

Optimisation of Fluid Process Engineering by a Complementary Modelling Approach

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Today, optimisation of Fluid Process Engineering is largely associated with process intensification, which results in rising process complexity and higher requested accuracy of process description. This is often beyond the capabilities of conventional modelling methods. A new concept called complementary modelling has recently been suggested, which uses different modelling approaches in combination, while their rigor and complexity stretch over a wide range. Among these approaches are a direct application of the equations of fluid dynamics, the hydrodynamic analogy method and the rate-based approach. In this contribution, the complementary modelling is highlighted and illustrated with a case study related to CO₂ capture.

1. Introduction

Fluid Process Engineering is involved in numerous production cycles of chemical process industries, automotive and energy sectors as well as of many other application areas. The process and equipment optimisation within the Fluid Process Engineering is crucial for the success of sustainable production. Today, it is largely dominated by the idea of process intensification leading to substantially smaller, cleaner, safer and more energy efficient process technology (Reay et al., 2013). Among the ways to realise more intensive operations are *process integration*, implying both functional combination (e.g., reaction and separation) and jointed equipment, *miniaturisation* of equipment units and their contact elements as well as the use of *innovative energy sources*. In all these cases, the complexity of intensified processes rises and becomes much higher than that of conventional processes. Furthermore, growing process intensity calls for exact unit design, and thus, for a break with the common way of using much larger equipment than necessary. As a consequence, process description has to become more accurate and reliable necessitating a step change in the modelling concepts. Above all, the knowledge on process kinetics, with respect to both transport phenomena and chemistry, is necessary; hence, the equilibrium concept, popular during the past century, cannot be properly used for the design and optimisation of intensified equipment units. The growing computational power as well as the need to understand and implement physicochemical backgrounds of the processes shifts the modelling focus to the kinetics-based approach.

But this is not at all easy. The application of rigorous theoretical concepts is hindered, because of complexity of the systems and phenomena under consideration. Taking fluid separation systems as an example, we may encounter multiphase flows, multicomponent systems, complex thermodynamics, complex column unit design and geometry, intricate column links and a substantial scale difference between the characteristic dimensions of the phenomena involved. These features make rigorous modelling of fluid separation processes extremely difficult.

Recently, we suggested a complementary modelling approach based on an efficient combination of different modelling methods (Kenig, 2008). We believe that this approach represents a good alternative to conventional description and enhances the chances for predictive modelling of complex intensified systems. In this paper, the complementary modelling approach is explained and illustrated with a case study from the area of CO₂ capture.

2. Classification of kinetics-based modelling methods

To build a framework for the complementary modelling, we first classify the modelling methods available in Fluid Process Engineering, focusing on methods directly considering process kinetics. Such a classification can be done based on different principles, depending on the specific aims and criteria. Here, we suggest to characterise the models according to their rigour and to relate them to the fluid dynamics complexity and scale of the processes or phenomena under study. This choice can be justified by the crucial importance of the fluid flow pattern and its impact on the very possibility to develop rigorous mathematical process models.

The most rigorous approach to the description of a process or a phenomenon in a fluid system is based on the classical equations of fluid dynamics. These equations are partial differential equations supplied by the corresponding initial and boundary conditions. When solved, such models yield local velocity, pressure, temperature and concentration fields which can further be used for the determination of all relevant process characteristics. The solution of the equation system is realised numerically, with the aid of different solution techniques and software tools. Altogether, this combines in a branch of fluid mechanics called *Computational Fluid Dynamics* (CFD).

CFD modelling presumes that, generally, the phase boundaries are known (spatially localised) which is possible for processes and phenomena taking place in geometrically simple flows. However, this seldom occurs in large industrial equipment, with complex unit and internals geometry and, consequently, in an extremely intricate, sometimes virtually chaotic flow pattern. Even for the regular geometry provided by some column internals (e.g. corrugated sheet structured packings), the exact localisation of phase interfaces represents a difficult problem, due to intricate interphase interactions. For such large-scale applications, CFD modelling is hardly applicable. Rather, it can be used for small-scale equipment or for parts of larger equipment (cf. Figure 1).

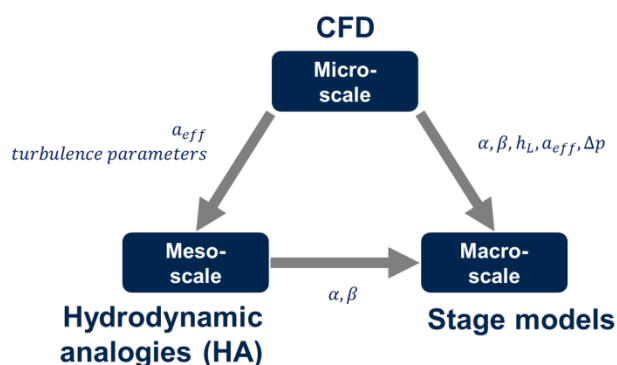


Figure 1: Classification of the kinetics-based modelling approaches

Problems on a meso-scale can be solved using some simplification of real fluid dynamics. One of such approaches proposed recently is called *hydrodynamic analogy* (HA, Kenig, 2008). It rests on the analogy between complex flow patterns encountered in industrial practice and geometrically simpler flows, e.g., films, cylindrical jets, spherical drops, as well as their combinations (Figure 2). This approach represents a certain compromise between rigor and simplicity.

For the processes in which fluid-dynamic patterns are too complex to be described by either CFD or by the HA, further assumptions and simplifications of a real fluid flow picture are required. For instance, large industrial separation units are usually modelled by a proper sub-division of a column unit into smaller elements. These elements (called stages) are linked by mass and energy balance equations. The stages are related to real trays for tray columns, and to packing segments for packed columns. They can be described using different theoretical concepts, with a wide range of physicochemical assumptions and accuracy (Noeres et al., 2003). Stage-based models directly considering process kinetics fall within the so-called *rate-based approach* (RBA). Equilibrium-based stage modelling remains an important tool for the basic design issues; it can also be useful for the generation of initial values during the simulation with the RBA.

2.1 Model complementarity

Figure 1 depicts some parametric links illustrating possible ways of complementary application of the modelling approaches described above. CFD-based simulations belong to *the first principle methods* and are independent of any engineering/design lump parameters like mass transfer coefficients. Therefore, they can be used for the estimation of such parameters based on the local data on field variables (e.g. velocity, temperature, concentrations). This can be done particularly efficiently for periodic systems, for instance,

structured packings or heat exchangers. In this case, a small piece of a corresponding structure has to be identified in such a way, that the property evaluation is possible. The engineering/design parameters thus determined can be transferred, in form of correlations, to other modelling approaches, HA and RBA. Similarly, CFD can support application of HA approach, by estimating and delivering turbulent mixing parameters. In this way, not only the number of necessary real hydrodynamic and mass transfer experiments – a frequent source of parameter correlations – can be reduced, but also column internals can be optimised directly “on screen”, without the need to manufacture them for validation experiments. Furthermore, the HA approach does not require the knowledge of mass and heat transfer coefficients and hence can be used to determine correlations for these parameters and deliver them to the RBA. In this way the individual modelling approaches are linked into a truly complementary modelling concept.

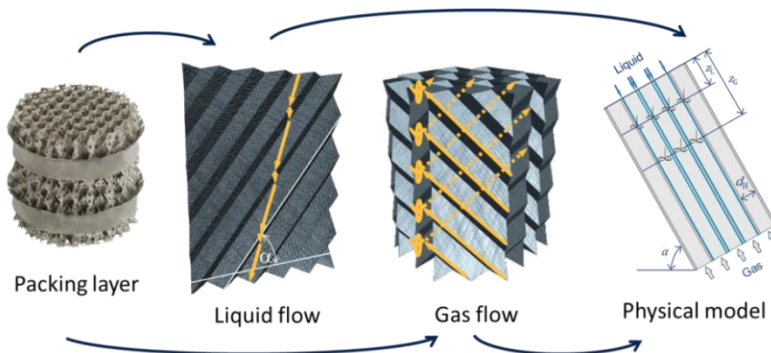


Figure 2: Development of a hydrodynamic analogy for a structured packing

3. Application to the post-combustion CO₂ capture

Post-combustion CO₂ capture was investigated in the context of the EU-funded project *CAPSOL* (Design Technologies for Multi-scale Innovation and Integration in Post-Combustion CO₂-Capture: From Molecules to Unit Operations and Integrated Plants, FP7-ENERGY-2011-282789). In this project, a holistic approach combining activities at the molecular, unit operations and pilot plant levels was applied. The tasks of our group within *CAPSOL* were to carry out virtual experiments with new solvents and innovative internals, to select the best performing solvents and internals, and to perform experimental investigations at pilot scale. The benefits of the complementary modelling approach could be best exploited during the development of new column internals (structured packing), in collaboration with the project partner Julius Montz GmbH. Here, we use it as a good illustration example.

3.1 Validation of individual approaches

All three approaches are to be tested with respect to their accuracy and reliability. CFD simulations were performed using the commercial software tool STAR CCM+ by CD-adapco. Rigorous simulations could be performed for one-phase gas-phase flow, while neglecting the influence of the thin films at the packing surface. Furthermore, the *inherent periodicity of structured packings* can be used in the fluid dynamic studies. Figure 3 illustrates the choice of the representative periodic element and shows the corresponding velocity field in it. Based on the post-processing of this local data, evaluation of the specific pressure drop in the packing can be done. This allows a reasonable validation of the method by comparison with experimental pressure drop data of Julius Montz (Figure 4) showing a good agreement for two different packing geometries.

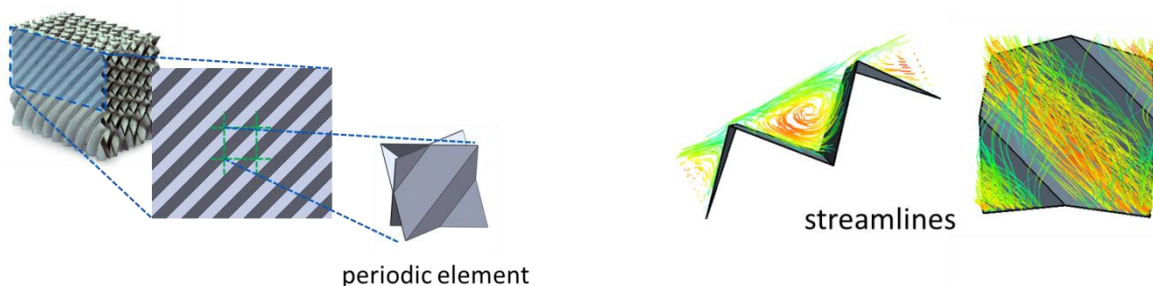


Figure 3: Cutting of a representative structured packing element (left) and corresponding streamlines (right)

Next testing was performed for the HA method. Here, we used the data from the comprehensive CO₂ absorption study by Notz (2009) who worked with standard solvent *aqueous monoethanolamine (MEA)* and *Sulzer Mellapak 250.Y* packing. Parameters describing turbulence in the two-phase flow were determined – in a complementary way – with the CFD simulations (see Yazgi and Kenig, 2013), while the correlation for the specific interfacial area was taken from Tsai et al. (2011). Good agreement of simulated and experimental data is clearly visible in Figure 5.

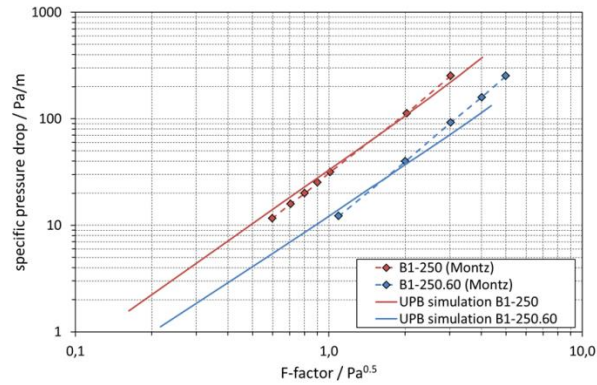


Figure 4: Comparison of specific pressure drop values for two different packing types determined by CFD-simulations and by measurements (UPB denotes the abbreviation of Paderborn University used in the CAPSOL project)

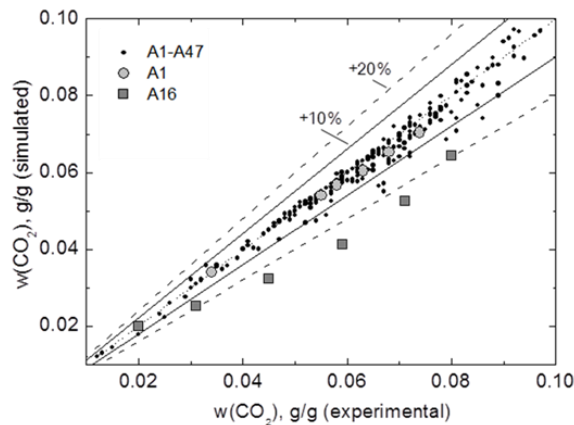


Figure 5: Comparison of CO₂ mass fractions in the liquid phase determined by HA-simulations and measured by Notz (2009)

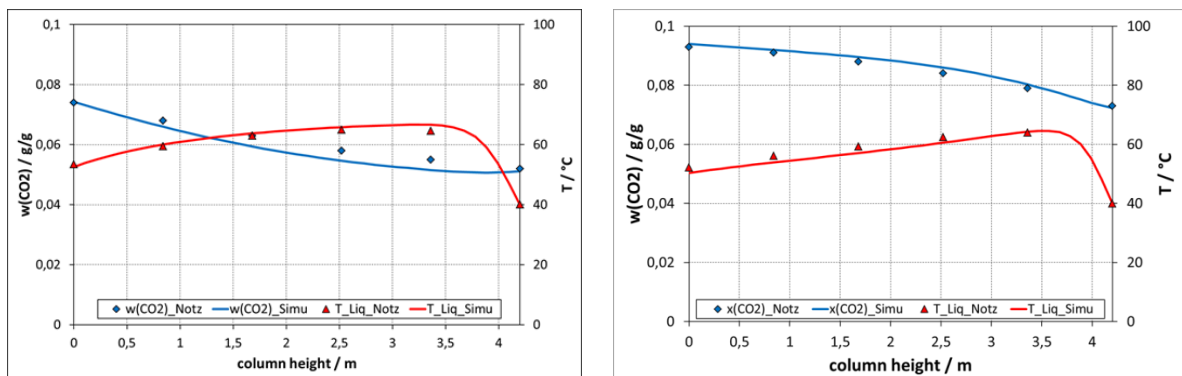


Figure 6: Concentration and temperature profiles in the liquid phase obtained by RBA-simulations and measured by Notz (2009) for two different experiments

Finally, a validation of the RBA tool available in our group was carried out using, again, the extensive data pool from Notz (2009). Parameter correlations, such as pressure drop, holdup, transfer coefficients and specific interfacial area were taken from Billet and Shultes (1999) and Tsai et al. (2011). Figure 6 shows concentration and temperature column profiles and demonstrates a very good agreement between simulated and experimental values, which was also confirmed for all investigated experiments.

3.2 Development of a novel structured packing

The models validated as shown above were used to develop a new structured packing for the CO₂ capturing with improved properties. Most often, two criteria are used to evaluate the packing appropriateness, separation efficiency and pressure drop, both depending on the packing geometry. We first used the CFD-based modelling, varied the packing inclination angle and analyse the results. As can be clearly seen in Figure 7, the inclination angle indeed strongly influences the pressure drop, but only up to the value close to 75°. For inclination angles above 75°, only marginal reduction of pressure drop can be encountered.

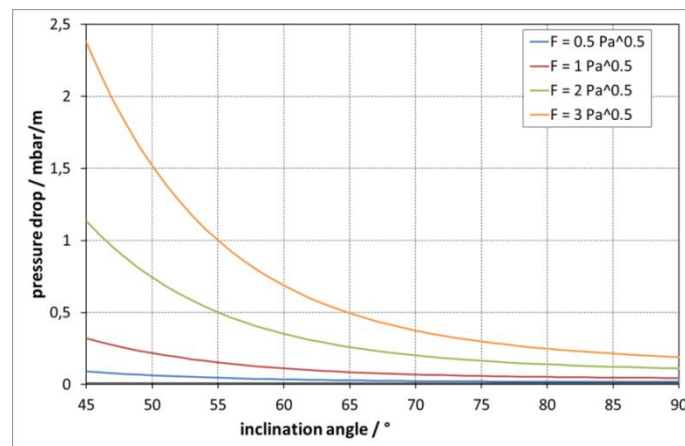


Figure 7: Pressure drop dependence on packing inclination angle and gas-phase load (represented by the gas capacity factor F) obtained by CFD-based simulations

In the second step, we used the HA modelling method allowing the separation efficiency to be evaluated. Inclination angles of 45° (standard for many commercial packings), 20° and 70° were studied. Absorption efficiency for higher angles decreased, which was expected. However, this reduction was rather insignificant (e.g., from 75% to 66% for the experiment A1 by Notz (2009)). Such a reduction can be overcome by using higher columns. Based on these results, a decision was taken to manufacture the new structured packing with the inclination angle of 75°, which was accomplished by Julius Montz (cf. Figure 8).

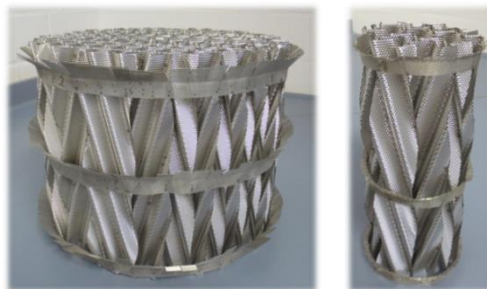


Figure 8: New structured packing with the inclination angle of 75° manufactured by Montz GmbH for the investigations in the pilot plant of Paderborn University, with DN300 and DN100 columns

3.3 Experimental testing and large-scale studies

The new packing was tested experimentally in the pilot plant recently built at the Paderborn University (cf. Hüser and Kenig, 2014). CO₂ absorption by aqueous MEA solution was studied. The new packing shows a dramatic reduction (over 90%!) of pressure drop as compared to conventional packing with 45° inclination angle (cf. Figure 9), thus fully confirming the expectations based on the modelling. In contrast, the corresponding loss in separation efficiency was found rather limited (Hüser et al., 2014).

Further tests of the new packing were performed with the RBA modelling, this time for the CO₂ capture system on industrial scale. The data from the industrial partners in CAPSOL were used to investigate bituminous coal fired power plant (power output of 650 MWe) and natural gas fired combined cycle (power output of 420 MWe). For the new packing, parameter correlations from the literature were adjusted based on our own experimental data, and it was found that the efficiency drop did not exceed 5%. Thus, both pilot plant experiments and large-scale simulations prove that the new 75° packing represents a good alternative to standard packings for the amine based CO₂ capture.

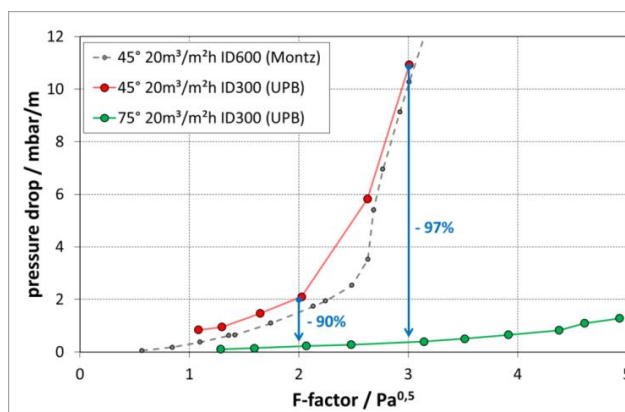


Figure 9: Pressure drop of irrigated packing with 20 m³/m²h liquid load. Here both a validation of the UPB experiments with conventional packing and a comparison with the new packing are given

4. Conclusions

Optimisation of Fluid Process Engineering calls for high model accuracy and reliability, while the process complexity rises. To address this challenge, the complementary modelling concept can be applied, based on a reasonable interrelated application of models with different rigour and complexity. More rigorous models should be used for small-scale simulations to determine process parameters and to deliver them to less rigorous models applicable for large-scale applications. This paper gives a detailed description of the complementary modelling framework and illustrates it with a representative example from the area of post-combustion CO₂ capture. The complementary modelling was applied within a EU-Project CAPSOL to develop a new structured packing for CO₂ absorption with improved properties and to test it. The new packing with inclination angle of 75° show over 90% reduction in pressure drop with only limited efficiency loss, which makes it attractive for the application in the amine based CO₂ capture.

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