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Development and Application of the TUM-WelChem Cell Model for Prediction of Liquid Distribution in Random Packed Columns

Florian Hanusch[a,*], Volker Engel[b], Robert Kender[a], Sebastian Rehfeldt[a], Harald Klein[a]

[a] Technical University of Munich, Department of Mechanical Engineering, Institute of Plant and Process Technology, Boltzmannstr. 15, 85748 Garching, Germany
[b] WelChem GmbH, Brunnenweg 40, 83666 Waakirchen, Germany
florian.hanusch@tum.de

Liquid maldistribution is, next to the prediction of interfacial phase area and mass transfer coefficients, one of the bigger uncertainties in random packed column design. In a joint project, “Cell Model for Packed Column and Liquid Distributor Design” supported by the Bavarian Research Foundation, liquid maldistribution experiments were conducted in three packed columns with diameters of 0.4, 1.2 and 2.0 m at Technical University of Munich (TUM), RVT Process Equipment GmbH and Linde AG. Experiments covered varying experimental and operating parameters – gas/liquid system, type of packing, packing height, type of liquid distributor, liquid load, and gas load. An evaluation of the acquired database provided insight into influencing factors on liquid distribution. (Hanusch *et al.*, 2017)
In 2007, Wild and Engel first presented their *WelChem Cell Model*. The original model predicted liquid distribution in random packing from cell layer to cell layer based on directional dispersion coefficients, deduced from virtual 3D irrigation simulations with a CAD model of one random packing element (Wild and Engel, 2007). Further development at TUM included implementation of the influencing factors liquid load and gas load, considering local loading effects and increasing liquid dispersion. Wall effects were refined by distinction of packing elements and voids at the column wall. Liquid distribution profiles predicted with the *TUM-WelChem Cell Model* are in good agreement with experimental data.
WelChem GmbH implemented the TUM-WelChem Cell Model in their column design software *TrayHeart*, thus making the research results directly accessible for *TrayHeart* users. Application of the TUM-WelChem Cell Model ranges from prediction of maldistribution in random packed columns, through liquid distributor design, considering interactions with random packing, to process simulation, considering maldistribution in parallel column models (Schultes, 2000).

1. Introduction

Mass transfer calculations for random packed columns generally assume even distribution of gas and liquid over the column cross-section. However, liquid channelling and an increased wall flow are well-known liquid maldistribution phenomena, resulting in uncertainties in random packed column design (Mersmann *et al.*, 2011). Experimental investigation of liquid maldistribution reaches back to the late 19th century, when Hurter measured the liquid distribution in a coke tower (Hurter, 1893). An extended review of liquid maldistribution experiments and observations on important influencing factors is given in Hanusch *et al.* (2017).
Insight gained via experimental investigations can be used for the development of theoretical models for the prediction of liquid maldistribution in packed columns. One approach to describe the liquid distribution in random packing applies the mathematical laws of probability (Tour and Lerman, 1944). Another type of model, derived from the probability approach, characterises liquid distribution as a diffusional process (Cihla and Schmidt, 1957). The aforementioned models consider liquid distribution on a differential scale. Cell models on the other hand discretise the packing with a resolution of the size of single packing elements or bigger (Crine

and Marchot, 1984), whereas zone stage models divide the packing into macroscopic volumes (Zuiderweg *et al.*, 1993). Prediction of liquid distribution is used to reduce column design uncertainties, for example by implementing mass transfer calculations in liquid distribution models (Higler *et al.*, 1999). Another approach in process simulation is the use of a parallel column model, where a single column is implemented as two or more parallel columns, with the column cross-sections and liquid flows being split dependent on liquid distribution (Schultes, 2000).

2. Materials and Methods

Based on the experimental data and knowledge gained of liquid maldistribution influencing factors (Hanusch *et al.*, 2017), the so called *WelChem Cell Model* by Wild and Engel (2007) was further developed and validated at the Technical University of Munich (TUM). With this tool for prediction of liquid distribution in packed columns in hand, applications of the model in column design as well as process simulation are proposed.

2.1 TUM-WelChem Cell Model

The TUM-WelChem Cell Model discretises the packing by layers of honeycomb cells, each cell representing one packing element. Cell dimensions are deduced from the packing bulk density and packing elements' proportions. Liquid is distributed from one cell to the centre and neighbouring cells in the layer below. A set of directional dispersion coefficients defines the split of the volume flow between the seven cells. Directional dispersion coefficients are deduced via virtual 3D irrigation simulations, with a CAD model of one packing element being placed in a cell at different rotations, resulting in sets of directional dispersion coefficients. During initialisation of the model, a random rotation and thus a set of directional dispersion coefficients is assigned to each cell. At the top of the packing, liquid is distributed according to the liquid distributors drip point coordinates. From there on, liquid distribution is processed layerwise from top to bottom. Wall cells are treated differently to consider the wall effect, reducing the flow from the wall back to bulk cells. (Wild and Engel, 2007)

The original *WelChem Cell Model* predicts liquid distribution in random packing only based on the geometric shape of the packing elements, without considering any column fluid dynamics. Further development at TUM introduces additional distribution effects, considering local liquid and gas loads in the packing. High local liquid loads, occurring i.e. for centre feed distribution, result in an increase of radial liquid distribution (Hanusch *et al.*, 2017). Packing blocks part of the column cross-section and poses an obstacle for liquid flowing downward. In the model, this effect is described by the liquid flowing through projected free cell areas of the CAD model. In each cell, a liquid flow $\dot{V}_{L,i}$ builds up a liquid level $h_{L,i}$, following Torricelli's law. At low liquid loads, the liquid can exit the cell through the projected free area. For a high liquid load, on the other hand, the liquid level building up can exceed the cell height, thus causing cell overflow. Excess liquid is distributed to the neighbouring cells in the same layer, considering their free capacities.

The gas load is considered to have the biggest influence on liquid distribution. An increase of the gas load results in an increase of radial liquid distribution (Kouri and Sohlo, 1987). Gas loads below the loading point improve liquid distribution over the column cross-section, while gas loads from loading to flooding point lead to an increase of maldistribution and wall flow (Yin *et al.*, 2000). Observations by Hanusch *et al.* (2017) indicate a strong dependency of liquid distribution and fluid dynamics in packed columns. The model implements the influence of the gas load by considering local gas loads in each cell, with hydraulic calculations based on the pressure drop model presented by Engel (2000). First, the local dynamic liquid holdup $h_{dyn,i}$ in each cell is calculated from the local liquid load B_i and local gas load F_i, with the global gas load F as the initial value. The local gas volume fraction $\varepsilon_{G,i}$ is then calculated via Eq(1) from the local liquid holdup $h_{dyn,i}$ and the packed bed void volume ε.

$$\varepsilon_{G,i} = \varepsilon - h_{dyn,i} \tag{1}$$

The model assumes the gas load to distribute itself according to the local gas volume fractions $\varepsilon_{G,i}$, resulting in the local gas loads F_i, estimated by Eq(2), where cells with a higher gas volume fraction $\varepsilon_{G,i}$ than the average gas volume fraction $\bar{\varepsilon}_G$ also have a higher gas load, and vice versa.

$$F_i = \frac{\varepsilon_{G,i}}{\bar{\varepsilon}_G} \cdot F \tag{2}$$

Lastly, the liquid holdup $h_{dyn,i}$ is calculated via an iterative approach with the local gas load F_i. Liquid holdup calculations already contain the local pressure drop Δp_i, which is now used to estimate the local flood factor Φ_i by Eq(3), where $\Delta p_{d,i}$ is the dry pressure drop for the gas load factor F_i and $\Delta p_{d,FP}$ the dry pressure drop at the flooding point for the corresponding liquid load B_i. (Engel, 2000)

$$\Phi_i = \sqrt{\frac{\Delta p_{d,i}}{\Delta p_{d,FP}}} \tag{3}$$

The flood factor Φ_i is used to describe the gas load dependent radial liquid distribution, with a $1 - \Phi_i$ part of the liquid remaining in a cell, while the rest is distributed evenly to neighbouring cells. At flooding conditions ($\Phi_i = 1$), all liquid is distributed to neighbouring cells.
An additional model adaption concerns the wall flow. Wall cells are now randomly designated as either packing elements or voids. While packing elements show standard distribution behaviour, as described above, void wall cells cause no radial distribution at all, passing the liquid on to the centre cell below. Assuming even initial distribution, more liquid flows to the wall than back into the packing bulk, as the random void cells keep the liquid at the wall. With the liquid trickling downwards through the packing, the wall flow increases up to an equilibrium state, in which the flows between packing bulk and wall equalise.

2.2 Liquid Distributor Design

With the TUM-WelChem Cell Model in hand, established column design guidelines can be reconsidered. In liquid distributor design, the approach by Moore and Rukovena (1987) is commonly used for estimation of the distribution quality. Liquid distributor drip points are represented by distribution circles. The distribution quality is calculated from graphical analysis of the column cross-section, considering the area not covered by distribution circles as well as overlapping of distribution circles. In conclusion, Moore and Rukovena (1987) recommend a minimum drip point density of 65/m^2. Parameters such as liquid and gas loads, column diameter or type of packing are not taken into account in this and other approaches (Perry *et al.*, 1990).
A method is proposed to utilise the TUM-WelChem Cell Model in liquid distributor design, in which operating parameters are considered. Liquid distributor, and (generally speaking) column internals, design is one of the last steps in column design. Liquid and gas loads, column diameter and type of packing are available input parameters for liquid distribution simulation. The only remaining free design parameter is the liquid distributors' drip point density. To find the optimum, minimum required drip point density, liquid distribution simulations are conducted for varying drip point densities and the resulting liquid distributions in the packing are evaluated via a maldistribution factor.

2.3 Process Simulation

Another field of application of the TUM-WelChem Cell Model is in process simulation. State of the art process simulation tools, e.g. Aspen Plus®, offer standard unit operations for distillation and absorption. Even hydraulic conditions in columns can be considered, using rate-based models for mass transfer calculation. Nevertheless, mass transfer calculations assume uniform distribution (plug flow) of gas and liquid phase. Thus, they are not able to take efficiency losses caused by liquid maldistribution into account.
A parallel column model divides a column, theoretically, into two or more parallel columns. An uneven split of the liquid flow into the parallel columns considers liquid maldistribution. Mass transfer calculations are conducted for each of the parallel columns, with the combined results showing an efficiency loss compared to the single column. Schultes (2000) applies the parallel column model on process simulation examples for distillation, absorption and desorption, using CHEMCAD software and an equilibrium model for mass transfer calculations. Different liquid loads in the parallel columns are set via a theoretical variation factor, which describes the degree of maldistribution. Following this approach, an ammonia desorption process example is set up in Aspen Plus®. Instead of a theoretical variation factor, the TUM-WelChem Cell Model is applied to predict the liquid distribution in the column. The number and column cross sections of the parallel columns are adapted to the degree of maldistribution, while the liquid is split according to the liquid distribution simulation results. Mass transfer is calculated using the rate-based approach, thus considering the hydraulic conditions influence on mass transfer in each of the parallel columns.

3. Results and Discussion

Liquid maldistribution experiments conducted in a Ø1.2 m packed column (air/water system) at TUM provide a large database with varying experimental and operating parameters – type of packing, packing height, liquid distributor, irrigation density, and gas load (Hanusch *et al.*, 2017). TUM-WelChem Cell Model simulations are validated against experimental data. Furthermore, the TUM-WelChem Cell Model is applied to estimate the optimum drip point density of a liquid distributor. Column design results are then used as input for a parallel column model of an ammonia desorption process.

3.1 Model Validation

Experimental liquid distribution data is available in the form of distribution spectra, displayed in Figure 2a, representing a liquid collector below the packing. The collector is divided in rings R1–6 of equal distance and ring W, which collects the wall flow. Additionally, the rings are subdivided in three circular sectors. Colouring of the collector's segments is according to the local liquid load B_i. Figure 2b displays the corresponding simulated distribution spectrum, which represents the honeycomb structure of the bottom cell layer in the packing. While centre feed distribution experiments pose an additional challenge for the TUM-WelChem Cell Model, due to high local liquid loads, Figure 2 shows that experimental and simulated data are in good agreement.

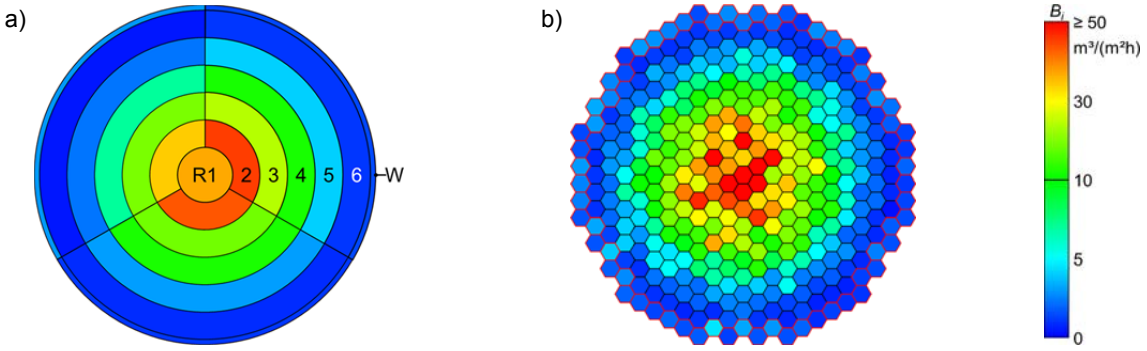

Figure 2: a) Experimental and b) simulated distribution spectra for RMSR 70-5, column diameter D_c = 1.2 m, packing height H_P = 3.0 m, centre feed distribution, liquid load B = 10 $m^3/(m^2h)$, gas load F = 1.5 $Pa^{0,5}$.

Comprehensive validation of the model is conducted by use of parity plots for different types of packing and initial liquid distribution. Liquid distribution data is plotted by means of simulated and experimental volume flow in the collector's rings 1–6 and wall. Figure 3 shows the parity plots for Hiflow® ring 90-7 plastic packing in the TUM Ø1.2 m packed column for various experimental and operating parameters. Both parity plots, Figure 3a for even distribution and Figure 3b for centre feed distribution, represent the trends for other types of packing (Raflux ring 35-5 and 50-5 metal, RMSR 50-4 and 70-5, Hiflow® ring 50-6 plastic) and show, that the TUM-WelChem Cell Model is well capable of predicting the liquid distribution in random packing.

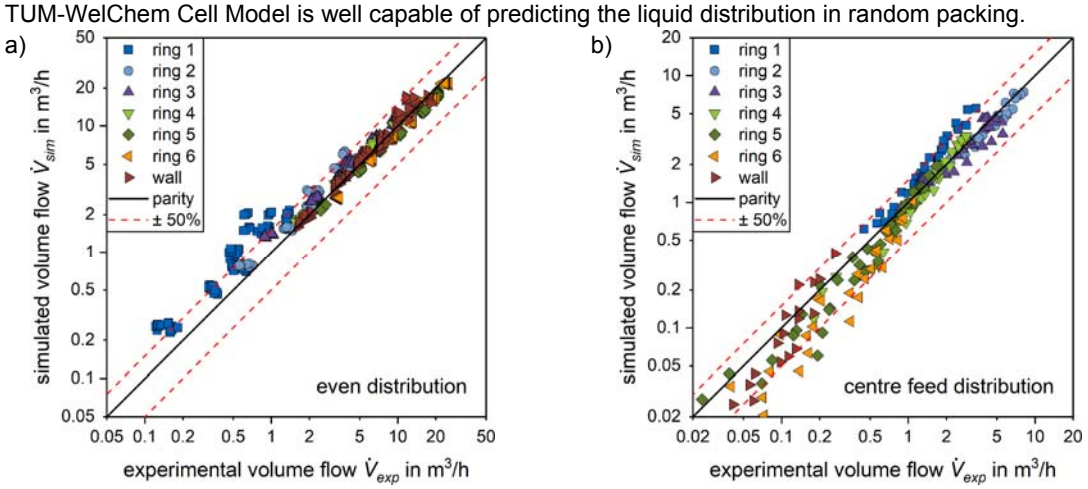

Figure 3: Parity plots of experimental against simulated volume flows for Hiflow® ring 90-7 plastic, column diameter D_c = 1.2 m, packing heights H_P = 1.0–3.0 m; a) even distribution, liquid loads B = 10–80 $m^3/(m^2h)$, gas loads F = 1.0–2.5 $Pa^{0,5}$; b) centre feed distribution, liquid loads B = 5–15 $m^3/(m^2h)$, gas loads F = 1.0–2.0 $Pa^{0,5}$.

3.2 Optimum Drip Point Density

In this section, application of the TUM-WelChem Cell Model in liquid distributor design is explained. An exemplary column design provides the following specifications: column diameter D_C = 1.0 m, packing height H_P = 5.0 m, liquid load B = 12.7 $m^3/(m^2h)$, gas load F = 1.78 $Pa^{0.5}$, air/water system. The optimum drip point density is estimated for Raflux ring 50-5 metal packing. Simulations are conducted for drip point densities of 4–100/m^2, each simulation providing data on local liquid loads $B_i(h)$ discretised over the packing

height for each cell layer. Information on liquid distribution at a certain height can now be summarised by means of a maldistribution factor $M_f(h)$, calculated from the local liquid loads $B_i(h)$ via Eq(4), with the number of cells n in a cell layer. Figure 4a shows the profile of the maldistribution factor $M_f(h)$ plotted against the packing height h for drip point densities of 20/m^2 and 100/m^2.

$$M_f(h) = \frac{1}{n} \cdot \sum_{i=1}^{n} \left| \frac{B_i(h) - B}{B} \right| \tag{4}$$

Finally, the degree of maldistribution is described by the mean maldistribution factor $\overline{M}_f$ for each simulation case, which is the average of $M_f(h)$ over the total height of the packing. Figure 4b displays the maldistribution factor $\overline{M}_f$ plotted against the drip point density, which tends towards a minimum maldistribution factor $M_{f,\min}$ at high drip point densities. One goal in liquid distributor design is to find the minimum drip point density at which a sufficient liquid distribution in the packing is still maintained. In this case, a sufficient liquid distribution is defined by a tolerance for the maldistribution factor $\overline{M}_f$ exceeding the minimum maldistribution factor $M_{f,\min}$ by 5%, resulting in an optimum drip point density of 56/m^2 for the exemplary column design with Raflux ring 50-5 metal packing.

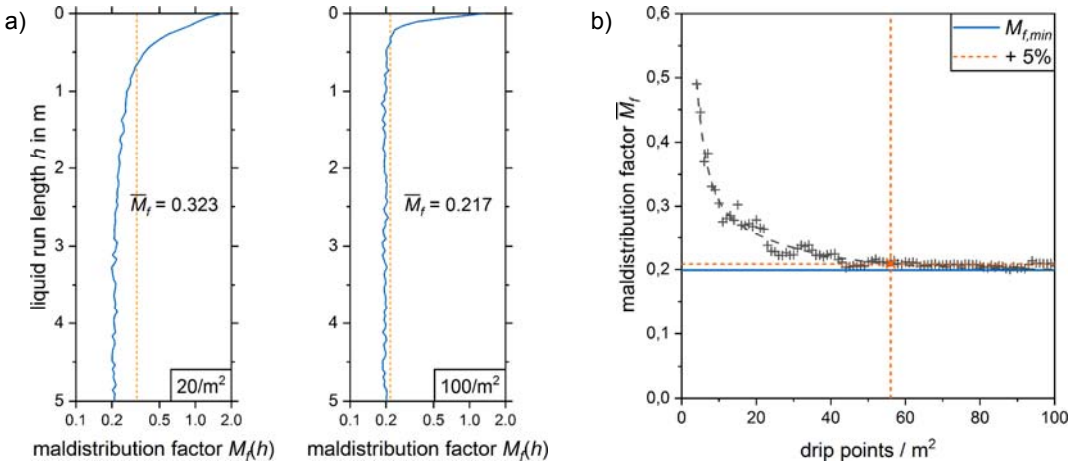

Figure 4: a) Simulated maldistribution factors $M_f(h)$ against liquid run length h for drip point densities of 20/m^2 and 100/m^2 and b) mean maldistribution factors $\overline{M}_f$ against varying drip point densities for the exemplary column design with Raflux ring 50-5 metal packing.

3.3 Mass Transfer Efficiency

Column design results are used as input parameters for a parallel column model to estimate separation efficiency loss caused by liquid maldistribution. Schultes (2000) investigates the desorption of ammonia from water with humid air, applying a theoretical split factor for the liquid and performing mass transfer calculations with an equilibrium model. A similar case is set up in Aspen Plus®, using the column design specifications from section 3.2 with Raflux ring 50-5 metal packing. The property method used for the ammonia/water system is *ELECNRTL*. Desorption is carried out at p = 1 bar pressure and T = 70 °C temperature. The liquid load is set to $B_{L,in}$ = 12.7 m^3/(m^{2}h), composed of water $x_{H2O,in}$ = 99.2 mol-% and ammonia $x_{NH3,in}$ = 0.8 mol-%. Humid air enters with a gas load $F_{G,in}$ = 1.78 Pa$^{0.5}$, composed of air $y_{Air,in}$ = 70.4 mol-% and water $y_{H2O,in}$ = 29.6 mol-%. Process simulation of a single column, calculating mass transfer via the rate-based approach, results in a remaining molar fraction of ammonia $x_{NH3,out}$ = 2.1×10^{-4} mol-% in the liquid.
In a second simulation case, displayed in Figure 5a, liquid maldistribution is considered by setting up two parallel columns, representing the desorption column. Liquid distribution simulation with the TUM-WelChem Cell Model provides Figure 5b, which shows the local liquid load $B(r)$ profile averaged over the column height. At a column radius of r = 468 mm, the column is split into a bulk (index: b) and a wall (index: w) section. The split results in column diameters of D_b = 0.936 m and D_w = 0.352 m, with corresponding liquid loads of B_b = 11.6 m^3/(m^{2}h) and B_w = 20.4 m^3/(m^{2}h). Gas loads in the parallel sections equal the total gas load $F_{G,in}$ = 1.78 Pa$^{0.5}$. Parallel column process simulation with the rate-based approach returns a remaining molar fraction of ammonia $x_{NH3,out}$ = 8.6×10^{-3} mol-% in the liquid. Comparison to equilibrium-based process simulation shows that the single column case equals n_{th} = 12 theoretical stages, while consideration of maldistribution in the parallel column case reduces the separation efficiency down to n_{th} = 6 theoretical stages.

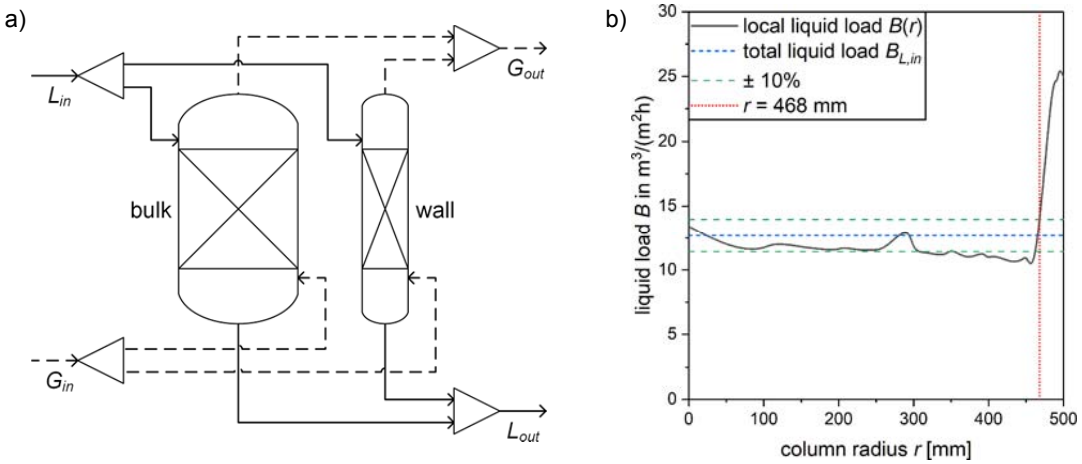

Figure 5: a) Parallel column process flowsheet; b) local liquid load B(r) against column radius.

4. Conclusions

The TUM-WelChem Cell Model is validated against a large liquid distribution database. Prediction of liquid distribution in random packing with the model provides various possibilities of application in process simulation and column design. Theoretical design studies have yet to be verified against actual process data. Nevertheless, optimised drip point densities could ensure sufficient liquid distribution at minimized materials usage, while consideration of maldistribution via the parallel column model could lead to reduced safety margins in process simulation.

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