/g(\rho_L - \rho_G)}}$$

$D^* = 184 > 52$

From which we understood that Taylor's bubbles cannot be sustained, therefore an heterogeneous churn flow is to be expected.



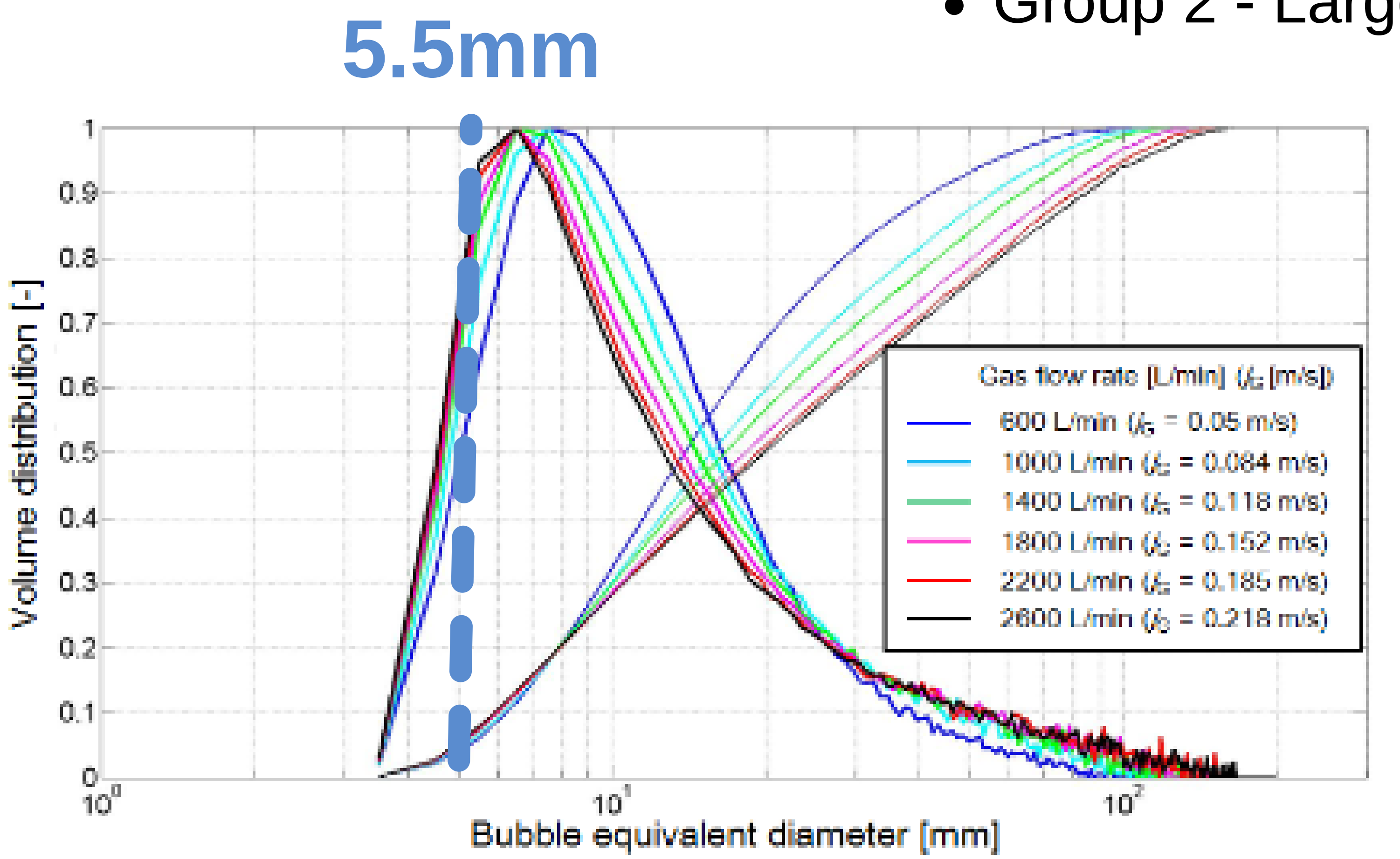
Preprocessing

Dispersed Phase Modeling

The experimental Bubble Size Distribution shows that the dispersed phase has to be modeled as an **adiabatic fixed poly-dispersed** flow.

For this purpose, the study was based on two main groups of bubbles:

- Group 1 - Small bubbles
- Group 2 - Large bubbles



	Small bubbles	Large bubbles
Mean diameter [mm]	4.762	12.877
Volume fraction [-]	0.07	0.93
Mass flow rate [kg/s]	0.0014	0.0186
Eotvos Number [-]	3.13	22.60

The specific parameters for each groups were evaluated through the BSD and its cumulative distribution function:

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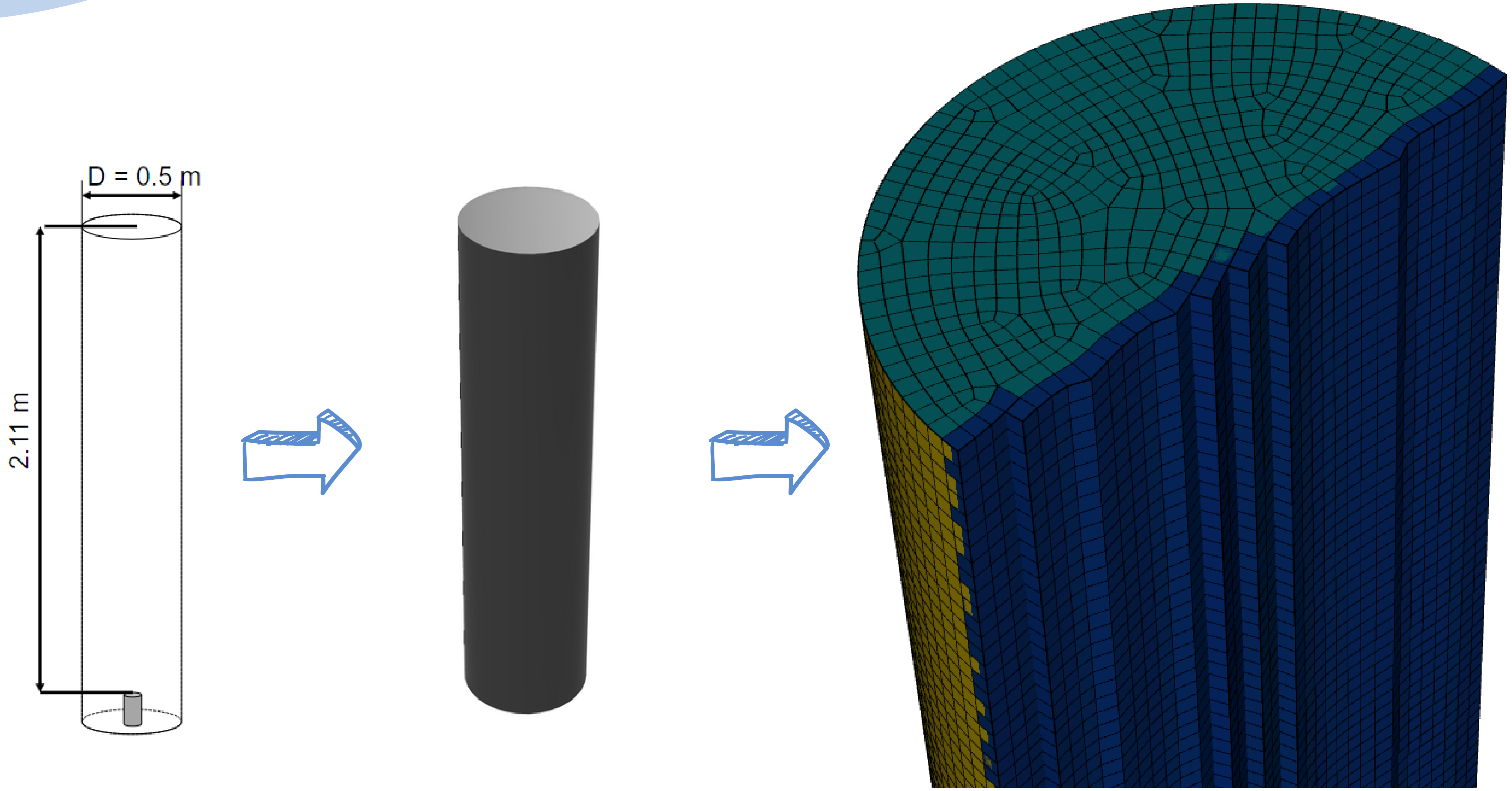
Meshing

From Real Geometry to Mesh

Our aim was to accurately capture the lack of a strong preferential direction for bubble movement, particularly near their generation point.



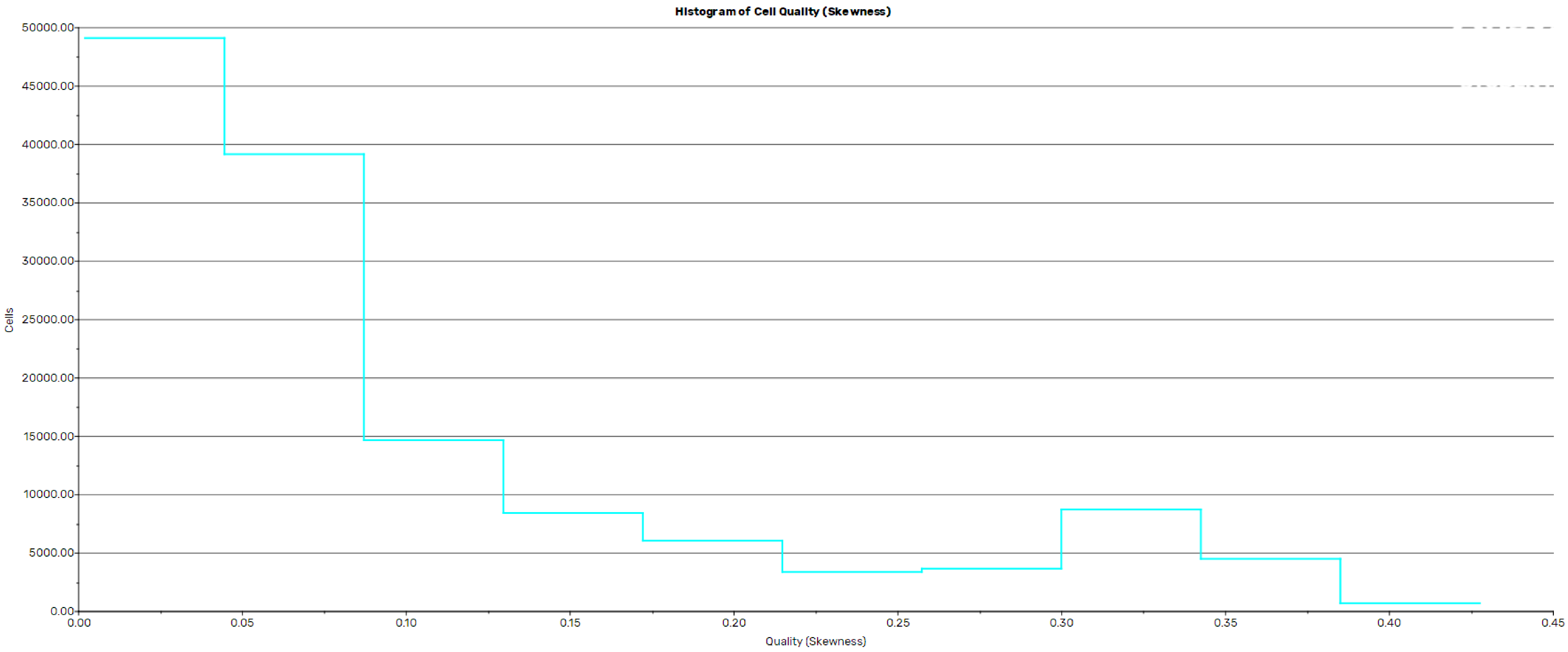
Our goals were:

- AR closest to 1 as possible
- High orthogonal quality

	AR	Orthogonal Q.	Swekness
min	1.76	0.903	0.002
avg	1.93	0.989	0.103
max	2.56	0.999	0.427

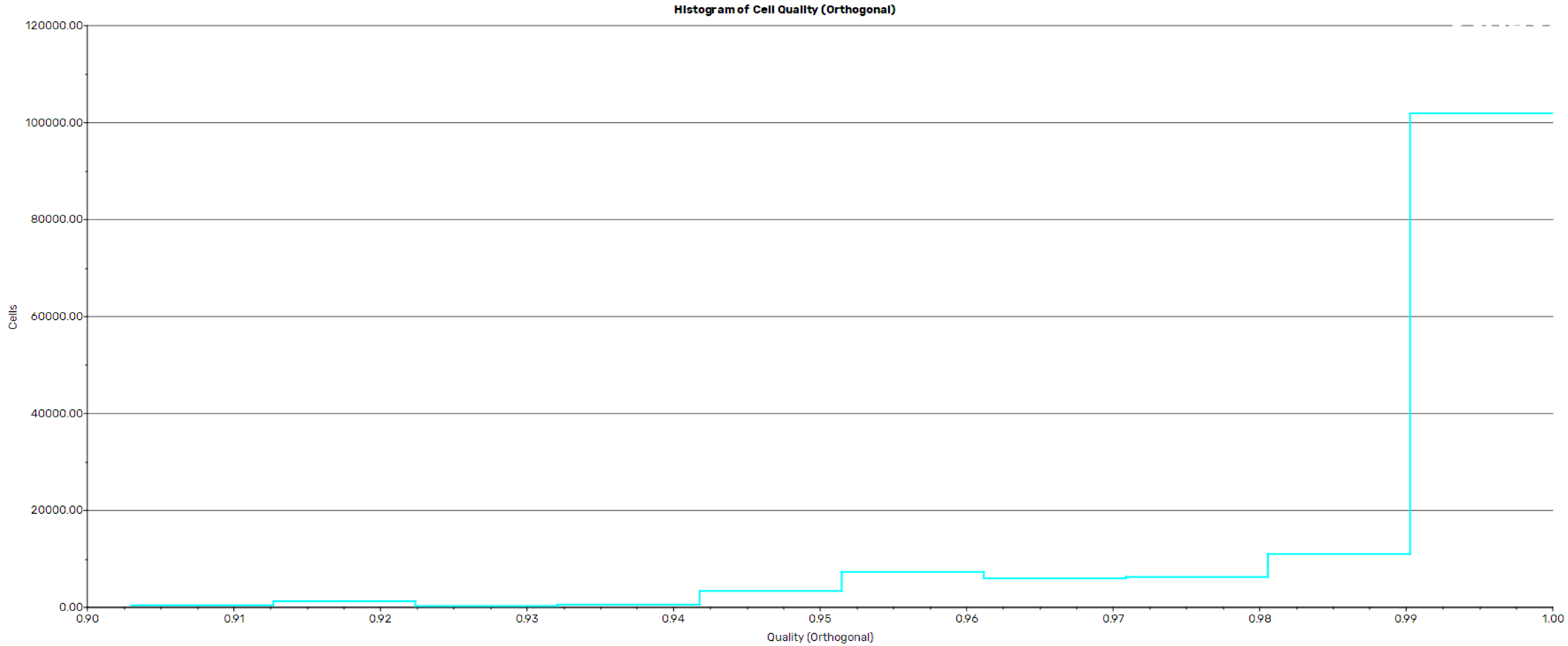
Meshing

Mesh stats - Skweness



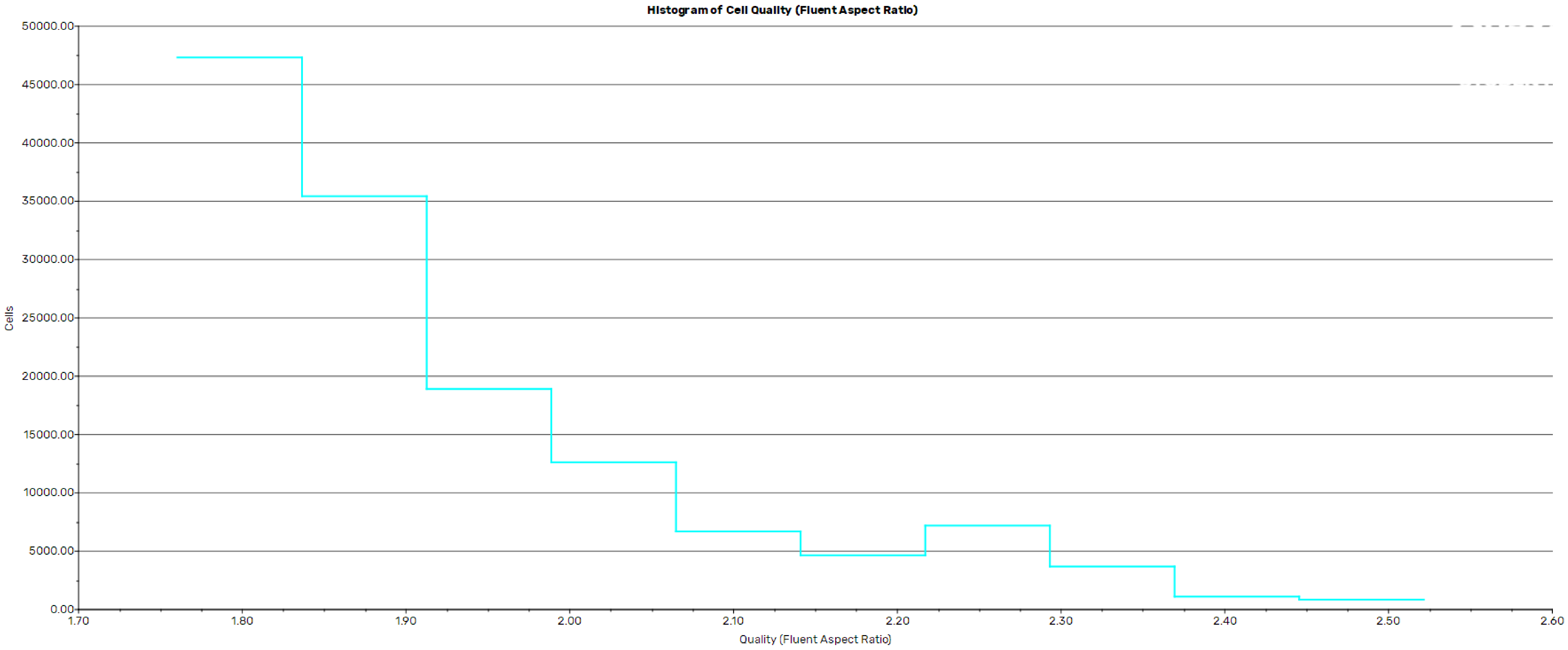
Meshing

Mesh stats - Orthogonality



Meshing

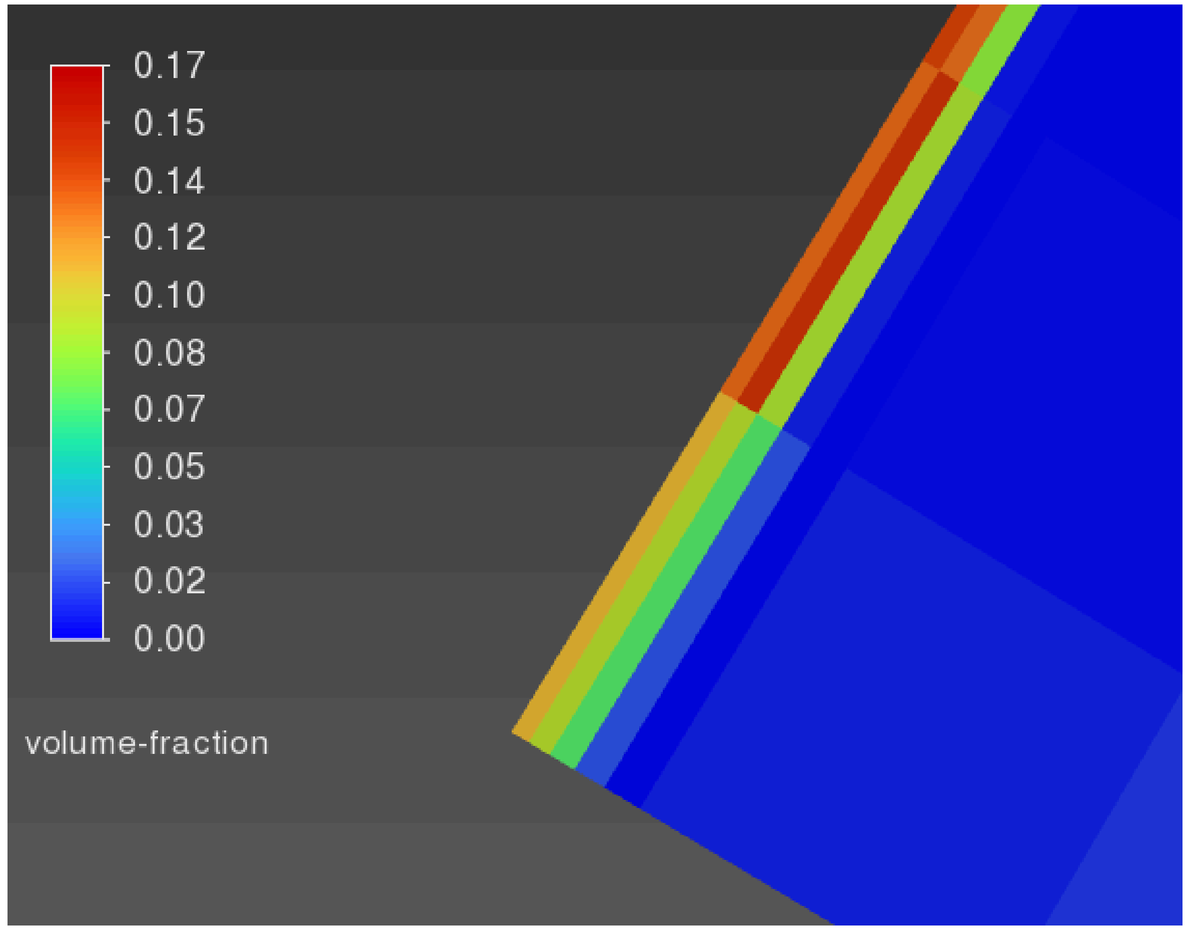
Mesh stats - Aspect Ratio



Meshing

Meshing Considerations - Boundary Layer

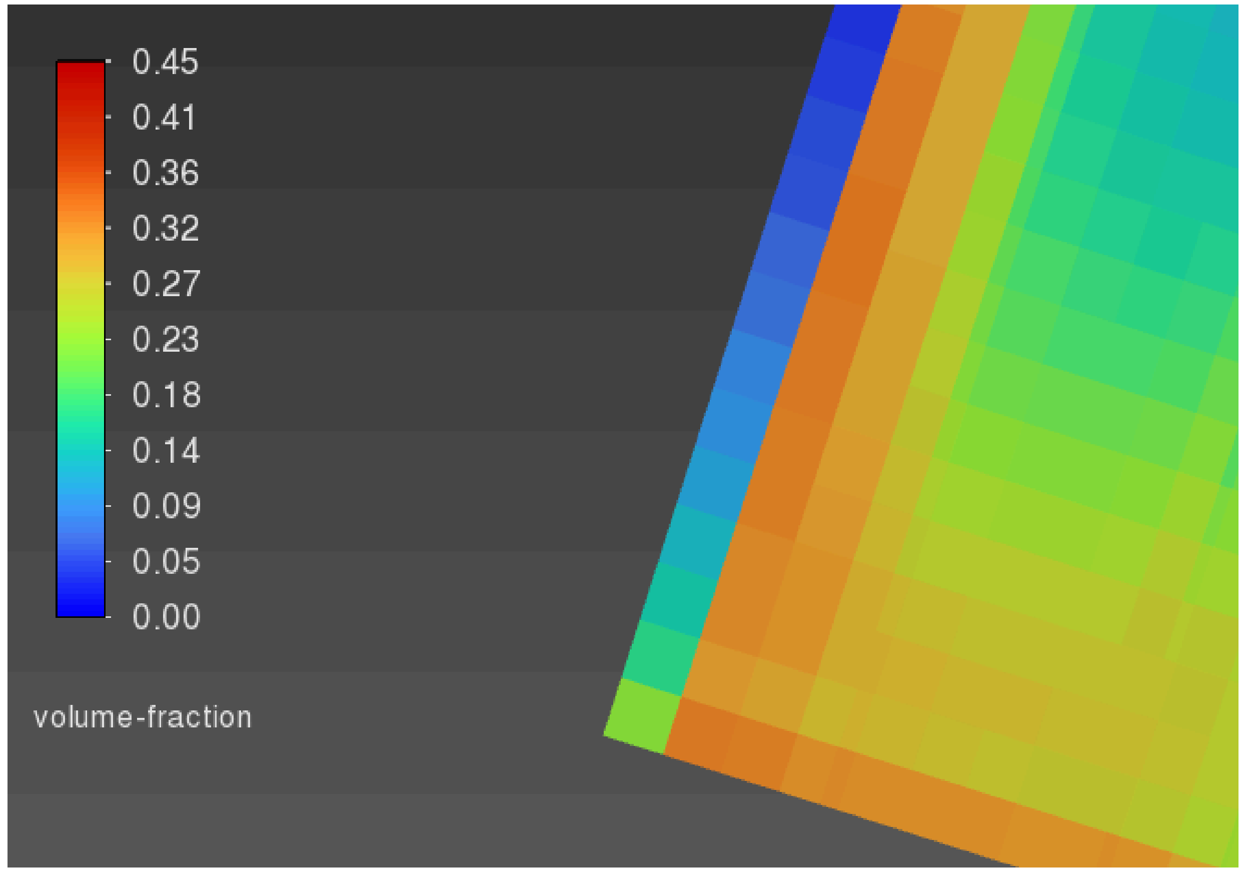
The wall boundary layer tends to "trap" the bubbles due to the preferential flow direction along the Y-axis, consequence of the large AR, while bubbles are also expected to exhibit consistent radial movement.



Volume fraction of **large** bubbles with Boundary Layer

As a result, many large bubbles remained confined within the boundary layer rather than migrating away from the wall.

Hence we chose to **remove the boundary layer**



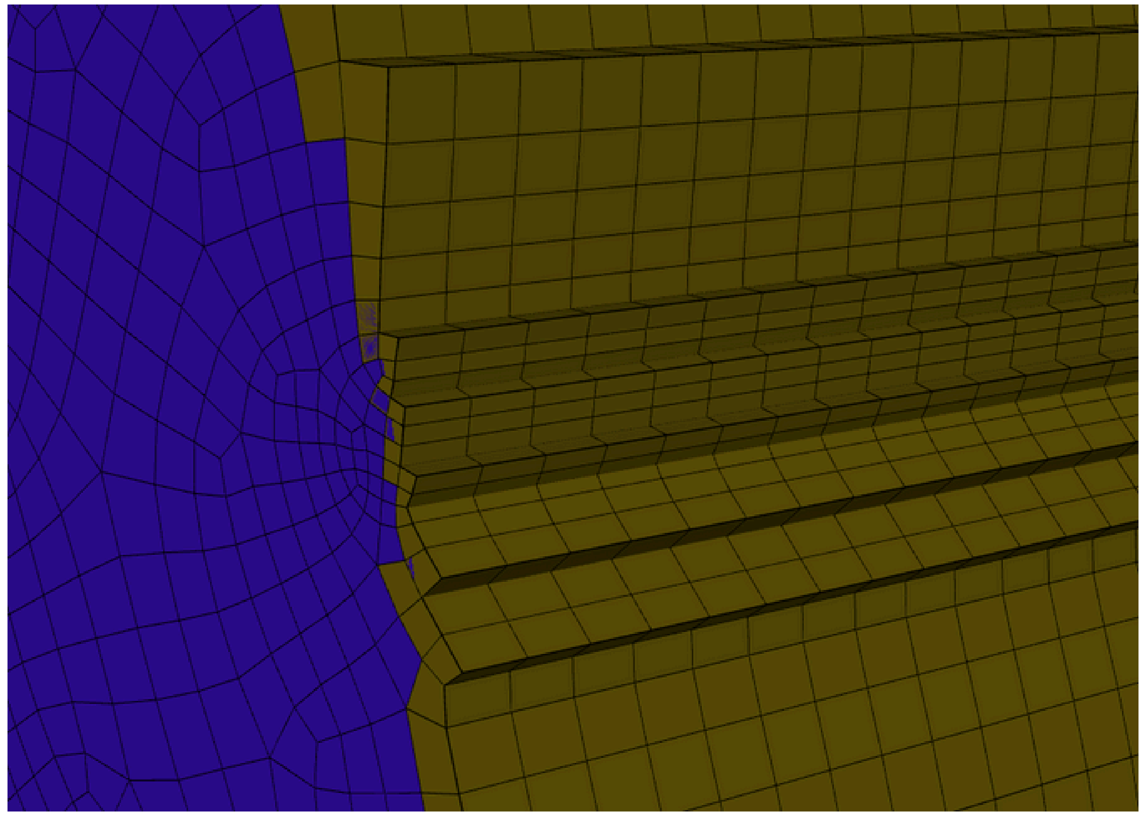
Volume fraction of **large** bubbles without Boundary Layer

Meshing

Meshing Considerations - Nozzle

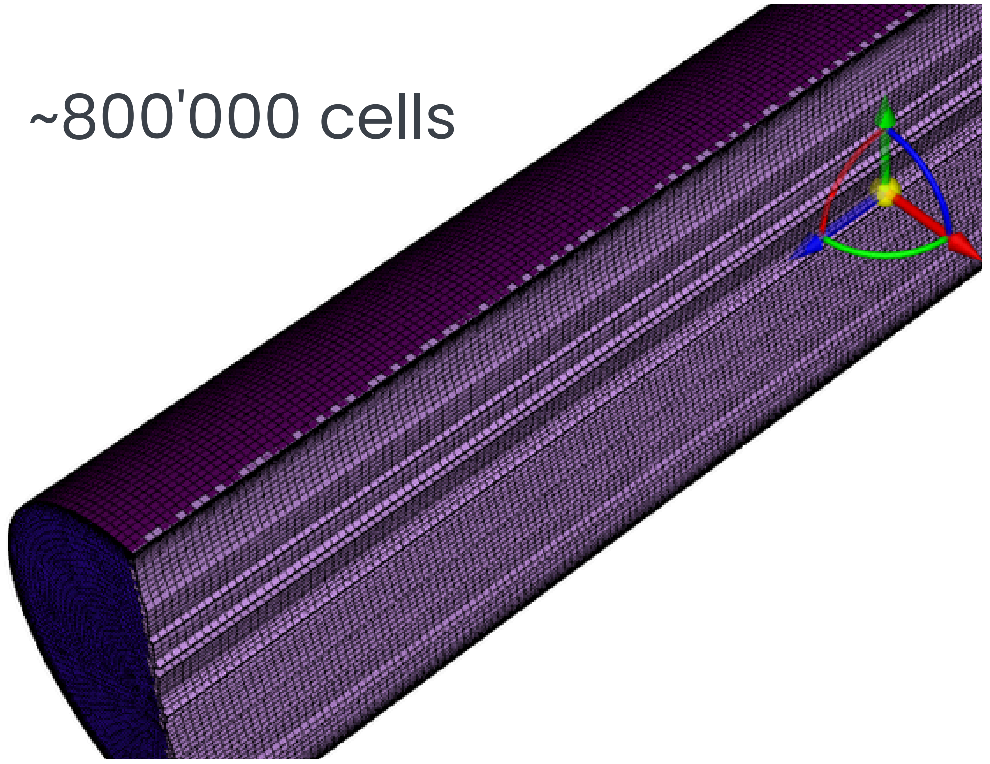
Modelling the nozzle as a part of the geometry caused meshing complication and caused the simulation to diverge rapidly.

We therefore chose not to model the nozzle as part of the geometry.



High AR on the cells above the nozzle

~800'000 cells



The Problem could have been solved with a finer mesh but to get satisfactory mesh quality the sacrifice in computational time was not acceptable.

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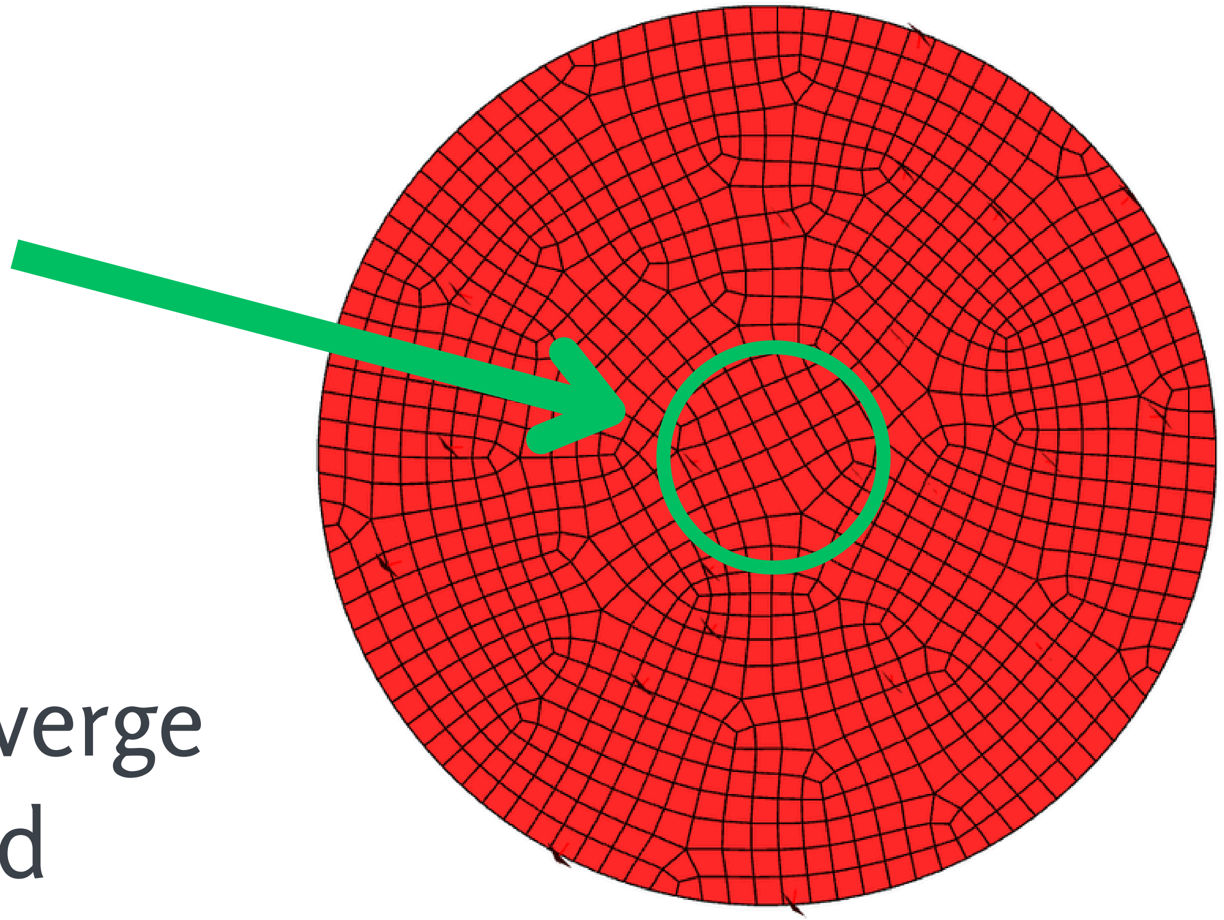
Modelling & Simulation

Modelling Choices - Boundary Conditions

if
$X^2 + Y^2 < r^2$
then
$v = 0.084\,{}^{m}/_{s}$
else
$v = 0\,{}^{m}/_{s}$

To model the whole bottom as a B.C. we defined an expression to limit the velocity intake to the points in a circle.



This caused some complications:

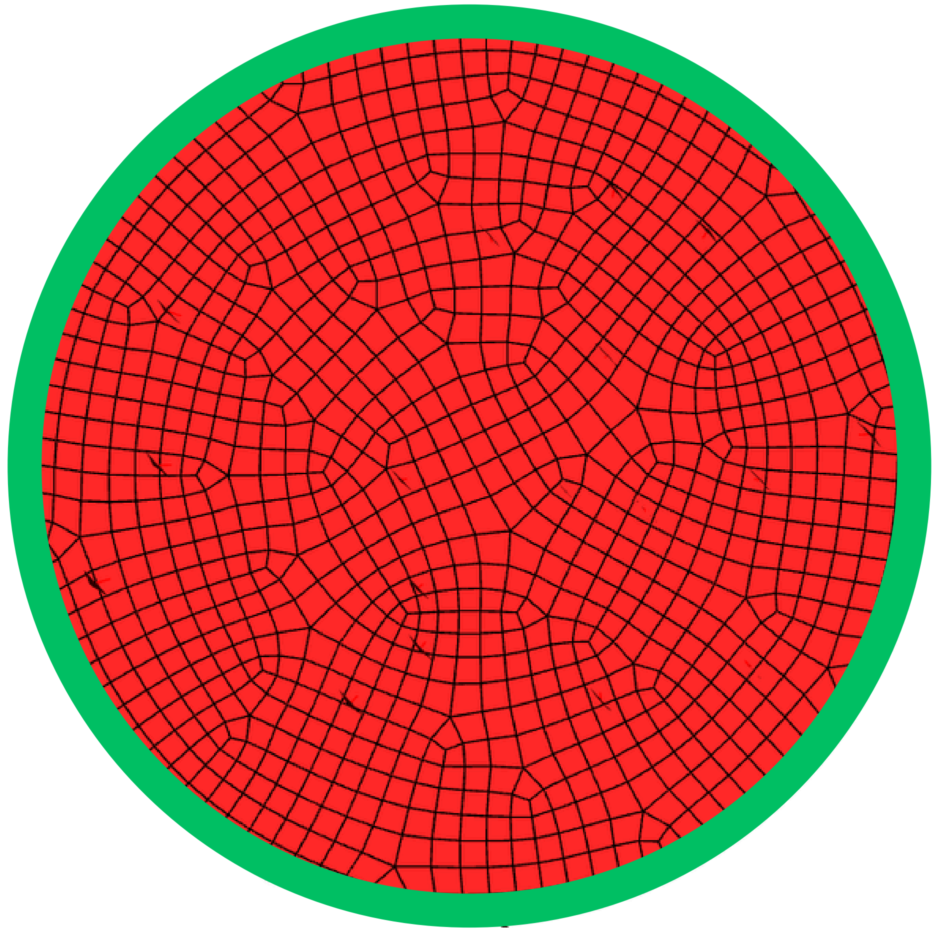
- By using the absolute gas velocity the simulation would diverge immediately as the air was accelerated to supersonic speed
- By using the **superficial** gas velocity, the simulation would run with reasonable results but the mass flow into the volume was coherently under the expected value.

Modelling & Simulation

Modelling Choices - Boundary Conditions

Therefore we chose to use the whole bottom surface as a velocity intake specifying the superficial gas velocitv.

By doing so we had correct volume and mass flow rate prediction and reasonable void fraction and phase velocities



We lost the information on the behavior of the bubbles at the bottom of the column but given that we are interested in average quantity at the top this was expected to not influence our results.

Modelling & Simulation

Transient Setup

The transient had to be initialized slowly to ensure proper initialization of the domain.

- with small time steps (1e-5 s)
- a lot of iterations per time step (300)
- low under-relaxation factors

After a couple of time steps we computed a characteristic time step:
Using the highest velocity in the domain and knowing the average cell dimension.
At first we used 1/10 of the this value, then 1/4.
This procedure was repeated until the main air front reached the top.

To run the final part of the simulation, from which we gathered data, we used the **adaptive time step** to ensure a multiphase Courant number below 2 (suggested value for multiphase flow in fluent)

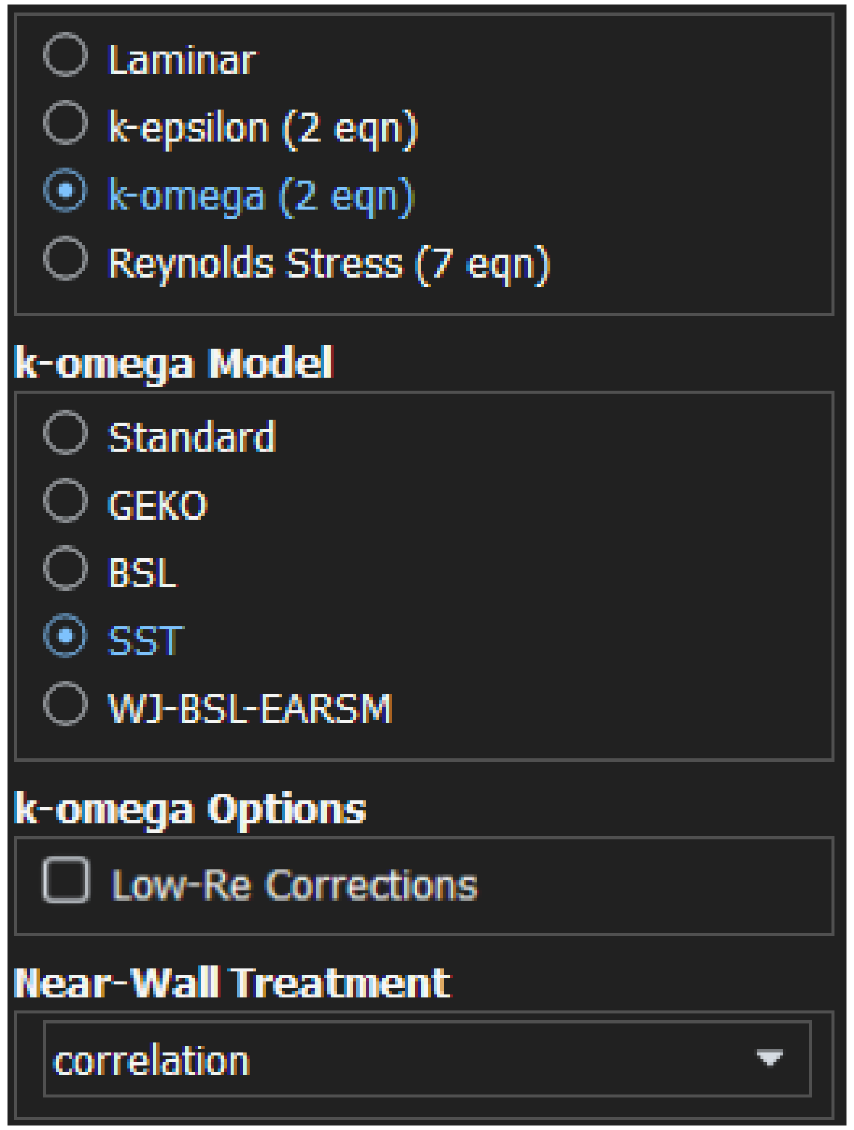
Modelling & Simulation

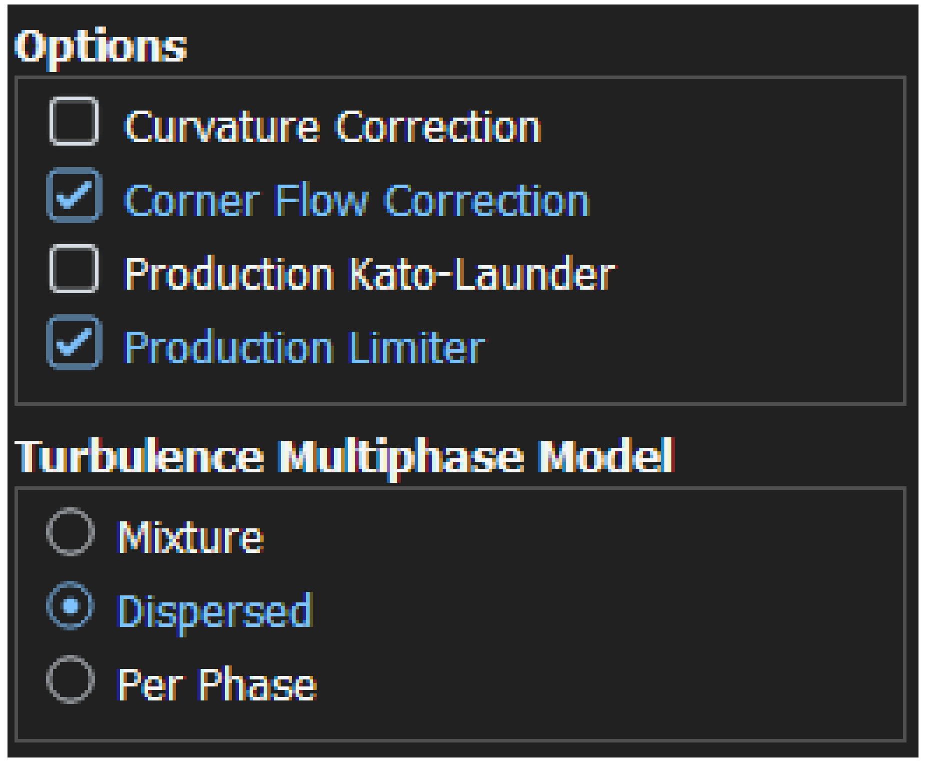
Turbulence Models

We chose k-omega SST dispersed.

We excluded laminar since we expected turbulence induced by bubbles.

We choose not to use k-epsilon since we did not model a boundary layer.





The dispersed turbulence model is an appropriate model when there is clearly one primary continuous phase and the concentration of the secondary phases are diluted: the secondary phase motion is influenced by the primary

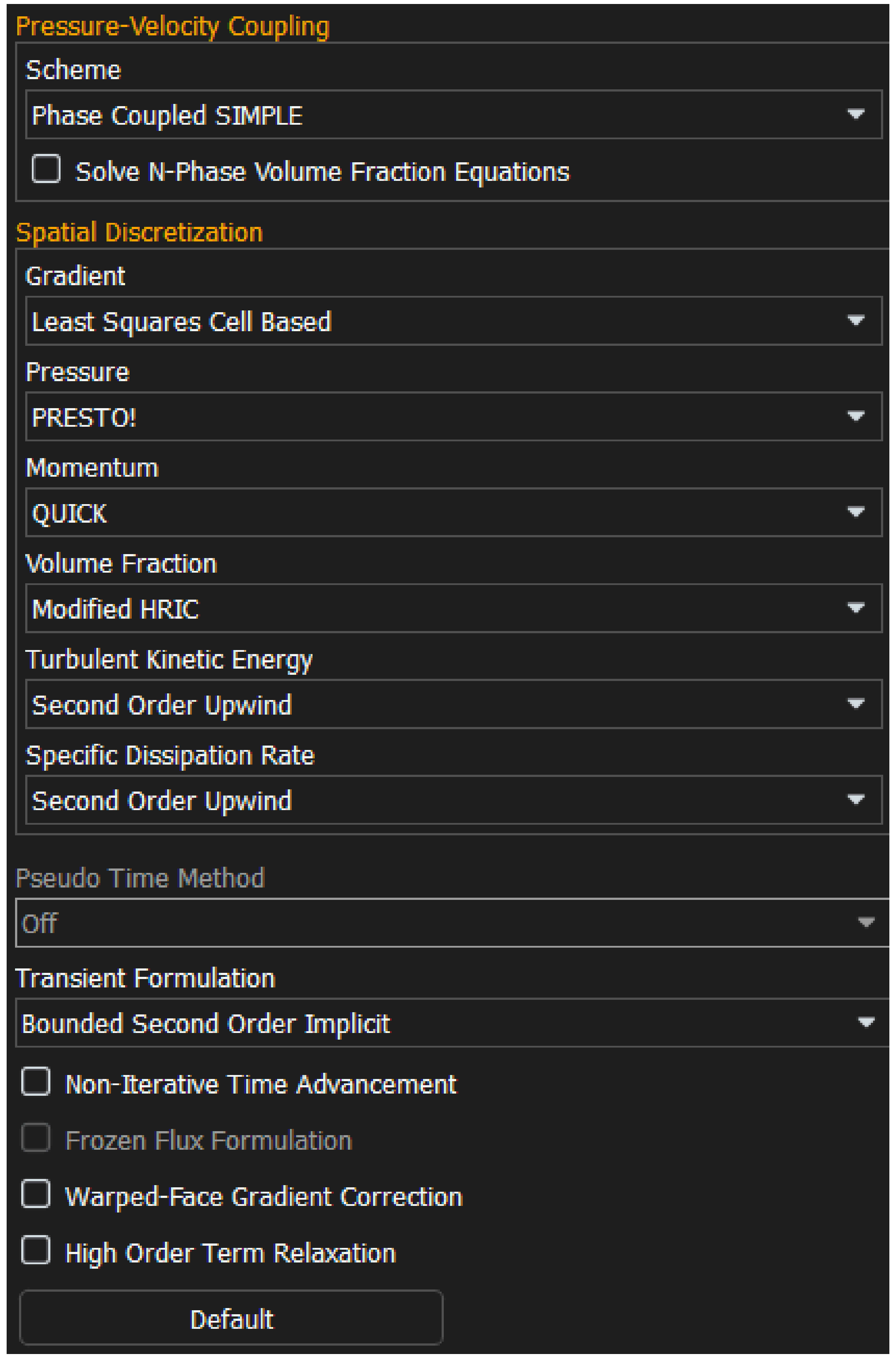
Modelling & Simulation

Simulation Methods & Monitors

We used a reasonable mix of high order of accuracy models and some faster approximations given that the simulation speed was greatly influenced.

The QUICK scheme for momentum was chosen for its higher order of accuracy.

The coupled scheme would cause each iteration to require x10 the time to be completed.



To monitor the behavior of the solution we set up the following monitors:

- **Volume fraction** of both gas phases
- **Maximum velocity** of all three phases
- Mass averaged **pressure** in the domain

Modelling & Simulation

Phase Interactions Models

We have looked into several models (all those that were mentioned during class) by reading the respective publications and while we simulated the column with just one set we did identified other models that could have been interesting to study.

Used Correlations	Small Bubbles	Large Bubbles
Drag	Tomiyama	Ishii & Zuber
Lift	Hessenkemper	Tomiyama
Wall Lubrication	Hosokawa	Tomiyama
Turbolent Dispersion	Burns et al.	Lopez De Bertodano

Other Possible Options	Small Bubbles	Large Bubbles
Drag	-	Tomiyama
Lift	Tomiyama	-
Wall Lubrication	-	Tomiyama
Turbolent Dispersion	-	Burns et al.

Virtual Mass was not considered, Turbolent interaction model was Sato and no further investigation on this matter. Surface tension constant to 0.072

Modelling & Simulation

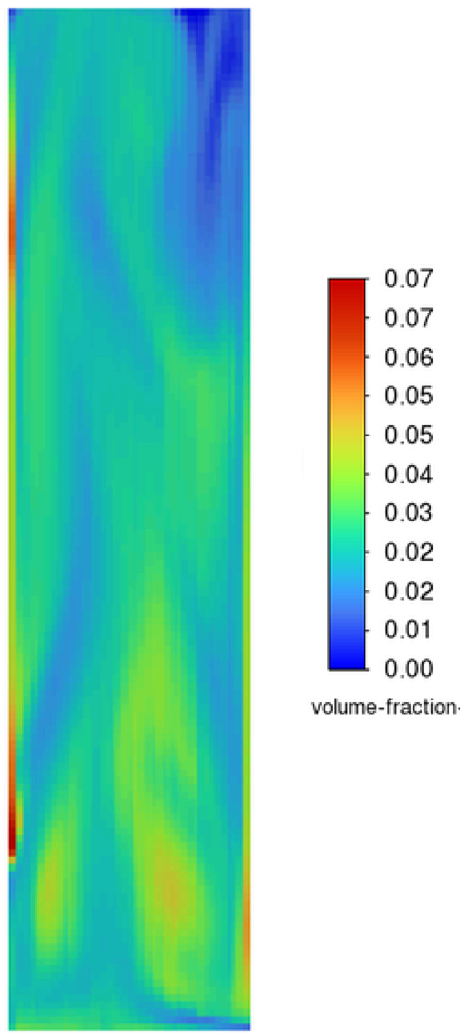
Phase Interactions Models

Body Force	Correlations	Considerations
Drag	Tomiyama Grace et al. Ishii & Zuber	Tomiyama and Grace models were developed for a single bubble but Tomiyama was found to be the default choice in a lot of studies. On the other hand Ishii & Zuber model was developed from observation of bubbly flow
Lift	Tomiyama Hessenkemper Ziegenhein	Tomiyama was chosen since is the only model developed for a large channel and for our large bubble diameter we fell in a region of noticeable disagreement between the three models. On the other hand, for the small bubble diameter the model would not greatly influence the coefficient, we therefore used the most recent correlation (Hessenkemper)
Wall Lubrication	Antal et al. Tomiyama Hosokawa	Tomiyama was developed for a pipe geometry and Hosokawa considered cases of large lift force which could have been the case for our very large bubbles. Antal et al. was excluded as it was focused on spherical bubbles and given the high Eotvos number we suspect noticable bubble deformation.
Turbolent Dispersion	Burns et al. Lopez De Bertodano	Burns models is focused on bubbly flow in a vertical pipe which could be acceptable for small bubbles. The Lopez model was chosen for the large bubbles as it is a special case of the Burns that takes into account medium size bubbles in non perfectly spherical shape

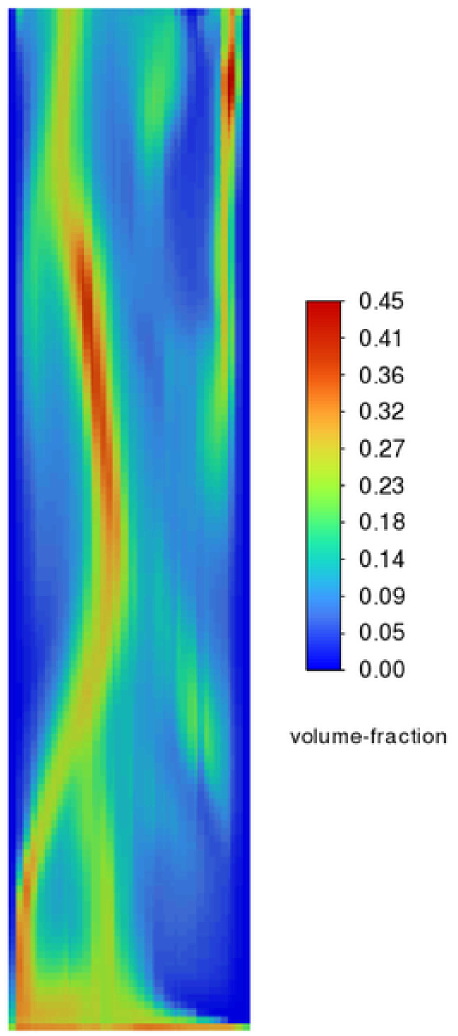
Modelling & Simulation

Simulation Results

Volume fraction of small and large air phases at the midplane and wall y+



Small Bubble Volume Fraction at the midplane

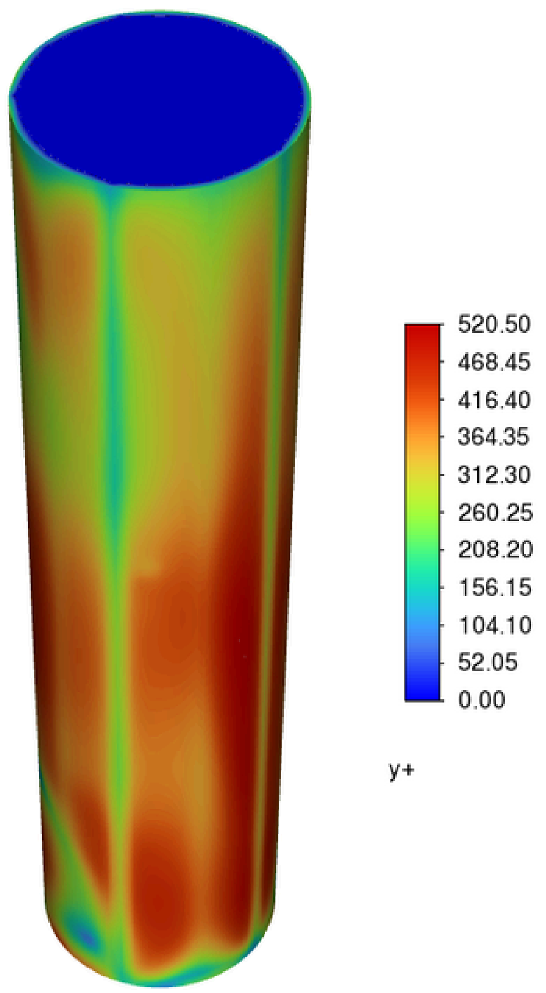


Large Bubble Volume Fraction at the midplane

We can see that the resolution of the volume fraction at the wall is unsatisfactory due to the coarse mesh.

For the same reason the wall y+ greatly above 1 in practically all wall adjecent cells.

These two factors show that a finer mesh and more attention to the boundary layer is required for better results

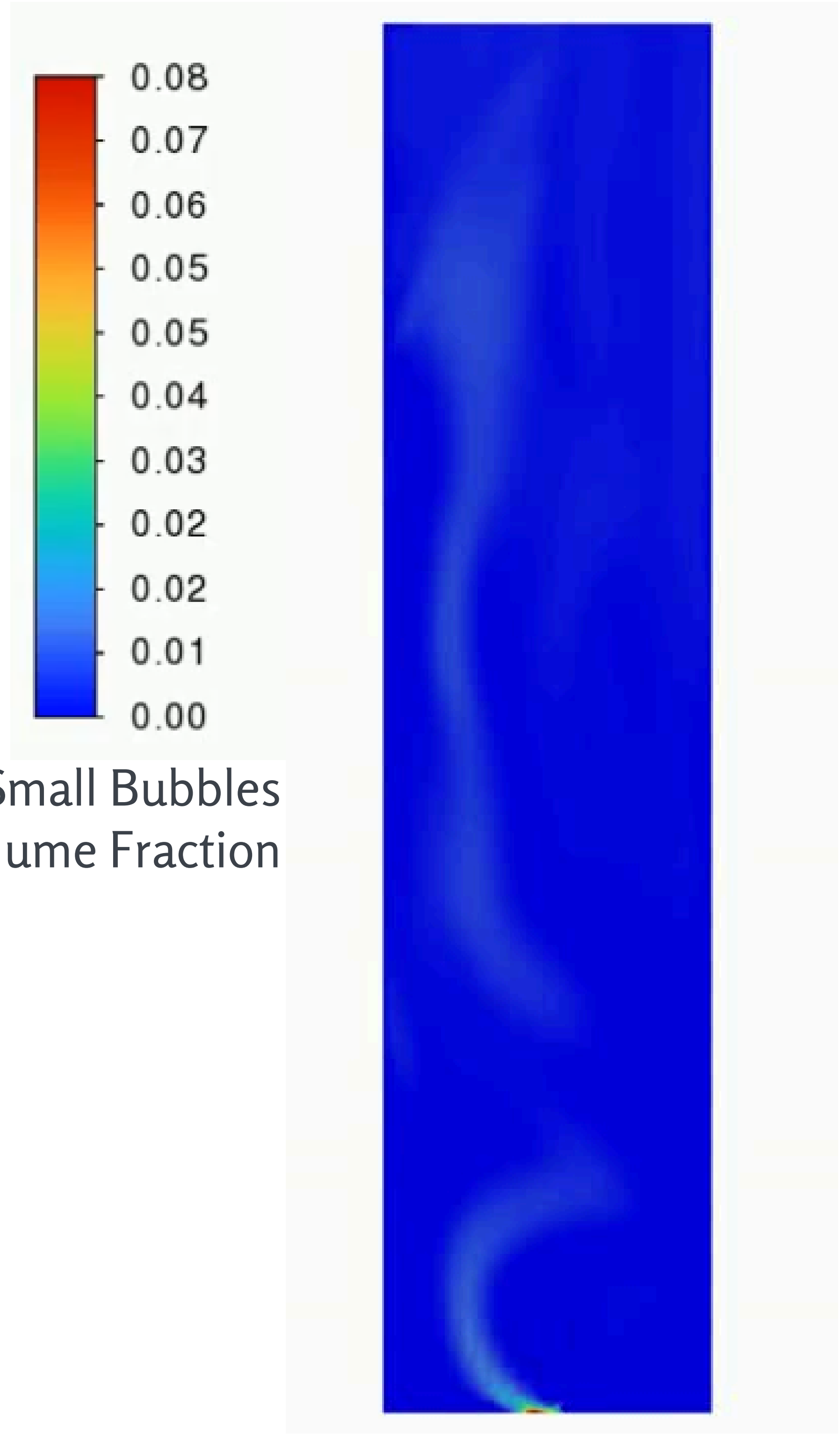


Wall Y+

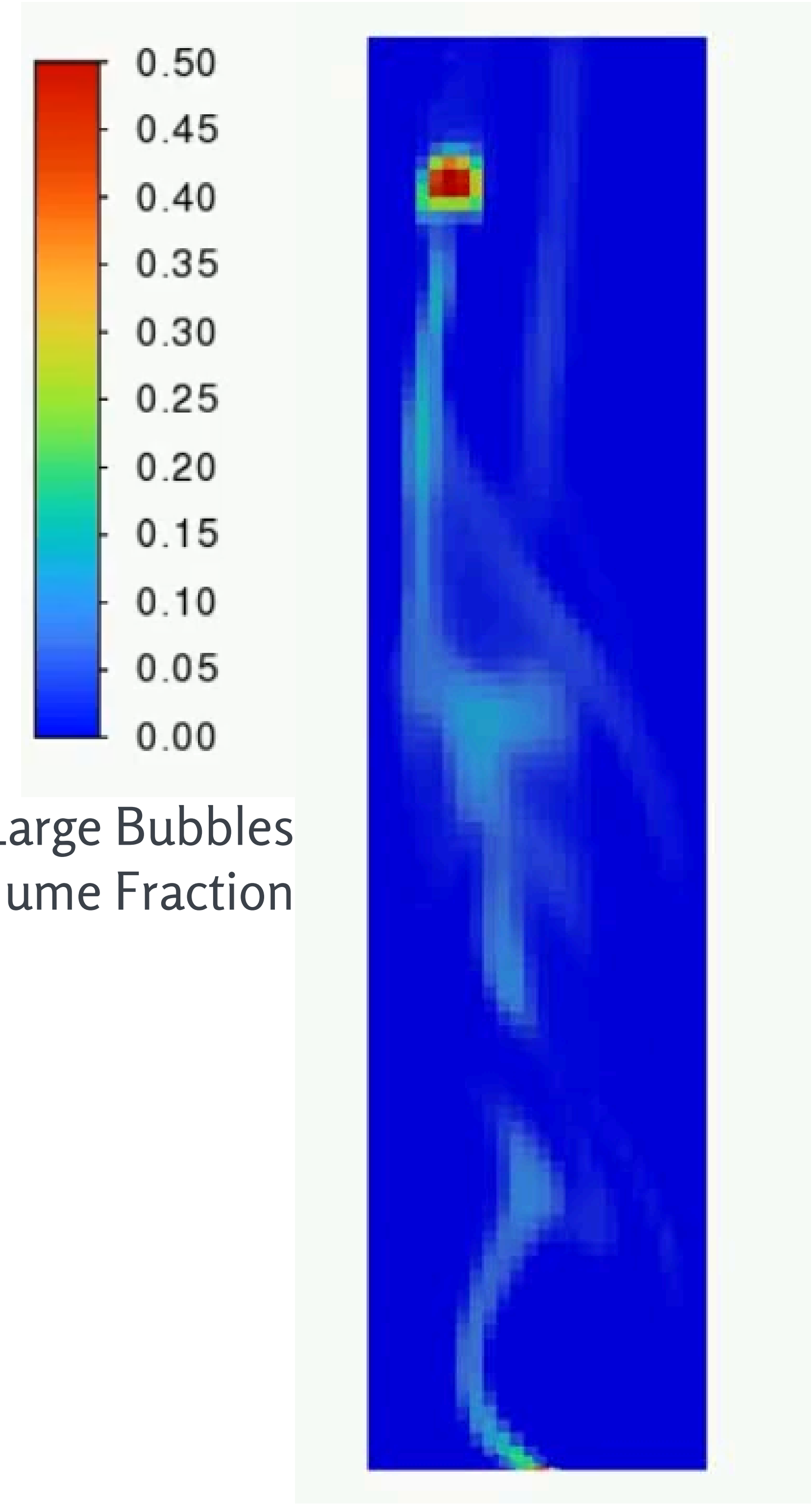
Modelling & Simulation

Initial simulation results: Nozzle issues

Animation of the volume fraction of small and large air phases at the midplane from the simulation in which we modeled the nozzle with the *if statement* on the bottom surface, using the superficial gas velocity



Small Bubbles Volume Fraction



Large Bubbles Volume Fraction

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- Preprocessing
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Postprocessing & Results

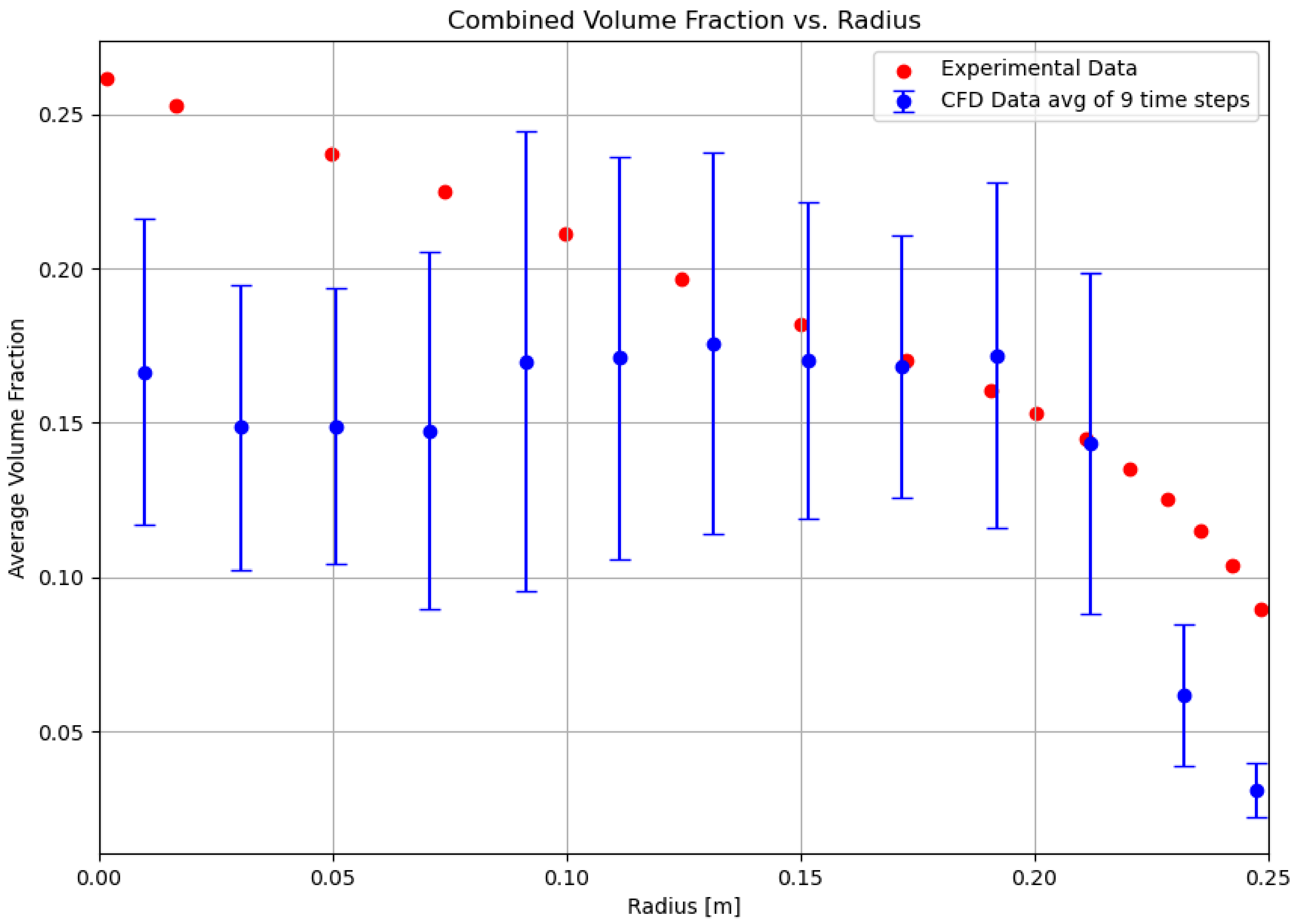
Simulation vs Experimental evidence

Average Experimental ε = 0.173
Average CFD ε = 0.146

CFD data comes form sampling the volume fraction distribution over the surface, which was then averaged into a smaller number of bins

We have observed that:

- **Near the wall** the simulation correctly predicts the general physical behavior
- **At the wall and in the bulk** the volume fraction is heavily underestimated

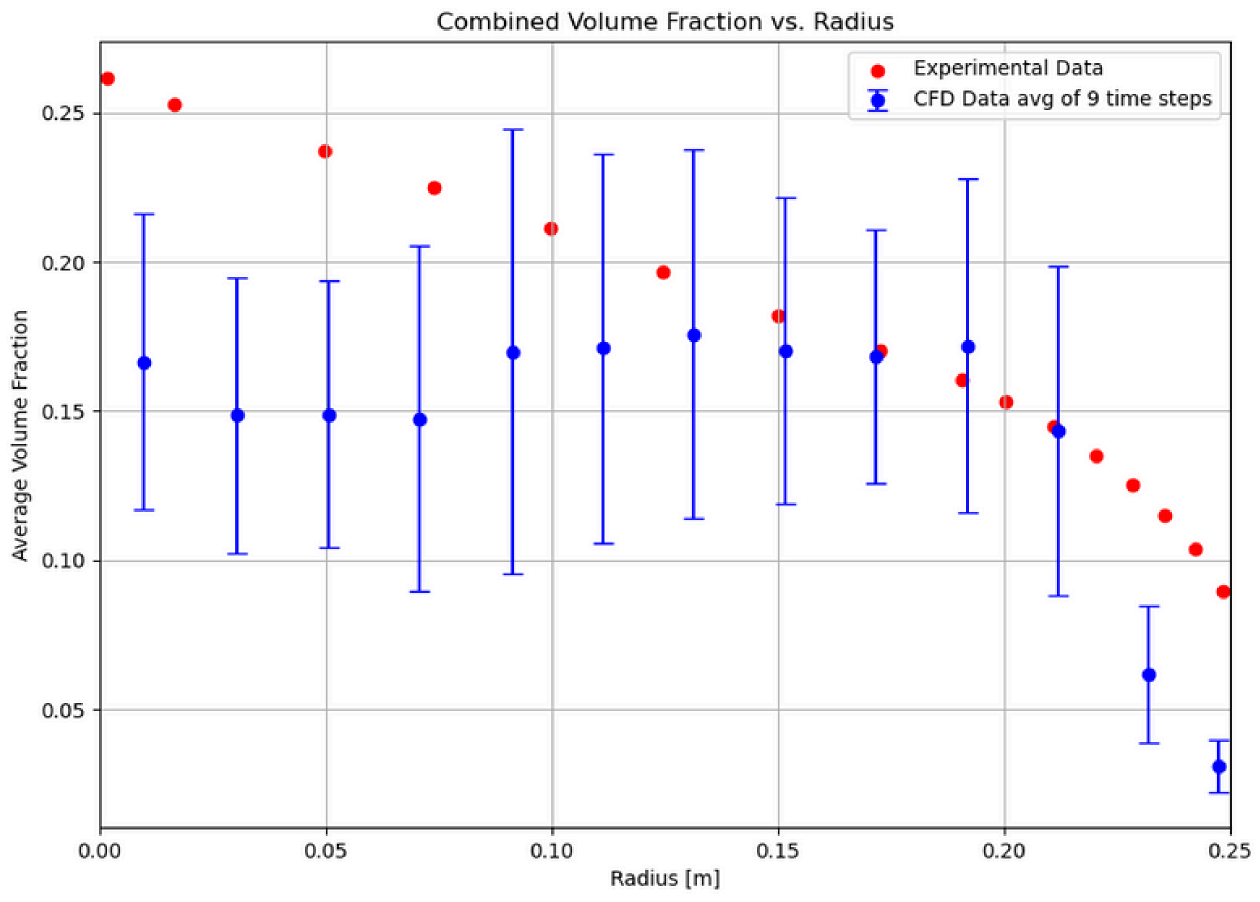


Postprocessing & Results

Simulation vs Experimental evidence

It is evident the the CFD results do not predict the real behaviour, this is caused by:

- Lack of boundary layer
- Order of accuracy
- Phase interaction models



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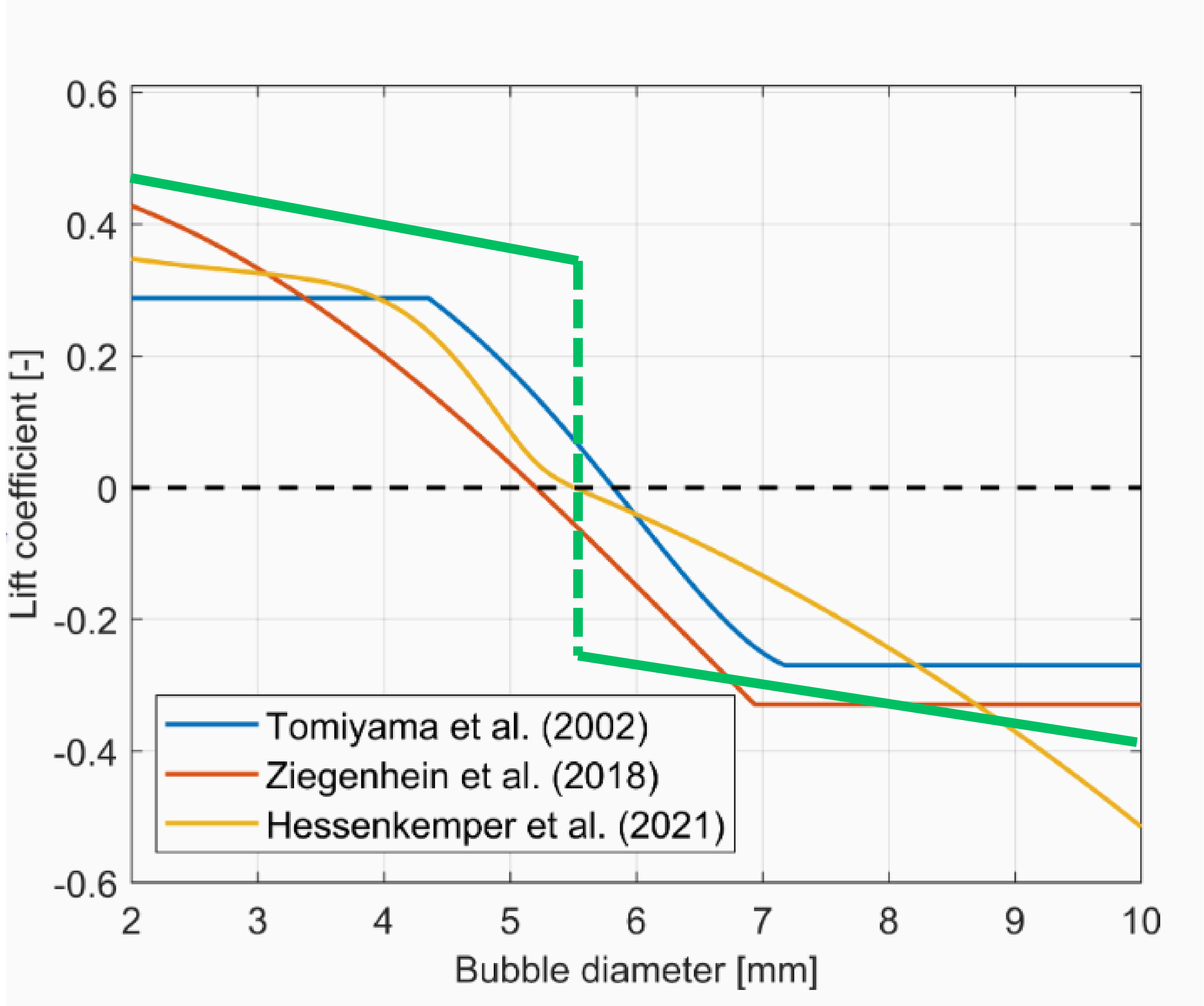
Conclusions

Proposal for Improvment

A possible improvement of the case study would include:

- Interactions between small and large bubble: breakup & coalescence
- A broader exploration of body force correlations
- Modification to **Lift Coefficent**



Our case is characterized by a low volume fraction of small bubbles (7%) and a significant proportion of large bubbles with a diameter of 13 mm. Based on our underestimated results and analyzing existing correlations we could improve our predictions by modifying the lift coefficient (LC) as follows:

- For small bubbles, having a greater LC could increase the volume fraction at the wall (higher than the one by Hessenkemper)
- We wouldn't change the critical diameter as it doesn't affect our case
- For large bubbles, Tomiyama's correlations is constant and doesn't scale much for very large bubbles whereas the Hessenkemper might look a bit too steep

Therefore our proposed target correlation would look like the green line.

Conclusions

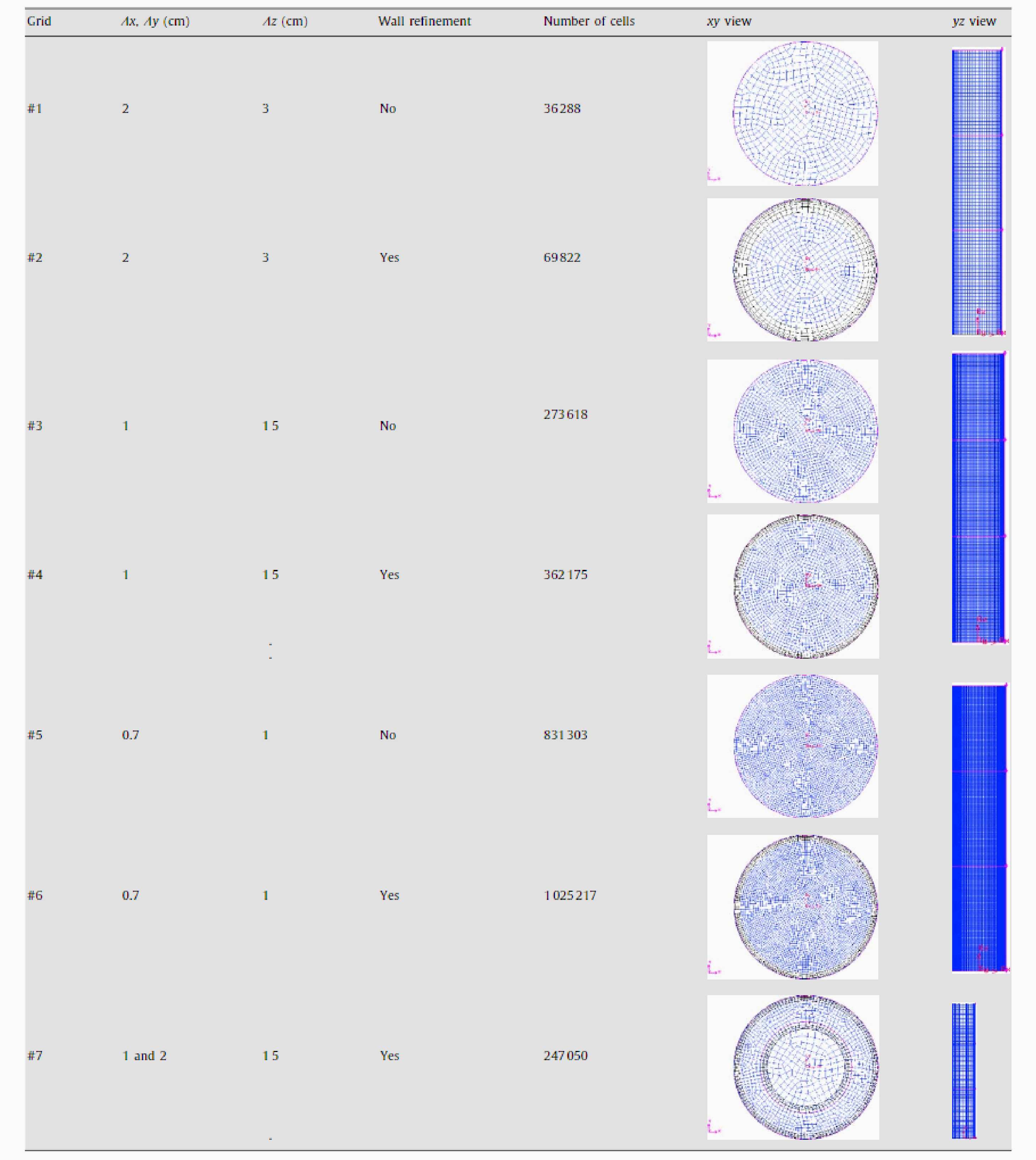
Literature Survey

We found a literature reference which could explain our underestimation of the volume fraction: **the boundary layer can greatly affect the void fraction distribution in the bulk.**

"CFD simulation of bubble column flows: Investigations on turbulence models in RANS approach"

Cédric Laborde-Boutet, Faiçal Larachi, Nicolas Dromard, Olivier Delsart, Daniel Schweich

Compares several meshing approaches and solution methods. States that the solution method greatly influences the final results, encourages to use high order of accuracy.



Grid	Δx, Δy (cm)	Δz (cm)	Wall refinement	Number of cells	xy view	yz view
#1	2	3	No	36288		
#2	2	3	Yes	69822		
#3	1	1.5	No	273618		
#4	1	1.5	Yes	362175		
#5	0.7	1	No	831303		
#6	0.7	1	Yes	1025217		
#7	1 and 2	1.5	Yes	247050		

Conclusions

Literature Survey

In another literature article we found an interesting comparison between the BSD at the inlet (sparger) and at the developed region. We noticed that our BSD is shaped much more like the one in the **developed region**.

We therefore conclude that our approach better fits the experimental data we were given and neglecting the nozzle region avoids biased BSD.

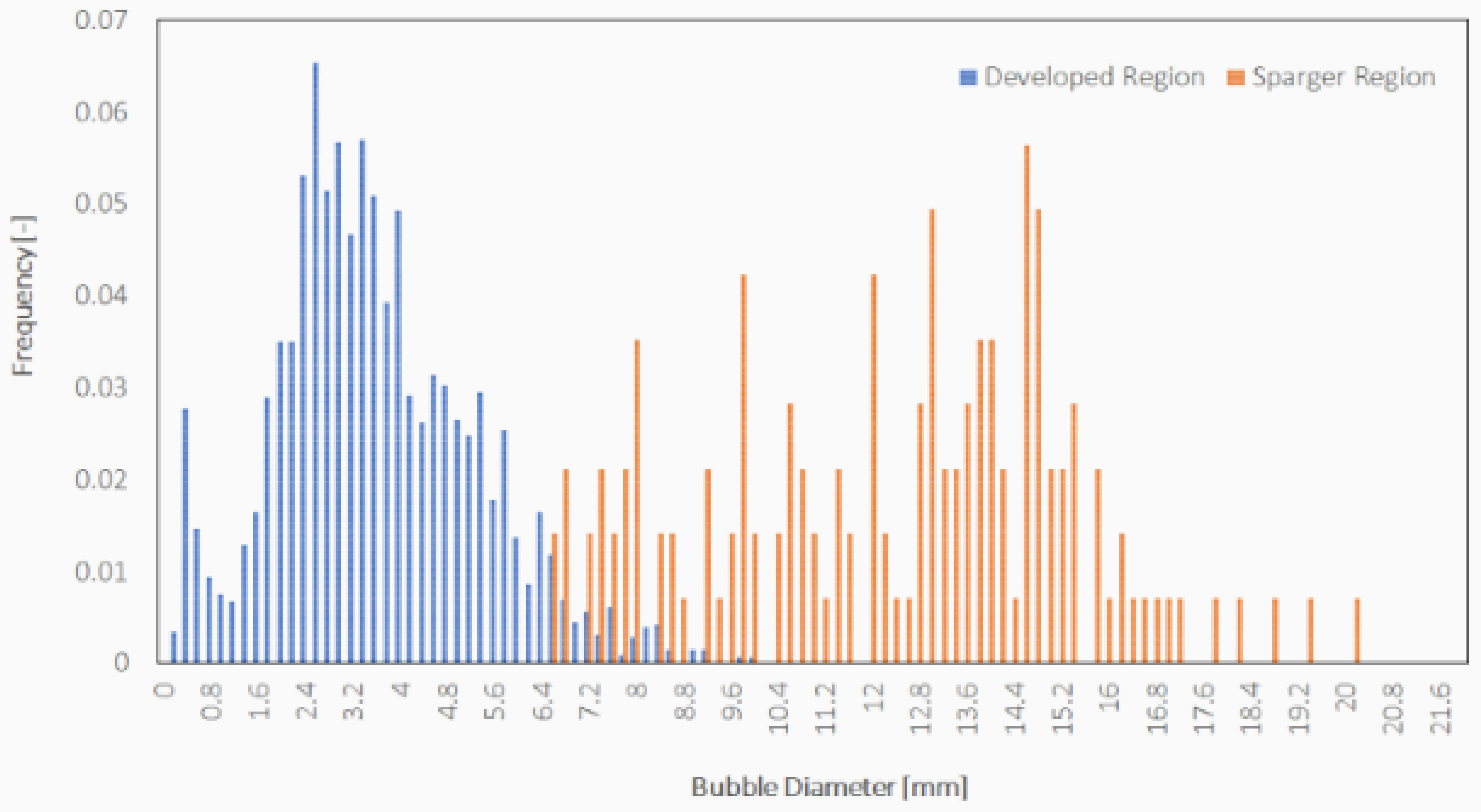


Fig. 5. BSD at the developed region and sparger for flow rate of 10 Nl/min (U_g = 0.003684 m/s).

"Multiphase numerical modeling of a pilot-scale bubble column with a fixed poly-dispersity approach"

Ashkan Hosseini, Riccardo Mereu, Salvatore Canu, Thomas Ziegenhein, Dirk Lucas, Fabio Inzoli

Showed that even if monodispered and bi-disperesed modelling do not affect the average volume fraction, the radial distribution is greatly affected and the bi-disperesed model has to be preferred.