Optimization of Trickle Bed Reactor Distribution: a Computational Fluid Dynamic Approach

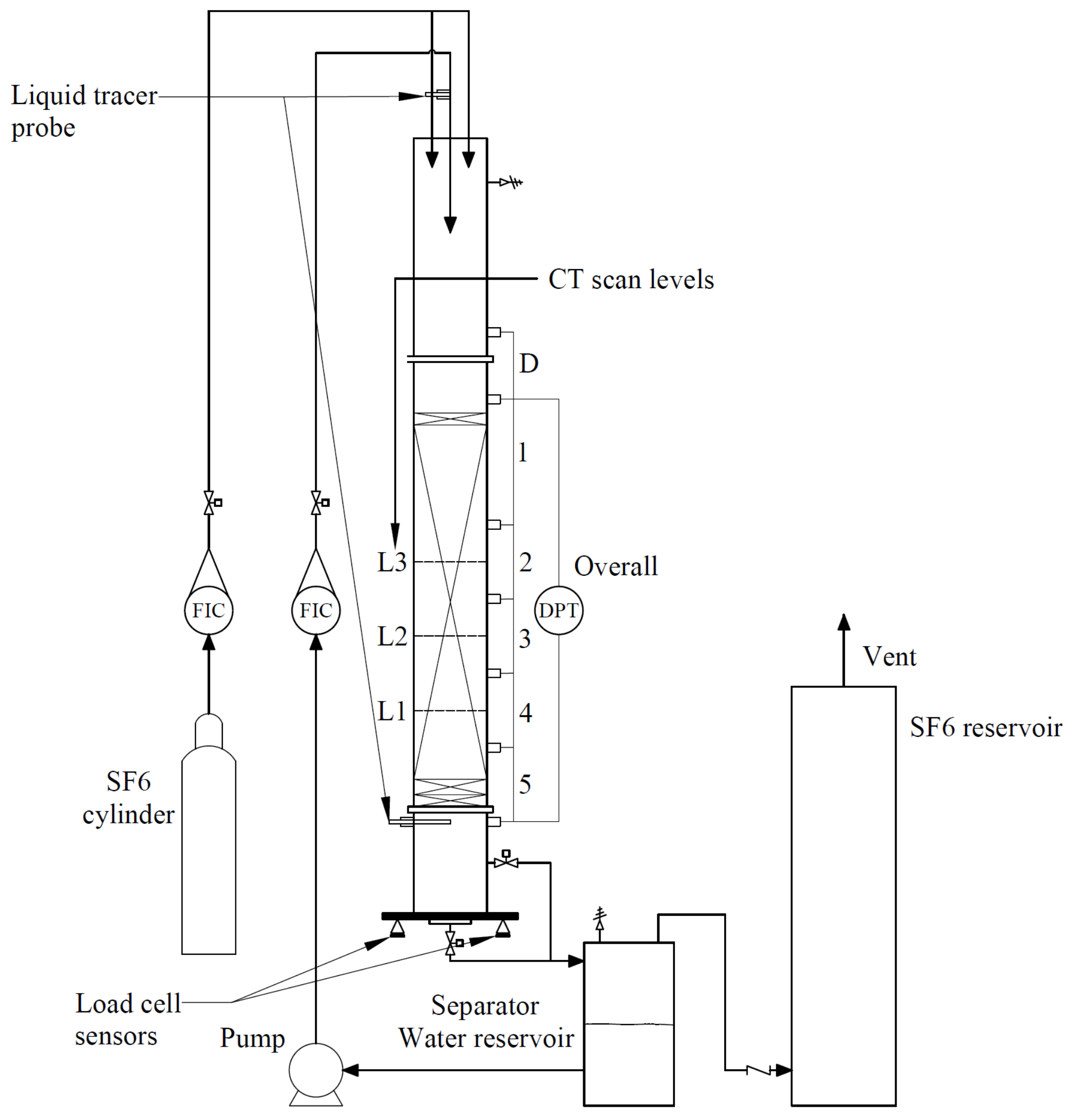
Carly Fox[1], Madison Holly[2], Sebastián Uribe[2*], Muthanna Al-Dahhan[2,3]

1 Mechanical and Aerospace Engineering
2 Linda and Bipin Doshi Department of Chemical and Biochemical Engineering
3 Department of Nuclear Engineering and Radiation Science

Doshi
Department of Chemical and Biochemical Engineering
College of Engineering and Computing

Introduction

Trickle bed reactors are widely applied across different chemical and biochemical industries. Despite the vast applications and uses of these systems, there is still a need to optimize these reactors in order to enhance their throughput and to enable the development of new processes. The present study is conducted to advance the knowledge in the optimization of the phases distribution in a TBR.



Schematic Diagram of the Experimental Setup

In order to optimize TBRs, and enable the design of new processes, it is of key importance to develop tools that allow the prediction of the phases distribution in the reactor, and that can assess the effect of internal structures and distribution plates over such distribution.In this study, the distributor plate design over the phase's distribution was analyzed using Computational Fluid Dynamic techniques.

Objective

General objective:

- **Study the two-phase hydrodynamics phenomena on the distributor section of a TBR to determine the effect of distributor plates over the downstream phases distribution**

Specific objectives

- **Implement an interphase tracking method for a two-phase (liquid and gas phases) flowing concurrently downward through the distributor plate.**
- **Determine the effect of the flow regimes over the maldistribution factor downstream from the distributor pla**
- **Perform a sensitivity analysis of the effect of design criteria of distributor plates, such as inlet tube diameters, side tube diameter and tube height, over the phases maldistribution, in order to optimize the distributor design**

Mathematical Modelling

STAR CCM+ is utilized to run simulations of the distributor plate to determine the maldistribution coefficient within the trickle bed reactor. A volume of fluids approach is used to approximate the fluid interactions.

Governing Equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \mathbf{u} \right) = 0$$

$$\frac{\partial}{\partial t}\left(\rho \mathbf{u} \right) + \nabla \cdot \left(\rho \mathbf{u}\mathbf{u} \right) = -\nabla P + \nabla \cdot \left[\mu \left(\nabla \mathbf{u} + \left(\nabla \mathbf{u} \right)^T \right) \right] + \rho \mathbf{g} + \mathbf{F}_{GL}$$

Volume of Fluids closure:

$$\sum_i \varepsilon_i = 1;\ \rho = \sum_i \rho_i \varepsilon_i;\ \mu = \sum_i \mu_i \varepsilon_i;\ \frac{\partial \varepsilon_i}{\partial t} + \nabla \cdot \left(\varepsilon_i \mathbf{u} \right) = 0 \quad i = L, G$$

Phase Interactions

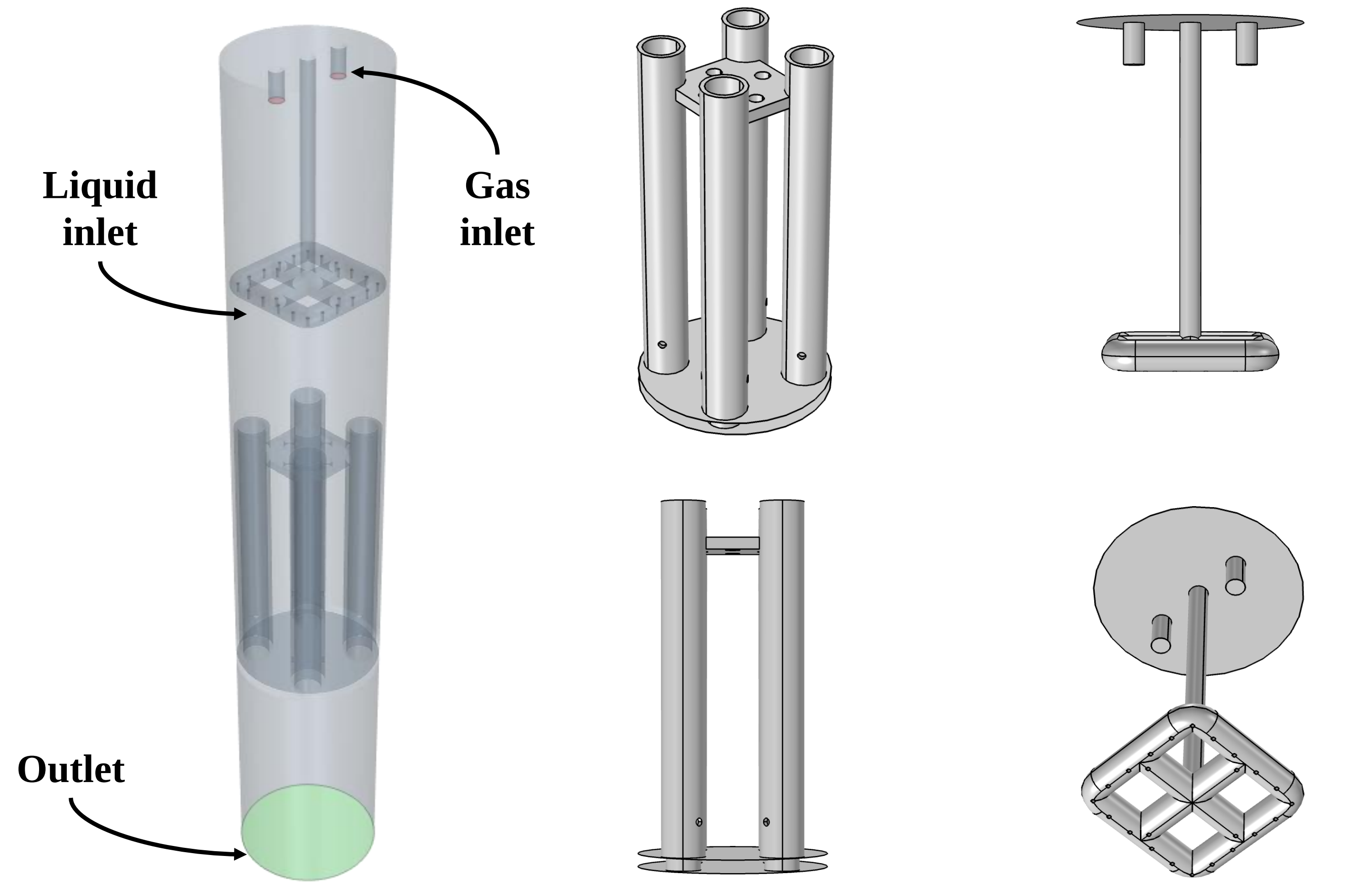
$$\mathbf{F}_{GL} = \mathbf{F}_{\sigma}^{n} + \mathbf{F}_{\sigma}^{t} = \sigma_{GL} \kappa \mathbf{n} + \frac{\partial \sigma}{\partial t} \mathbf{t}$$

$$\mathbf{n} = \nabla \varepsilon_i;\ \kappa = -\nabla \cdot \frac{\nabla \varepsilon_i}{\left| \nabla \varepsilon_i \right|}$$

$\mathbf{F}_{GL}$ considers the normal ($\mathbf{F}_{\sigma}^{n}$) and tangential ($\mathbf{F}_{\sigma}^{t}$) surface tension components. σ_{GL} and κ are the surface tension and surface curvature, respectively. n and t are the surface normal and tangential vectors, respectively

CAD Modelling

The geometrical representation of the distribution section was modeled using Siemens NX



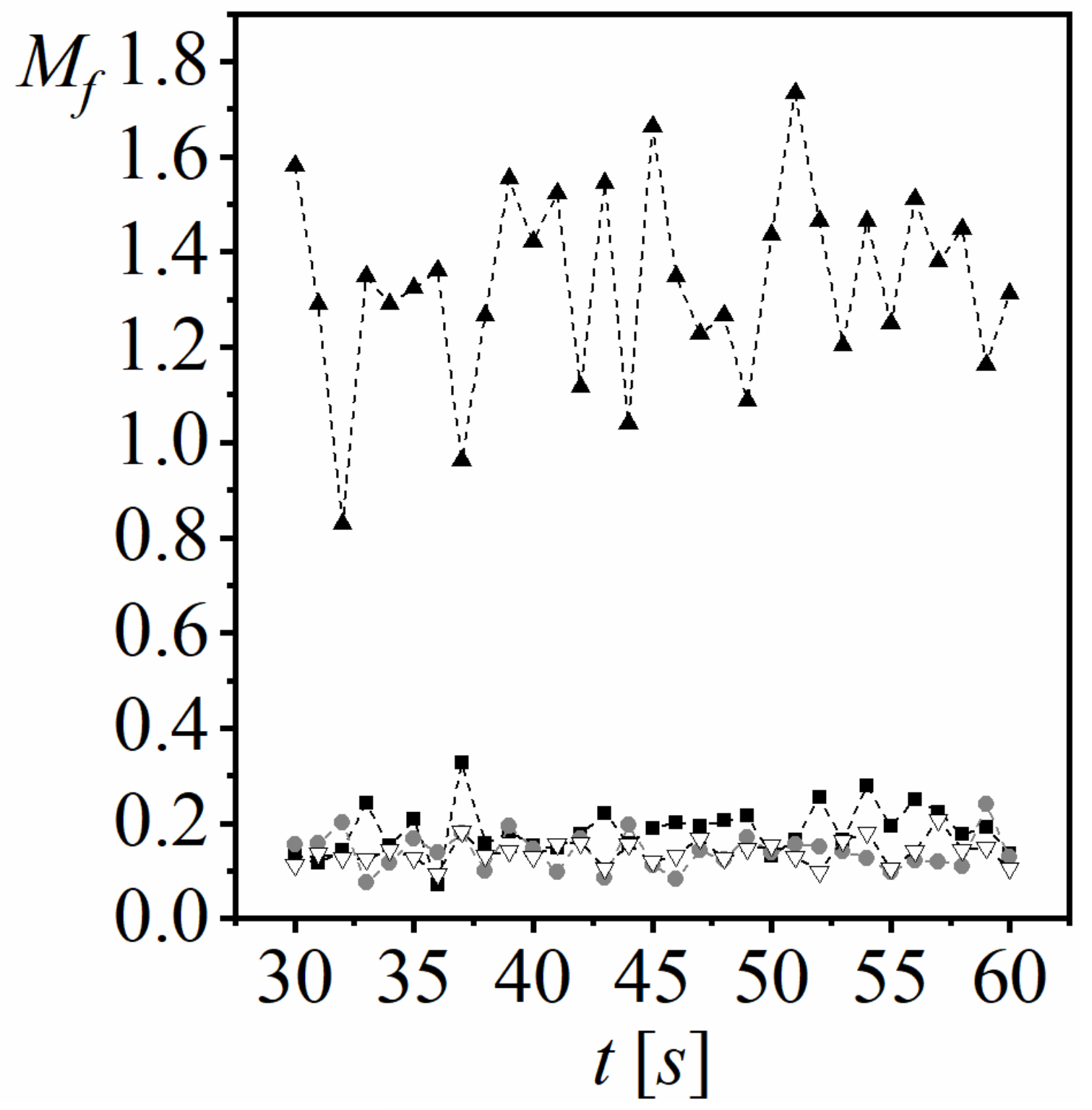
Full geometry

Distributor plate

Gas and liquid inlet

Details of the CAD model

Results & Discussion

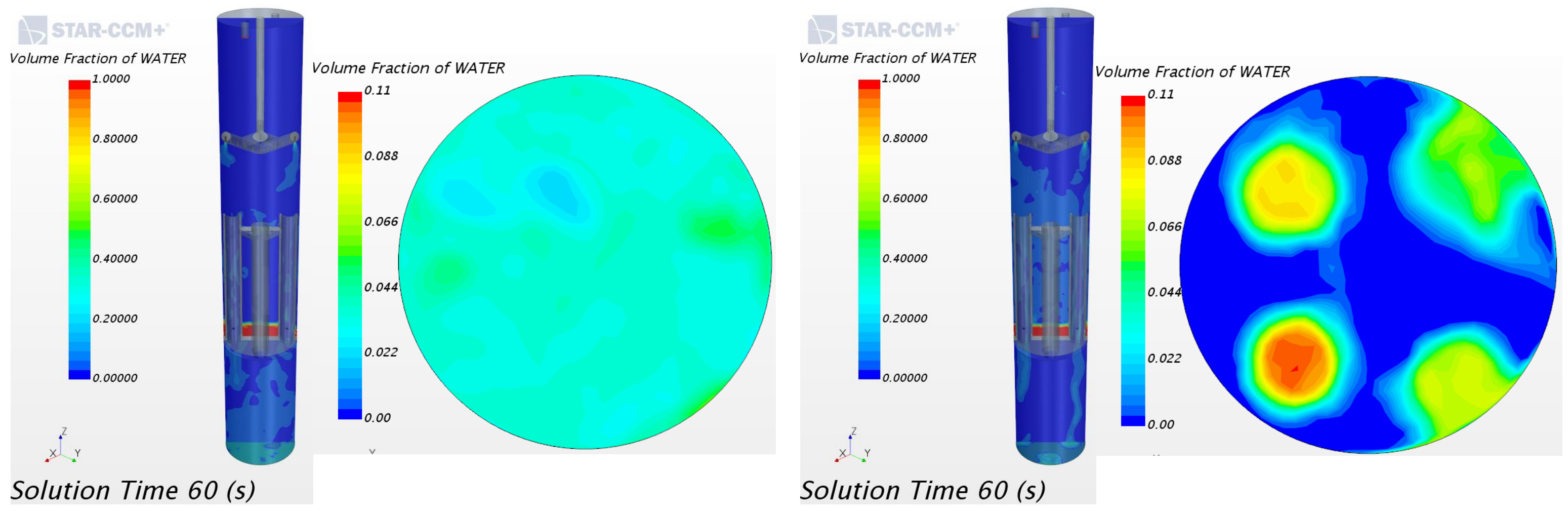


Liquid Maldistribution Factor:

$$M_f = \sqrt{\frac{1}{N\left(N-1\right)} \sum_{i=1}^{N} \left(\frac{\varepsilon_{L,i} - \bar{\varepsilon}_L}{\bar{\varepsilon}_L} \right)^2}$$

The maldistribution factors (M_f) were calculated from the simulation results at the outlet boundary at intervals of 1 *s*, for 30 *s*, at the interval 30<t<60 *s* to ensure steady state predictions

Time series and average maldistribution factors obtained at different flow rates



$L = 6.3\,kg/m^2s;\ G = 0.13\,kg/m^2s$

Good distribution

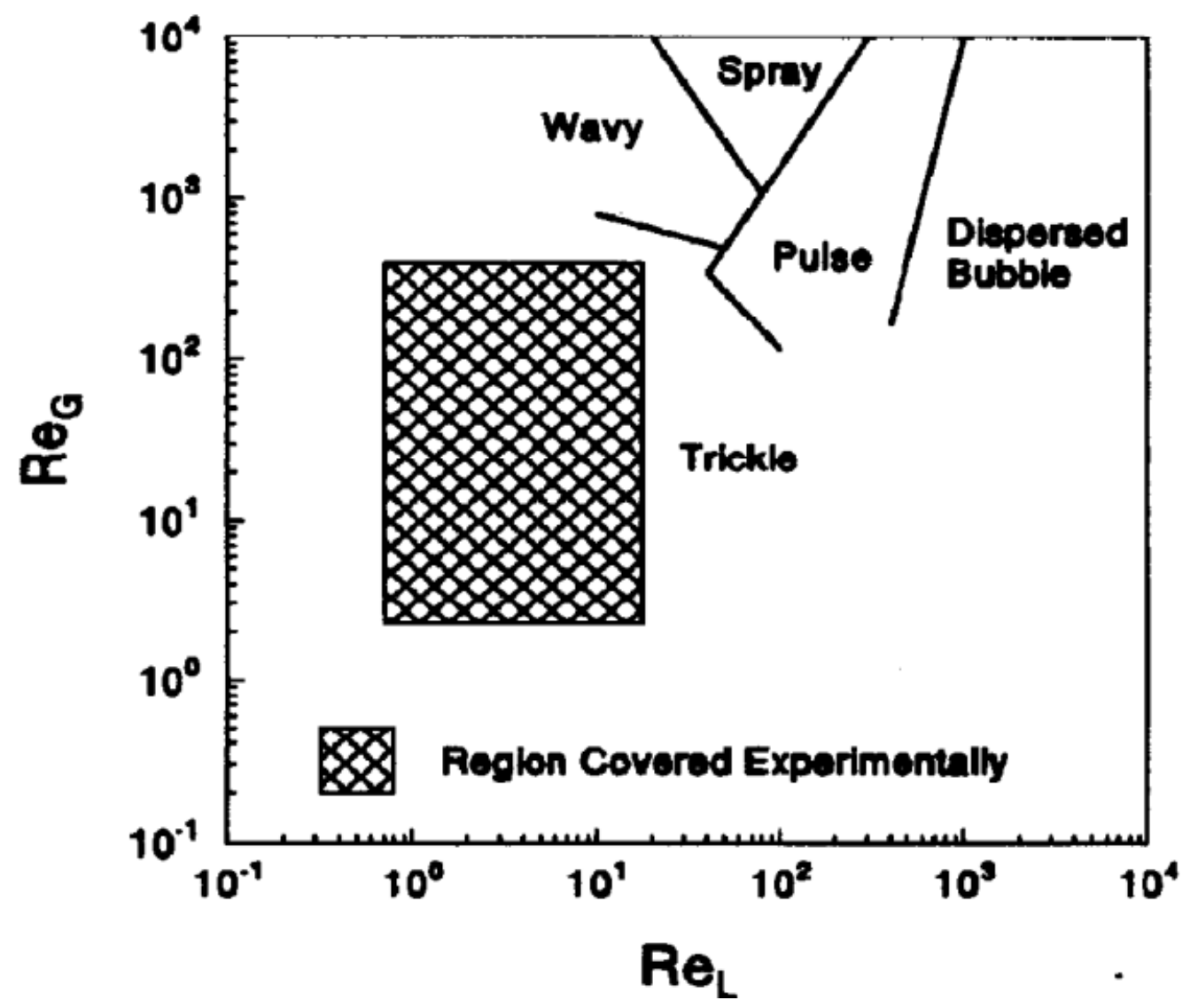
$L = 12.7\,kg/m^2s;\ G = 0.20\,kg/m^2s$

High maldistribution

Sample of distribution profiles predicted by the model

Remarks

- **Application of CFD techniques allows to properly predict the effect of the distributor plate and flow regimes over the maldistribution in a TBR**
- **Some flow conditions highly impact the maldistribution obtained. This could be an indication of a change in the flow regime**
- **Further analysis of flow conditions and distributor designs are needed**



(*Al-Dahhan & Dudukovic, 1994*)

References

Al-Dahhan, M. H., & Dudukovic, M. P. (1994). Pressure drop and liquid holdup in high pressure trickle-bed reactors. Chemical Engineering Science, 49(24), 5681-5698.

Al-Dahhan, M. H., Larachi, F., Dudukovic, M. P., & Laurent, A. (1997). High-pressure trickle-bed reactors: a review. *Industrial & engineering chemistry research*, 36(8), 3292-3314.

Qi, B., Farid, O., Uribe, S., & Al-Dahhan, M. (2020). Maldistribution and dynamic liquid holdup quantification of quadrilobe catalyst in a trickle bed reactor using gamma-ray computed tomography: Pseudo-3D modelling and empirical modelling using deep neural network. *Chemical Engineering Research and Design*, 164, 195-208.

Qi, B., Uribe, S., Farid, O., & Al-Dahhan, M. (2022). Random trilobe packing using rigid body approach and local Gas-Liquid hydrodynamics simulation through CFD with experimental validation. *Chemical Engineering Journal*, 435, 134481.