What's Going on Within the Big Guys in Chemical Plants?

DNS and Mesoscale Simulation of Gas Phase Concentration Transport Structurered Packings of Absorption and Distilation Columns

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In Short

- The concentration transport within distillation and absorption columns is important for the separation efficiency
- CFD simulations of industrial sized columns of meters in diameter is prohibitive in terms of computational resources.
- Direct numerical simulations will be conducted in a small excerpt of the column internals - a structured packing of metal sheets - in order to calibrate a mesoscale model for structured packings, which is computationally capable to simulate large scale columns.
- DNS has to be used since turbulence models showed to have insufficient precision in concentration transport in this type of geometry and typical flow regimes including also the transition from laminar to turbulent flow.

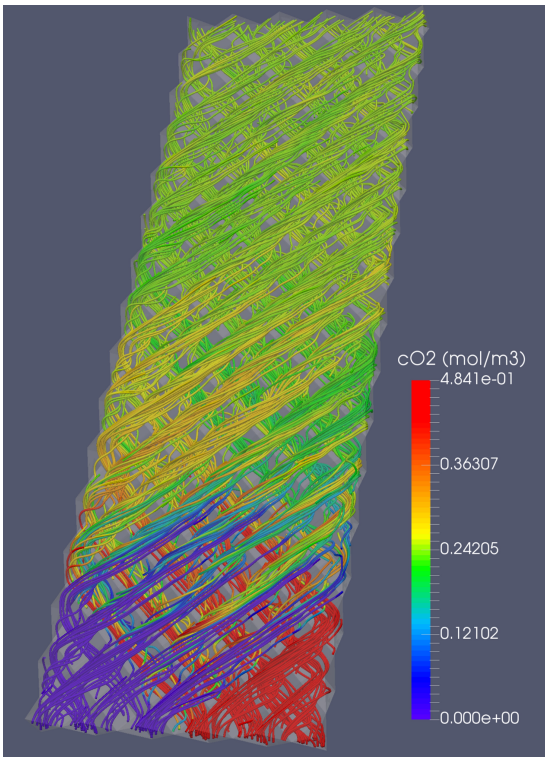

***Figure 1:** Structured packing gas flow CFD simulation with tracer concentration.*

Distillation and absorption columns are the most popular units for substance separation in chemical plants (Fig.1). An ever more popular column internal are so called structured packings of metal sheets which provide a high two phase interfacial area and mass transfer while keeping low pressure drops (Fig.1).

Especially in large scale columns of several meters in diameter the distribution of concentration within the columns is more non-uniform and has not been thoroughly investigated and understood in terms on its impact on the seperation efficiency of the distillation processes.

In times where energy consumption is more critical, the understanding and prediction of the three-dimensional concentration distributions becomes important to achieve more efficient column designs and operations in the future.

Since CFD calculations are practically prohibitive to simulate industrial sized distillation and absorption columns of meters in diameter, a new mesoscale model has been developed in order to simulate the concentration distribution in structured packings by [2]. The mesoscale model in its turn has to be calibrated with experimental data or CFD data (i.e. virtual experiments). In [2] the mesoscale model was successfully calibrated and validated within the laminar flow range against laminar steady-state CFD simulations.

In the turbulent and transition regime, however, as shown in [2] by comparision to experimental results, steady-state RANS models have a poor precision of the concentration transport in structured packings. Therefore, more expensive transient DNS calculations are necessary to yield good data to calibrate the mesoscale model in the turbulent regime.

Within this project DNS calculations are performed on a small periodic element (2X2X2cm) of the structured packing to calibrate the mesoscale model within the turbulent and transition regimes. Further, DNS calculations are conducted on a bigger excerpt of the structured packing (50X20X2cm) over the whole regime range to proove the mesoscale model's predictive power. All simulations include the concentration transport of a tracer component.

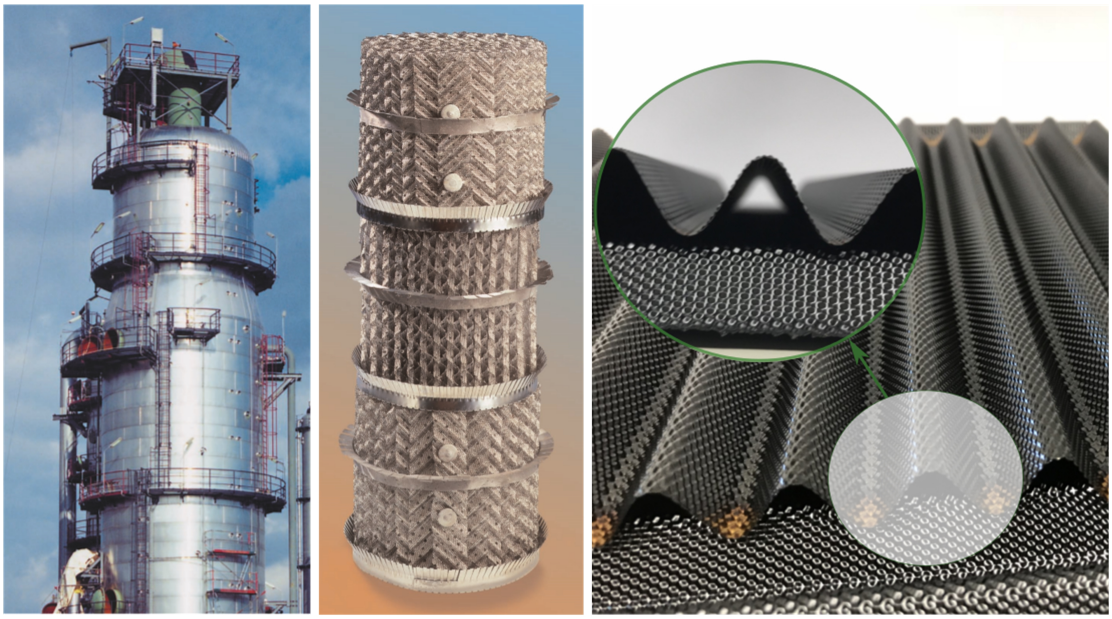

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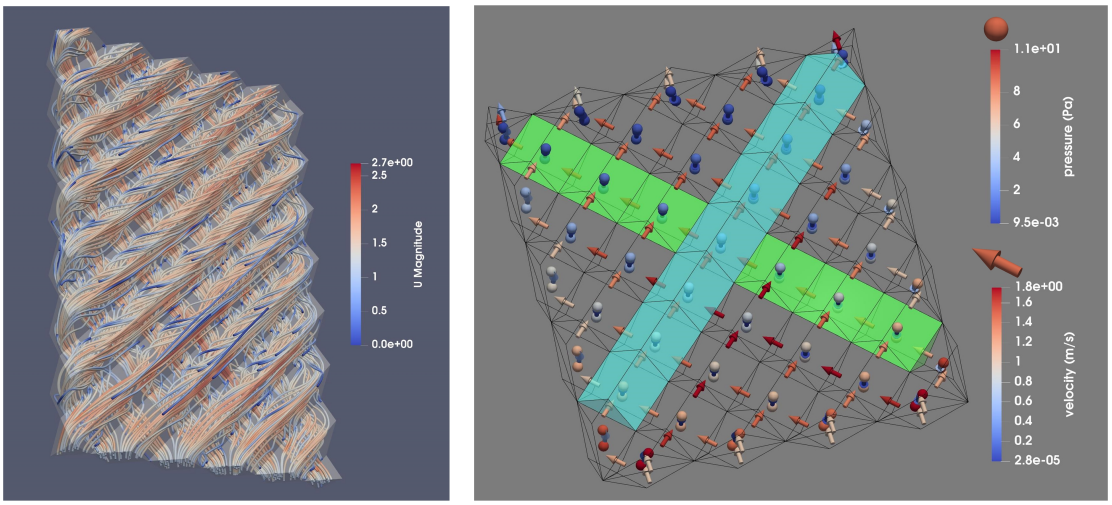
Figure 2: *(a) Industrial sized absorption column [2]. (b) Structured packing of metal sheets - a popular column internal [2]. (c) Geometry of structured packings [1].*



(a) (b)

Figure 3: *(a) streamlines of CFD simulation in a structured packing; (b) mesoscale simulation in excerpt of structured packing.*

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DA2010%20Sponsor%20Information/Montz/MONTZ%20Main%20Cataloque.pdf

More Information

[1] J. Sacher, J.-U. Repke, *Chem. Eng. Res. Des.* **147**, 430-442 (2019). doi: 10.1016/j.cherd.2019.04.032

[2] Montz main catalogue http://folk.ntnu.no/skoge/prost/proceedings/distillation10/