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RESEARCH ON MASS TRANSFER COLUMNS "OLD HAT OR STILL RELEVANT?"

Michael Schultes
Raschig GmbH, Mundenheimerstrasse 100, 67061 Ludwigshafen, Germany,
e-mail: MSchultes@raschig.de

Abstract
Research activities in Universities in the field of mass transfer columns have heavily decreased in the past years. This contribution tries to discuss the question of whether the current knowledge in the field of mass transfer technology for trays, packings and column internals is sufficient to design energy and cost-efficient systems. In the article, various points of view are described which have not been clarified from an industrial point of view and which should play an important role in the field of research in the future. Alongside the thermodynamics of industry relevant systems, this also includes the improved description of fluid dynamics and the mass transfer efficiency in trayed and packed columns. Research should not only deal with idealistic test mixtures, with the help of standardised test equipments and standardised test systems. The industrial parameters such as foams, solids, and chemical and catalytic mass transfer are also of great interest.

Keywords: Standard testing procedure, mass transfer column, trays, packings

1. Introduction to the layout of mass transfer columns

At the beginning of each layout process for mass transfer columns a technical specification is elaborated. This specification includes a list of mass components to be treated, as well as specifications of the column head and bottom product as targets. The mass flow rates, system pressure, and temperatures of the various feed flows are stipulated. This specification can be developed comprehensively from the sequence of a complete process simulation; see also table 1.

Table 1: Tasks and methods of solutions for design of mass transfer columns and the evaluation of reliability.

Task	Solution	Evaluation of reliability
Definition of external feed flows, component lists, and product specifications	Elaboration of a technical column specification via process simulation	Secured statements based on process simulation
Definition of phase equilibrium, physical properties, process pressure and temperatures	Thermodynamic model	Predominantly secured calculation approaches but experience necessary
Internal flow rates and number of theoretical stages	Column simulation with thermodynamic model	Predominantly secured calculation approaches
Fluid dynamics of "efficient" column internals: Column diameter, pressure drop, liquid hold-up	Individual calculation model or experiments	Predominantly good calculation approaches but experience necessary
Separation efficiency of "efficient" column internals	Individual calculation model or experiments	Limited reliable calculation approaches (experience necessary)
Selection of "non-efficient" separation column internals: liquid distributor, gas distributor, collector, droplet separator	Empirical layout methods	Limited reliable calculation approaches

If the column specification is available, the selection of a suitable thermodynamic model to describe the phase equilibrium takes place. A series of new and proven calculation modes are available for the process engineer. If experimental data is available, the engineer can validate the calculation results.

However, it is frequently the case that experimental equilibrium and physical properties are not available, so that a lot of experience is required in order to select the suitable thermodynamic model. After selection, a simulation run of the mass transfer column takes place with simulation programmes on the basis of the concept of theoretical separation stages. The results of the simulation are internal column flow rates and related physical properties as well as information about the required number of theoretical stages to achieve the product specification. The simulation results are generally reliable when the correct thermodynamic model has been used.

In the following stage, the mass transfer "efficient" column internals have to be specified for a certain column diameter and the column height has to be defined. To reach this approach the fluid dynamics (capacity, pressure drop, and liquid hold-up) as well as the separation efficiency of a mass transfer tray, structured or random packing has to be determined. There is often experimental data available from Universities and test institutes for the fluid dynamics of trays or structured and random packings, whereby the results are oriented towards numerous standard test mixtures. In contrast, reliable experimental data for the separation efficiency is usually only available for a few standard test mixtures. In industry, the component mixtures and phase flow ratios often differ greatly from those standard conditions, which is why the evaluation of the fluid dynamics and separation efficiency for industrial columns is getting more difficult. State of the art calculation of the fluid dynamics and separation efficiency of trays, random or structured packings is an alternative to extensive experiments. Published correlations are available to the process engineer for this. However, process engineers should be aware that these correlations only offer confidential results for the considered test mixtures and column internals taken into account during modelling phase.

Nowadays, lots of engineers avoid this conflict by using the operating experience of existing, older plants and generally avoid using modern column internals. Modern column internals therefore continue to find it very difficult to be used in industry on a short-term bases. Furthermore, high safety margins are considered for new separation processes, which lead to economic and ecological potentials being unconsidered. The influence of so-called “non-efficient” column internals on the function of a mass transfer column was frequently underestimated in the past and has not been considered in research up until now. Fig. 1 shows a typical mass transfer column which consists of several sections. The packed bed, only covers a fraction of the column volume. Column internals such as the droplet separator (demister), liquid distributor, support and hold-down constructions, annular channels, gas distributors, etc. have another significant share of the column volume. When dimensioning these components, one still have to rely upon the empirical layout knowledge of the internal manufacturers.

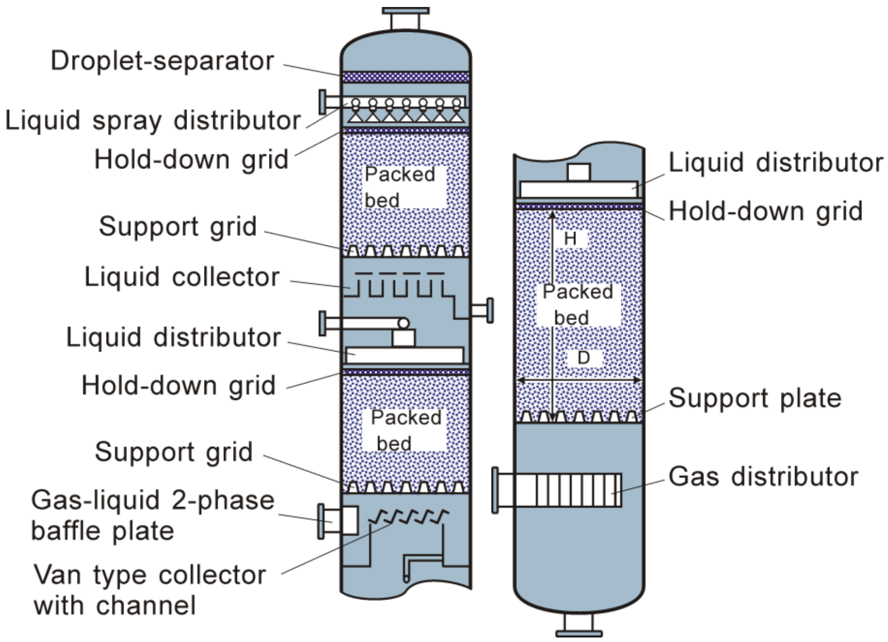

Figure 1. Layout of a mass transfer column with several feeds and bed sections, as well as various “non-efficient“ internals

2. Experiments and calculation modes for fluid dynamics and separation efficiency of "efficient" column internals

Calculation models can only be as accurate as the error range of the experimental data basis. If one compare measurements of the same product by different test institutes, one always receive different results. It is therefore necessary to standardise the experimental layout of test facilities in order to receive comparable test results. Simple standard test systems should be defined, with which the fluid dynamics and the separation efficiency of trays, random or structured packings can be established. Furthermore, one should agree on test systems with very different physical properties in order to be able to cover industrially relevant conditions. In all cases, the recommendations should be connected with a suitable thermodynamic model to describe the phase equilibrium and the physical properties.

Measurements of the fluid dynamics of trays, random or structured packings are generally the specific pressure drop, the specific liquid hold-up, and the flooding point. The accuracy of these measurements is around ±5 %, if one test system and one test facility is studied. If the experiments are carried out on different test facilities but with the same system, experimental differences of ±15 % can occur. If different test systems are used beyond this and one tries to correlate the results, 90% of all test data can be predicted with an accuracy of ±20 % with state of the art models. Significantly higher differences can occur if predictions are extrapolating experimental data.

Table 2. Mean deviations between the experimentally determined performance data and calculated values with state of the art models.

Fluid dynamic performance numbers			Number of known test systems	Mean deviation for interpolation	Mean deviation for extrapolation
Capacity / flooding limit		$F_{V,Fl}$, $C_{S,Fl}$	13	± 20 %	± 30 %
Specific pressure drop		$\Delta p/H$	25	± 20 %	± 30 %
Liquid hold-up		h_L	20	± 10 %	± 30 %
Mass Transfer	Absorption and desorption	$\beta_V a_{Ph}$ $\beta_L a_{Ph}$	31	± 20 %	± 50 %
	Rectification	HTU_{OV}, HETP	14	± 30 %	± 80 %
	Chemisorption	a_{Ph}/a	4	± 80 %	> ± 100 %

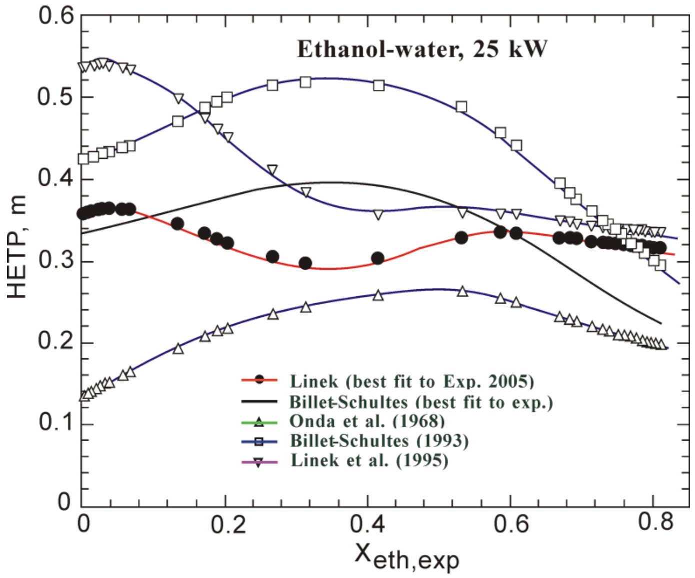

Figure 2. Measured HETP values for the rectification of the ethanol/water system and the calculated values according to different models[1] .

The measurement data on mass transfer efficiency of trays, random or structured packings is much more inhomogeneous which is why larger deviations result from precalculations. If the physical properties or flow rates in an industrial column differs from secured test systems correlations are extrapolating experimental data. In this case the uncertainty levels increase significantly. In the case of these types of extrapolation, one has to expect inaccuracy of up to ±80 % for the separation efficiency and over ±100 % for the effective mass transfer area using state of the art equations; see table 2.

The uncertainties of a prediction increase further if foaming or fouling systems are to be evaluated. The same applies to extreme physical properties such as highly viscose (ionic) fluids. If new packing elements or trays are introduced to the market, the prediction of their performance level is not possible, even for standard test systems, because the influence of all geometric data is not universally valid in any of the correlations.

The experimentally determined HETP values upon rectification of the ethanol/water system are shown in Fig. 2. Depending on the calculation method used, extreme differences to the experimentally determined values can occur.

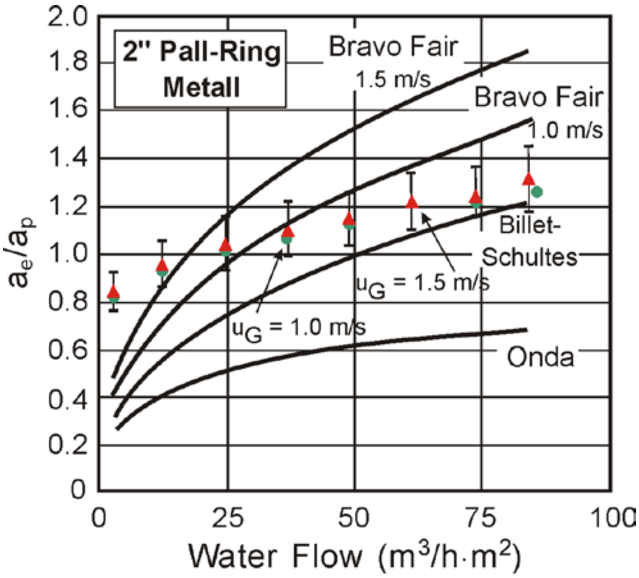

Figure 3. Experimentally determined, specific mass transfer area and calculated values from different correlations

If one tries to calculate the specific mass transfer area a_{Ph} /a in advance with the correlations known to industry, it results in the comparisons between the measurement results and calculations shown in Fig. 3 for the ideal CO_2 -air/sodium hydroxide test system. As can be taken from Fig. 2 and Fig. 3, there is currently no correlation which can safely calculate the separation efficiency and the specific mass transfer area in advance, whereby it has to be stated once again that different test institutes can come up with different performance figures.

3. Layout of "non-efficient" column internals

Alongside trays or random / structured packings as mass transfer efficient separation elements, each mass transfer column also has non-efficient tower internals such as liquid distributors, hold-down grids, support grids, gas distributors, or liquid collectors, etc.; refer to Fig. 1.

The correct function of these column internals is of essential importance for compliance with the performance figures of a mass transfer column. Up until now, there has been no general guideline for dimensioning these internals, which is why one has to rely on the manufacturer's know-how. There are generally heuristic rules available provided by the manufacturers which are to be followed to design the column internals. The calculation approaches are currently very rudimentary and contain numerous empirical parameters (origin is frequently unknown).

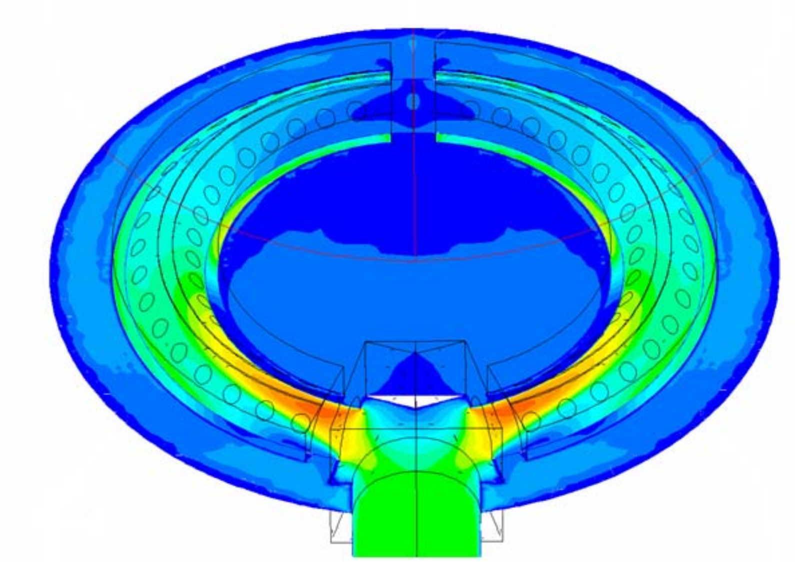

Figure 4. CFD model of a gas feed device[2].

The functional evaluation of non-efficient column internals is frequently served with CFD modelling (CFD = Computational Fluid Dynamics). CFD modelling provides flow profiles and can also be used for complex geometries; refer to Fig. 4. However, with this method it should be noted that the result of a CFD study can generally not be validated.

4. Future research tasks

As explained in the preceding chapters, one can see that research on mass transfer columns can certainly not be deemed to be completed - see table 3.

In the field of thermodynamics, good progress has already been made in the advance calculation of physical properties or the phase equilibria. In this field, intensive research activities will be necessary also in the future in order to be able to guarantee the prediction of the thermodynamic properties of modern fluids, e.g. ionic solvents, with new model approaches. Thermodynamics should continue to deal with reactive and catalytically active fluids, because the processes in industry will continue to be energetically optimised and additives will have to be added to the fluids to achieve targeted effects.

In the area of mass transfer columns, there is still a wide range of unanswered questions. Research should be oriented towards practical problems, such as the influence of impurities on fluid dynamics or the separation efficiency of trays and packings. The same applies to the description of the formation mechanism of foam and its influence on the effectiveness of mass transfer processes.

Modern fluids such as the ionic solvents have a high viscosity level and a high molecular weight. These properties also create questions oriented towards fluid dynamics and mass transfer. Can the former regularity for the prediction of diffusion coefficients and mass transfer coefficients still be used for highly viscose media?

As a result of the high demands in industry on energy-saving processes, the conditions set in mass transfer columns are becoming more and more extreme. This means that very high liquid loads are coupled with extremely low gas rates. The requirements of product purity levels also continue to increase so that more and more industrial columns are operating in the field of molecular rectification. This arises the question whether the mass transfer efficiency measured in the medium concentration range can still be applied.
The definition of standards for the setup of test facilities are also relevant for the determination of fluid dynamics and separation efficiencies[3]. Industry requires reliable data for the layout of its columns and has to rely upon the reliability of measurement data.

As described in the previous section, the calculation methods for determining the mass transfer coefficients and mass transfer areas must be developed further. High safety margins do not match the concepts for energy-saving measures. Industrial engineers not only require calculative results, but also the possibility of being able to analyse the simulation results. For example, figures must be developed which apply to any chemical reaction in mass transfer columns and which can be used for a plausibility test ($HETP_R$ or HTU_R?).

In the development of new mass transfer trays or packings, it has still not been possible to calculate the fluid dynamics or separation efficiency in advance. A wide range of complex tests must be carried out before a new product can be placed on the market. This results in considerable disadvantages for industry because potentials are identified and implemented too late. It would be preferable to develop criteria which drastically reduce this timeline of product development and introduction to the market.

The field of non-effective column internals is a completely new area of research. There are numerous empirical regulations; some of which do not have any physical justification. The development of internationally acknowledged and physically-based guidelines is very important for industrial practices.

Table 3. Preferable main areas of research in the field of mass transfer columns

Area of research	Focus of activities
Thermodynamics	- Description of new systems (e.g. Ionic Solvents) - New models for more accurate description of physical and equilibrium properties - Development of a universal decision tree for recommending a thermodynamic model for mass transfer systems
Fluid dynamics	- Description of standards for test equipments and the experimental testing procedure - Influence of foaming and fouling systems - Influence of industry relevant extreme physical properties and column loads - Further development of the calculation model with the use of modern analysis procedures / measurement techniques - Predictive description of modern trays and packings
Separation efficiency	- Description of standards for test equipments and the experimental testing procedure - Further development of the calculation models - Influence of foaming and fouling systems - Influence of industry relevant extreme physical properties and column loads - Separation efficiency at very high product purity levels - Development of generalized performance figures for systems with chemical reactions. - Predictive description of modern trays and packings
"Non-efficient" column internals	- Fluid dynamics and hard ware design criteria for distribution systems for: Liquids; Gases; Gas/liquid mixtures; Liquid-liquid systems; Solid-liquid systems; Collectors and redistributors - Influence of foaming and fouling systems - CFD modelling (with experimental verification)

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