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Influence of the turbulence model in CFD modeling of wall-to-fluid heat transfer in packed beds

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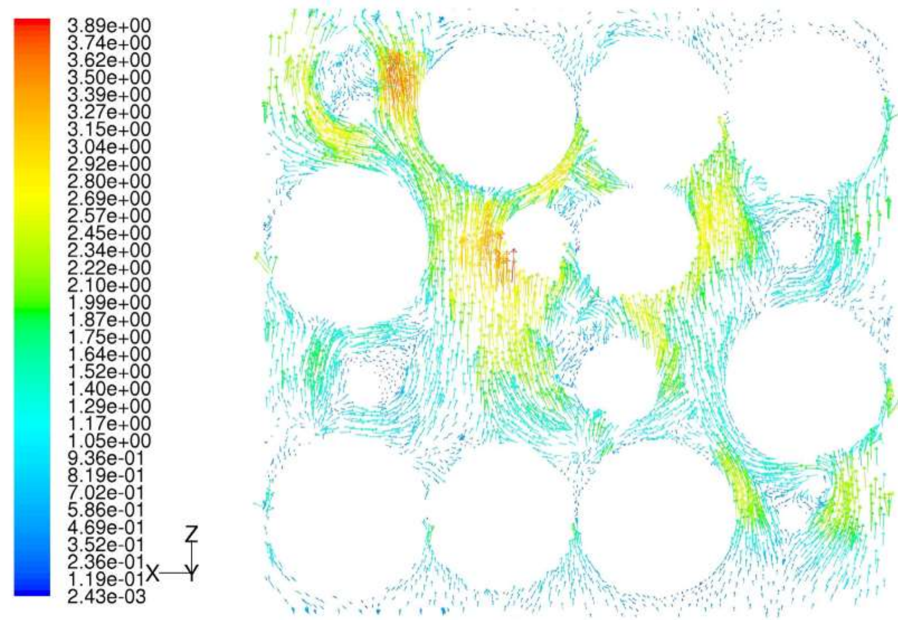
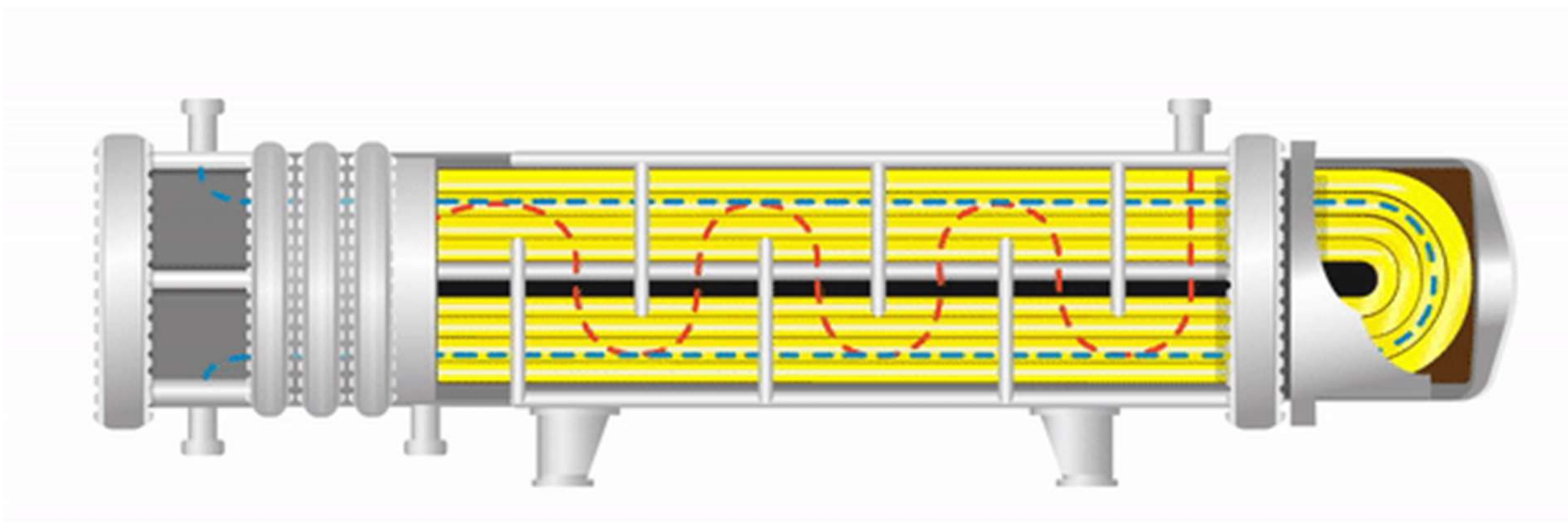


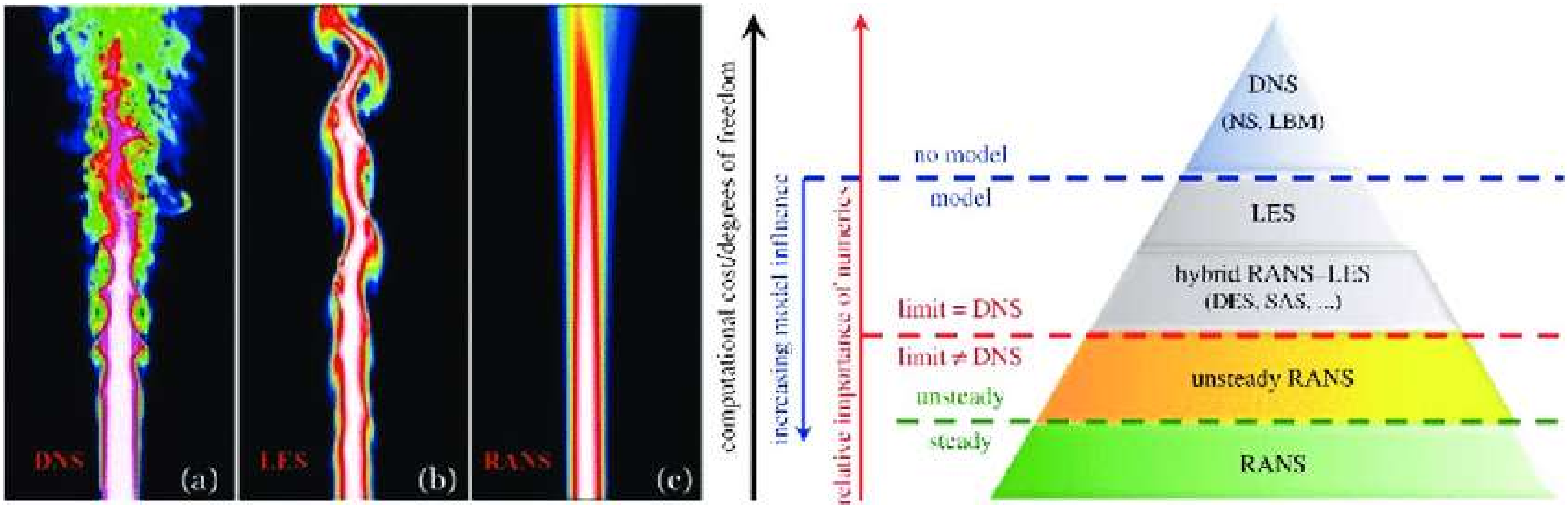
Figure 4.6. Velocity vectors profile in a cross section ($y = 0$) for $Re = 633$
Velocity profile is expressed in m/s

Introduction: Heat Exchanger

- Well designed packing structure and column geometry can lead to the desired fluid and mass transport characteristic for the desired behavior.
- Pressure drop along the bed, ΔP is a crucial parameter as it is directly related to the fluid flow resistance in the bed
- Low-pressure drop is typically preferable for heat exchangers as it minimizes resistance to fluid flow, ensuring efficient heat transfer.

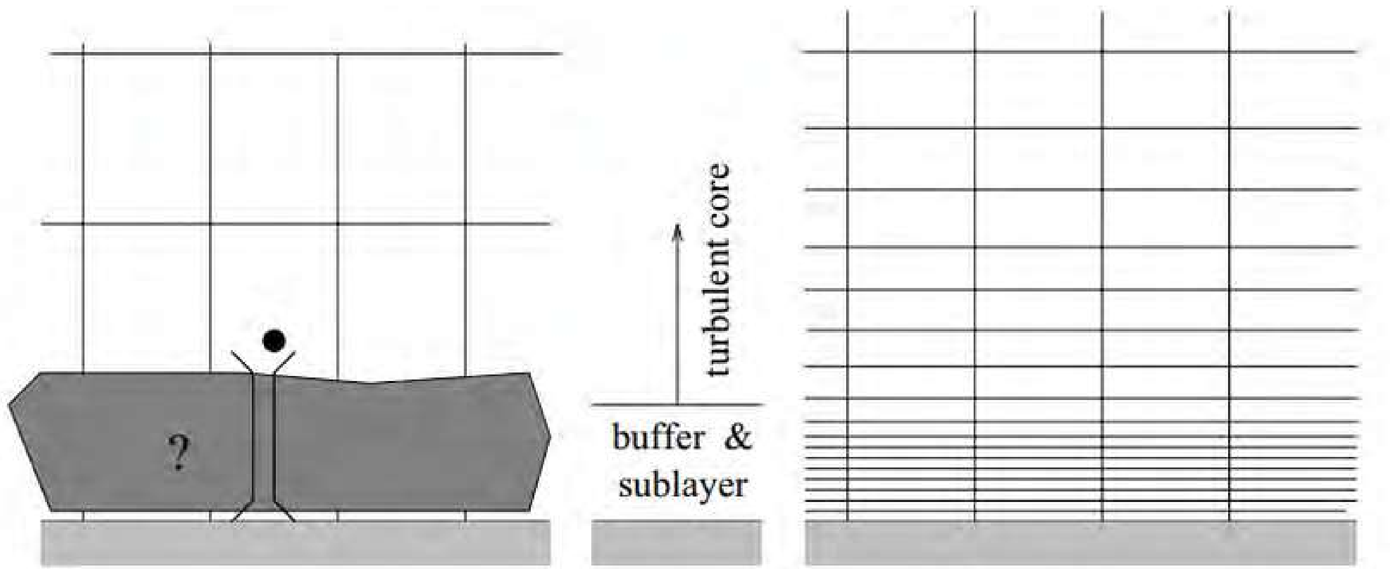


Introduction: Turbulence Modelling



- In most turbulent models, an additional term is included in the Navier-Stokes equation to account for the effect of turbulence.
- Add an empirical or semi-empirical turbulent viscosity term, which models the effects of turbulent mixing on the fluid's momentum and energy
- Inaccurate prediction can over/underpredict fluid flow.

Introduction: Meshing



Wall Function Approach

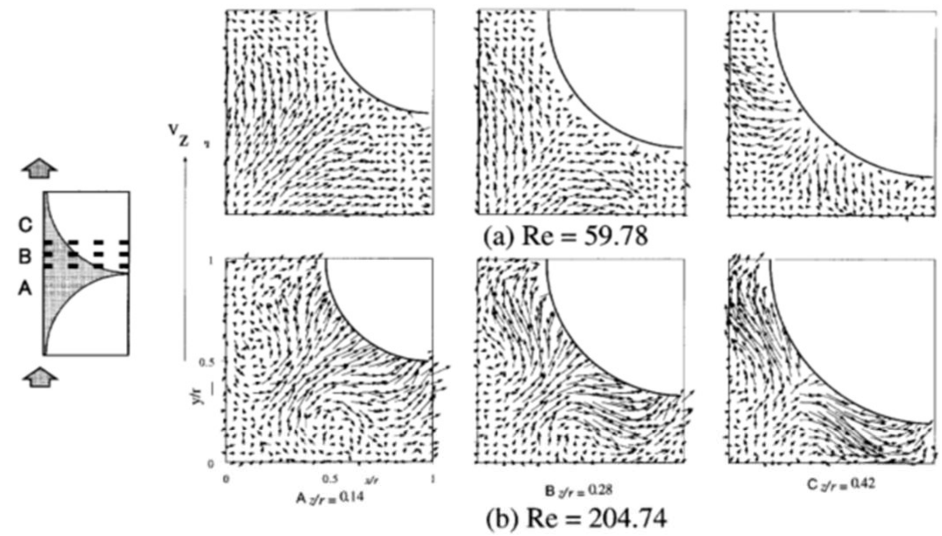
- The viscosity-affected region is not resolved, instead is bridged by the wall functions.
- High-Re turbulence models can be used.

Near-Wall Model Approach

- The near-wall region is resolved all the way down to the wall.
- The turbulence models ought to be valid throughout the near-wall region.

Motivation

- Computational fluid dynamics (CFD) can enable accurate view of temperature and velocity throughout the column
- Which turbulent model to choose?
  Spalart-Allmaras (SA)
  k-*ε* {Standard, Realizable, RNG}
  k-*ω* {Wilcox, Wilcox's modified, SST}
  Reynolds Stress Model (RSM)
  Large Eddy Simulation (LES)
  Detached Eddy Simulation (DES)
  …. And many more!
- Best model?



[6] **Figure 10. Horizontal flow at (a) *Re* = 59.78 and (b) *Re* = 204.74 in the downstream slices, where the cross-sectional area decreases along the main flow direction (see sketch at left).**

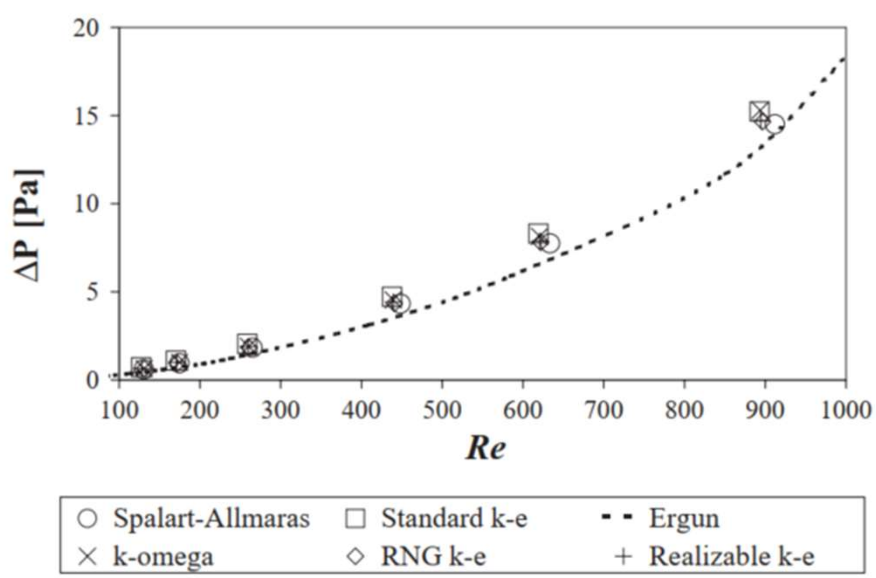
Length of the left arrow represents the magnitude of the main flow velocity v_z at the pore center ($x = y = z = 0$) of 8.66 and 29.78 mm/s for $Re = 59.78$ and 204.74, respectively.

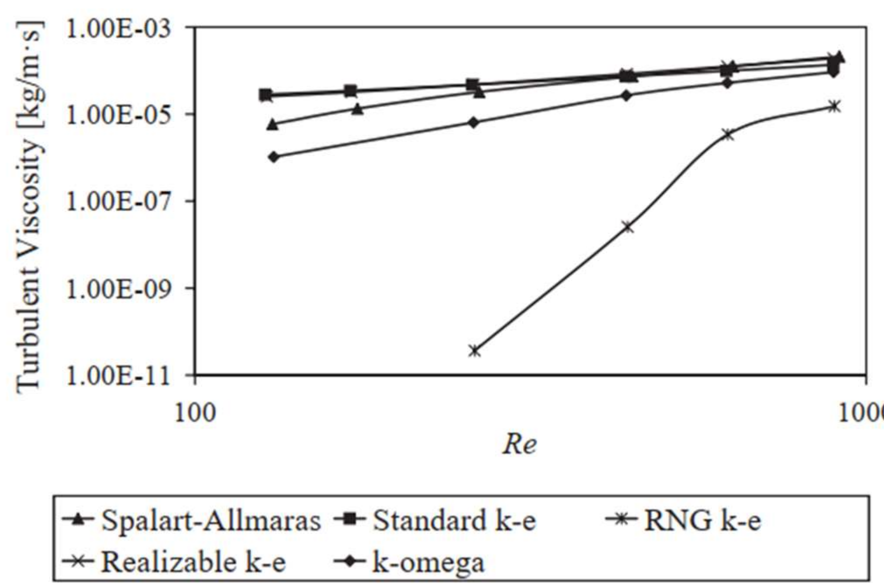
Problem Objective

1. Simulate steady state turbulent flow (inlet turbulence intensity of 4%) coupled with forced convection using standard SA and RNG k-ε turbulence model with inlet velocity of 0.525m/s and 0.75 m/s.

2. Evaluate the model performance by replicating pressure drop, ΔP vs Re_D plots.

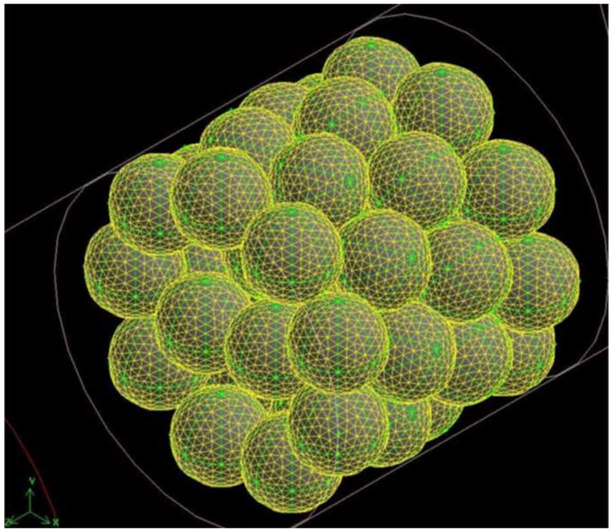
3. Evaluate the model performance by replicating turbulent viscosity vs Re_D plots.

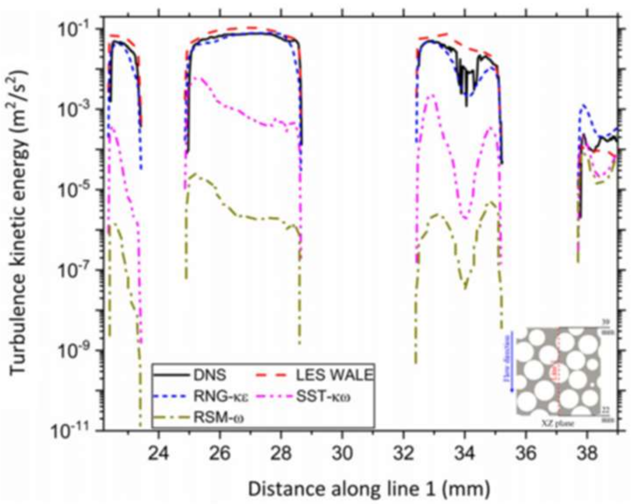




Literature Review

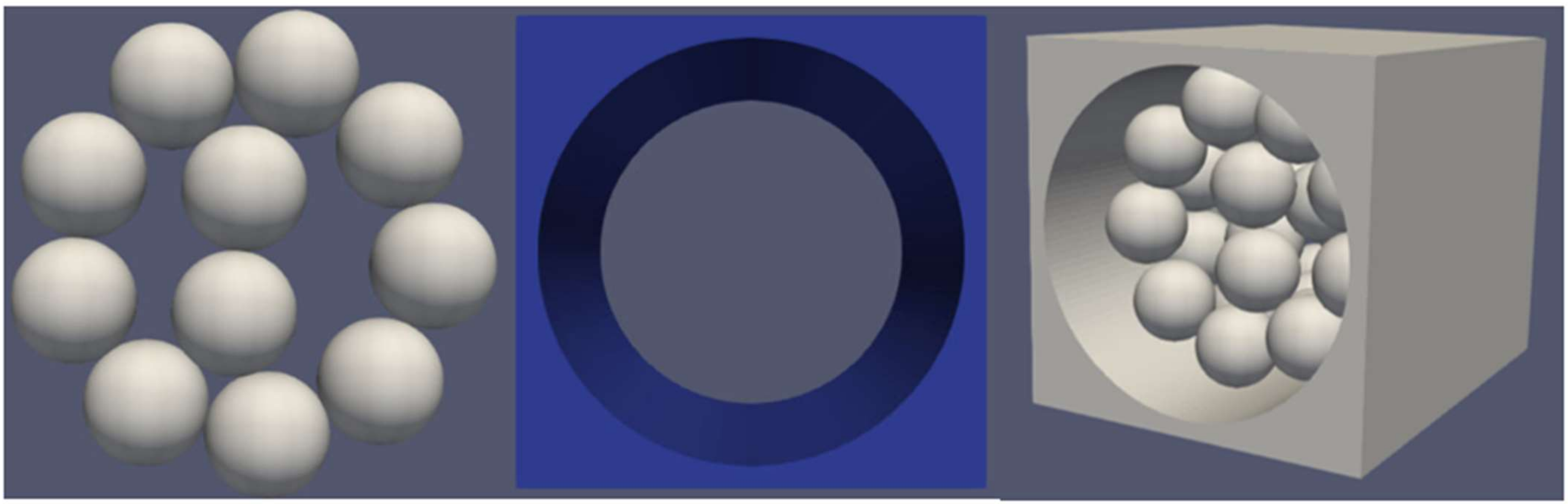
- Guardo *et al*. [1,2] simulated a packed sphere bed using 5 RANS model and found that SA was the best and RNG was fair.
- Wood et al. published presents a comprehensive review of the current understanding and modeling of turbulent flows in porous media. They report that that k-ω SST and Realizable k-ε is most widely used in the industry
- Ambekar et al. [5] simulated 113 randomly packed sphere bed using RANS, LES and DNS using lattice Boltzmann method (LBM). They found that RNG k-ε performed well compared to direct numerical simulation (DNS) showed that k matched DNS better than other RANS model.





Methodology: Mesh Generation

- Sphere Diameter =0.00186m
- Pipe Diameter=0.152m
- 11 sphere configuration with 1% overlap
- Sphere law is duplicated with 60˚ rotation for each layer



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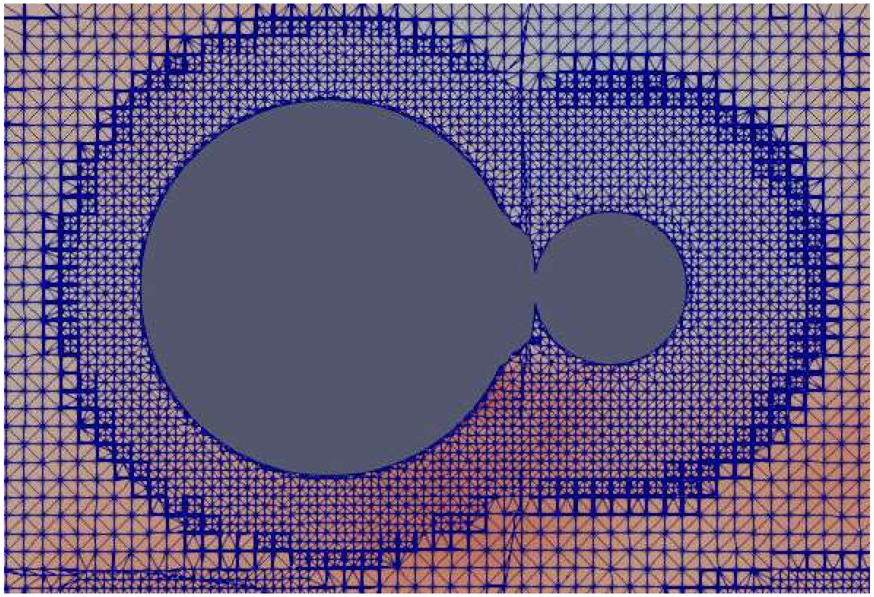
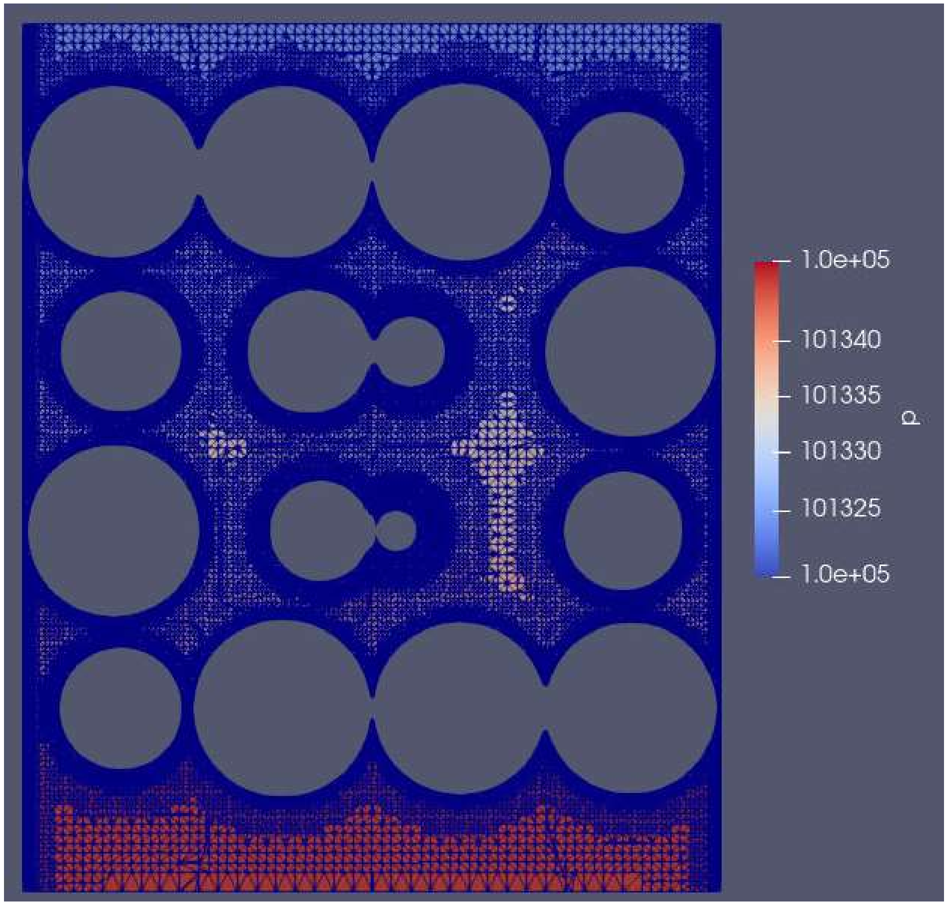
Methodology: Mesh Generation

- snappyHexMesh
- Average y+ value of 1.65 for the spheres and 1.86 for the pipe walls.
- The minimum y+ values were 2.6 and 3.3 for the spheres and pipe walls





Methodology: Case Setup

- CFD simulation was performed on OpenFOAM using Wichita State University high performance computing platform using up to 36 cores and 4Gb of RAM each
- Steady state, turbulent flow coupled with forced convection is simulated using buoyantSimpleFoam.

$$k = \frac{3}{2} U^2 I^2 \quad (1)$$

$$l = 1.32 d_h (\frac{U d_h}{\nu \psi})^{-0.75} \quad (2)$$

$$d_h = \frac{2\psi}{3(1-\psi)} d_p \quad (3)$$

$$\varepsilon = C_\mu \frac{k^{3/2}}{l} \quad (4)$$

$$\omega = \frac{\varepsilon}{C_\mu k} \quad (5)$$

$$v_t = \frac{k}{\omega} \quad (6)$$

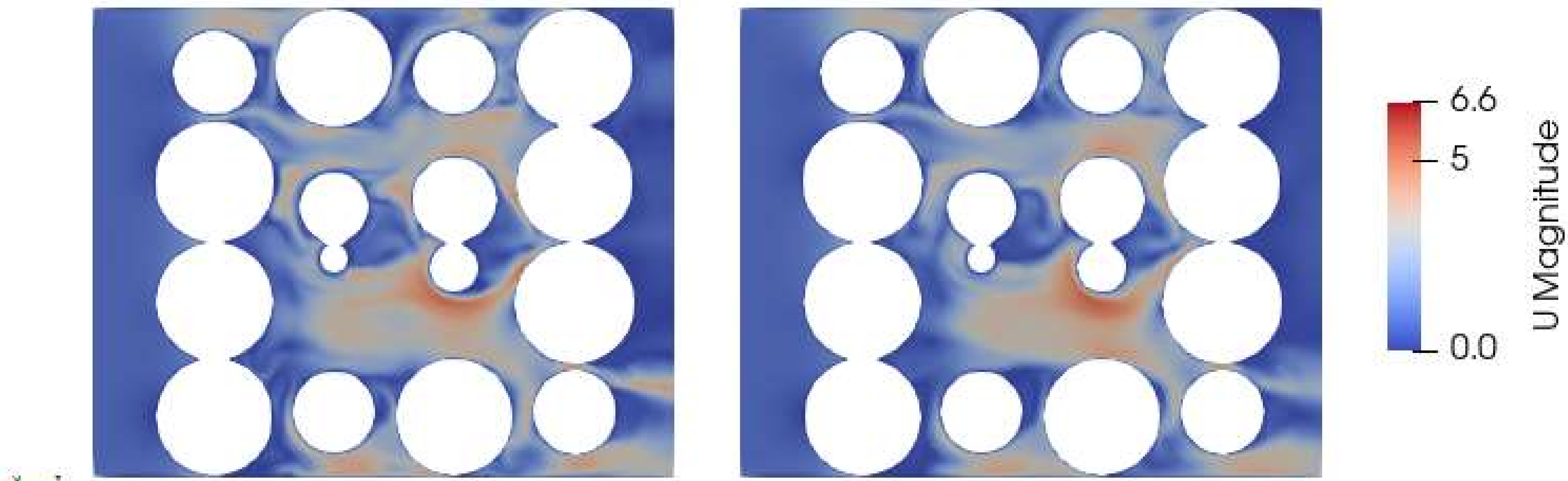
Methodology: Case Setup

- To simplify calculations, only the average fluid properties is used for Reynolds number calculation

$$Re = \frac{U\, d_p}{\nu} \quad (7)$$

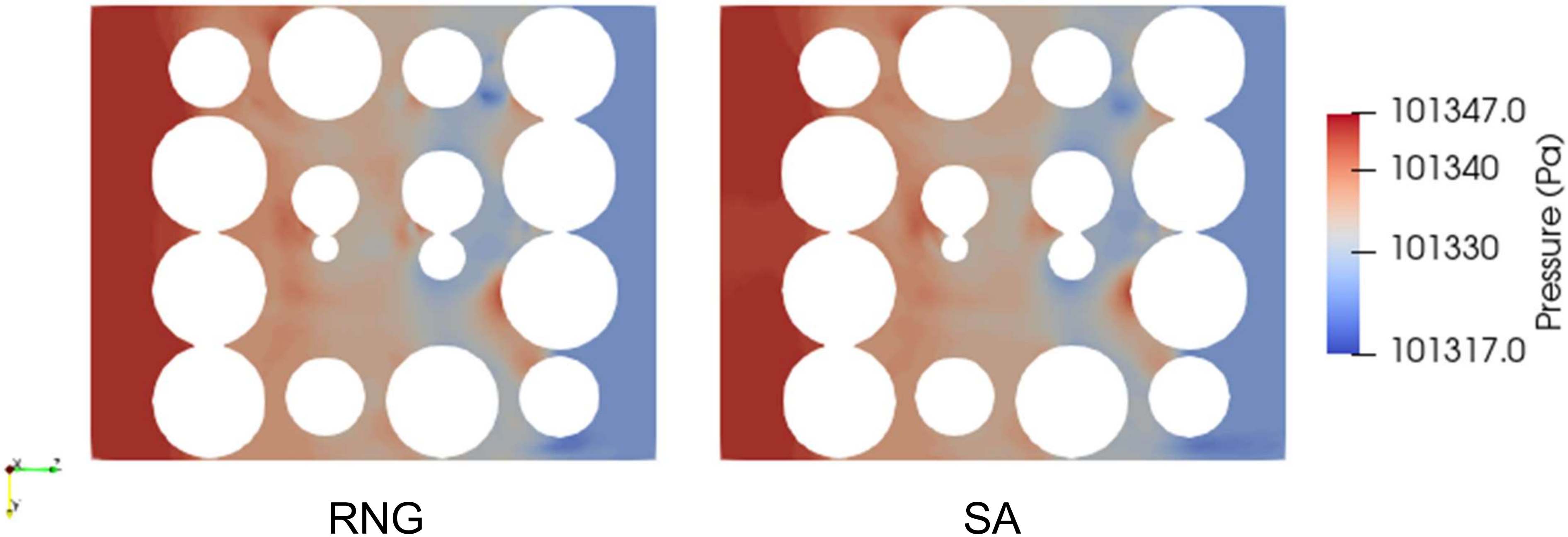
- The resulting Reynolds number of 0.525m/s and 0.75m/s was 630 and 900 respectively
- The initial simulation ran for 2000 iterations but after the first simulation, it was found that the simulation had converged at about 500 iterations

Results: Velocity Profile



RNG SA

Results: Pressure Drop



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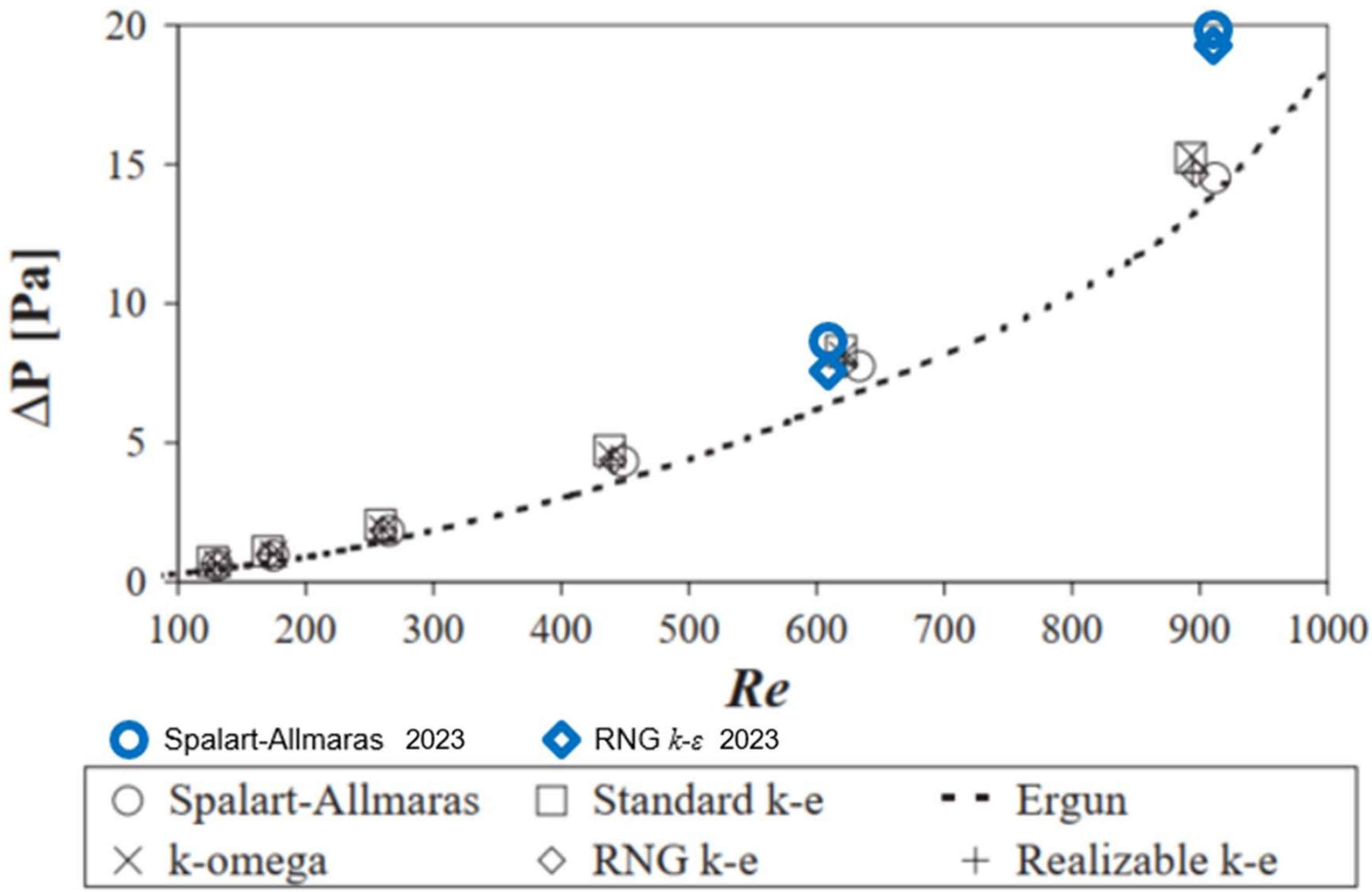
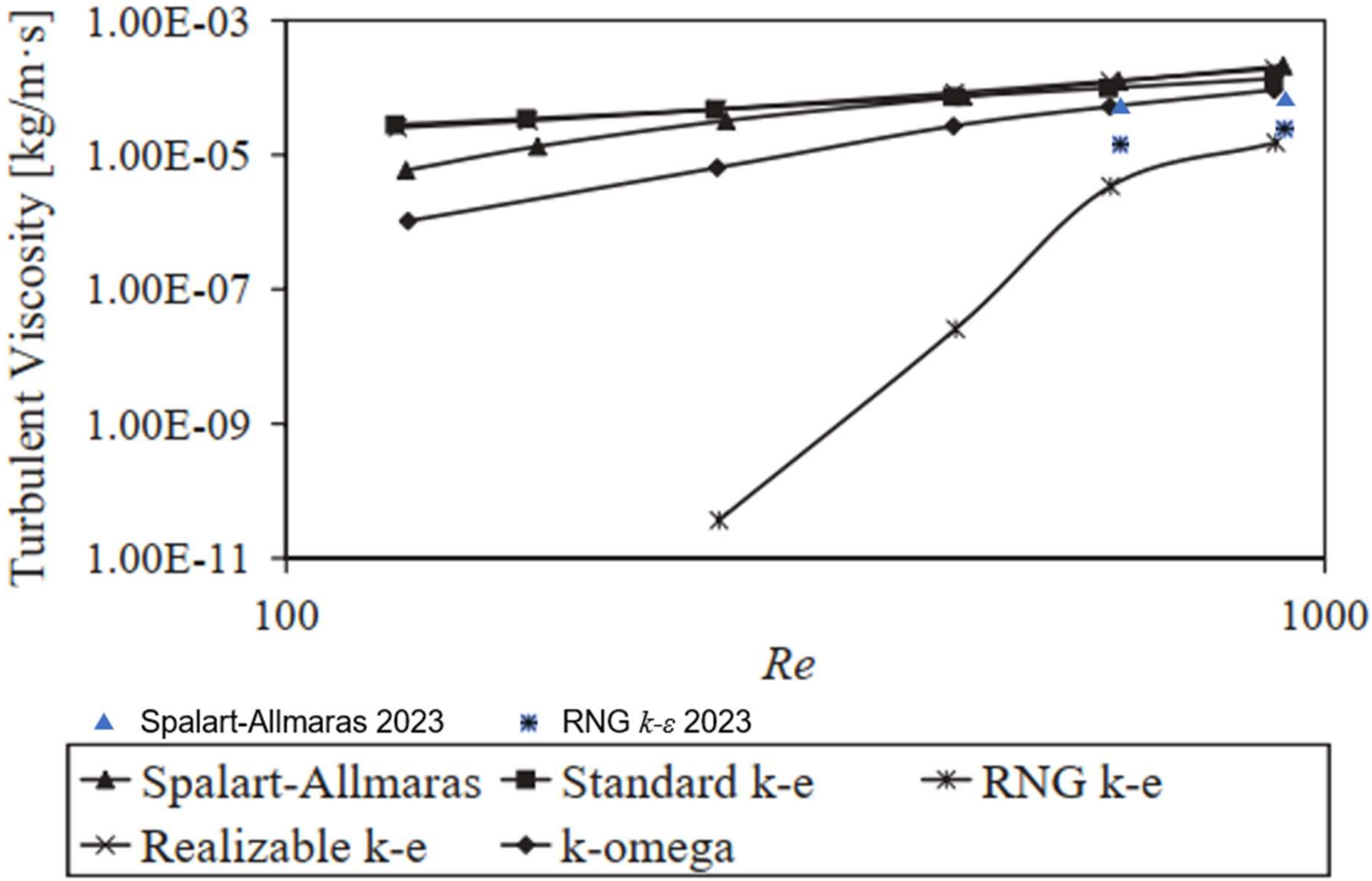
Results: Pressure Drop



Results: Turbulent Viscosity



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Limitations

Assumptions made in reproduction

- Forced convection only therefore natural buoyancy effect on fluid and heat transfer are ignored
- No developing volume prior to the packed beds
- Turbulent properties of boundary conditions may not reflect the original work
- Geometry of the pipe and STL may not reflect the original work

Limitations of the study

- A mesh independence study was not done and there could be numerical errors due to the grid size
- Only 2 inlet velocity is investigated and the results may differ with other Reynolds number
- Boundary conditions were calculated empirically and based on industry practices, using DNS data or experimental results would be better for this complex flow

Conclusion

- RNG k-ε performs slightly better than Spalart-Allmaras for pressure drop.
- Regarding turbulent viscosity, SA appears to be more accurate, although RNG k-ε has shown improvements compared to the 2005 study.
- This highlights the need for further research in this area, as the original 2005 study may be outdated

Future work

- Investigate additional turbulence models and more Reynolds number
- Include natural buoyancy effects

References

[1] A. Guardo, M. Coussirat, M. A. Larrayoz, F. Recasens, and E. Egusquiza, "Influence of the turbulence model in CFD modeling of wall-to-fluid heat transfer in packed beds," *Chemical Engineering Science*, vol. 60, no. 6, pp. 1733–1742, 2005.

[2] A. Guardo and A. Larrayoz, "Computational Fluid Dynamics Studies in heat and mass transfer phenomena in packed bed extraction and reaction equipment: Special attention to supercritical fluids technology," thesis, 2007.

[3] S. Ergun and A. A. Orning, "Fluid flow through randomly packed columns and Fluidized Beds," *Industrial & Engineering Chemistry*, vol. 41, no. 6, pp. 1179–1184, 1949.

[4] B. D. Wood, X. He, and S. V. Apte, "Modeling turbulent flows in porous media," *Annual Review of Fluid Mechanics*, vol. 52, no. 1, pp. 171–203, 2020.

[5] A. S. Ambekar, C. Schwarzmeier, U. Rüde, and V. V. Buwa, "Particle-resolved turbulent flow in a packed bed: Rans, Les, and DNS simulations," *AIChE Journal*, vol. 69, no. 1, 2022.