

INDUSTRIAL ABSORPTION CURRENT STATUS AND FUTURE ASPECTS

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Absorption is still one of the most important separation processes in chemical and petrochemical industry. Although absorption has reached a high level in theoretical understanding, process design and technical implementation, nowadays industrial work on this unit operation is full of economical, technical and scientific challenges. The current status and future developments of industrial absorption are described in this presentation.

KEYWORDS: absorption, column, column internals, mass transfer, rate based modelling

INTRODUCTION

Industrial absorption, its applications and theory are well described in historical and present textbooks [1], [2], [3], [4], [5]. Thus it is not the intention of this presentation to recapitulate the already known fundamentals but to highlight relevant aspects from the viewpoint of daily industrial absorption work.

Among others, absorption is a well established unit operation with a high level of technical implementation and maturity (Figure 1). Therefore further development is carried out by small steps on a high level. But the importance in industrial life, moving economical targets and new applications make “old fashioned” absorption attractive and dynamic for everyone, who has to deal with it in his daily work or research.

ECONOMICAL ASPECTS

In chemical industry absorption technology is used all along the value added chains:

- Feedstock preparation, e.g. synthesis gas treating with amine solutions
- Bulk chemical synthesis, e.g. nitric acid, sulphuric acid or formaldehyde production
- Gas purification in loop systems, e.g. CO₂-removal in ethylene oxide production
- Off-gas cleaning, e.g. scrubbing gases from vessels, reactors, tanks, dryers or flue gas cleaning

Therefore, absorption is still one of the most important separation processes. Interest in absorption grows for example by usage of new gaseous feedstocks [7] or as coal gasification becomes an alternative for chemical feedstocks with increasing oil and naphtha prices [8].

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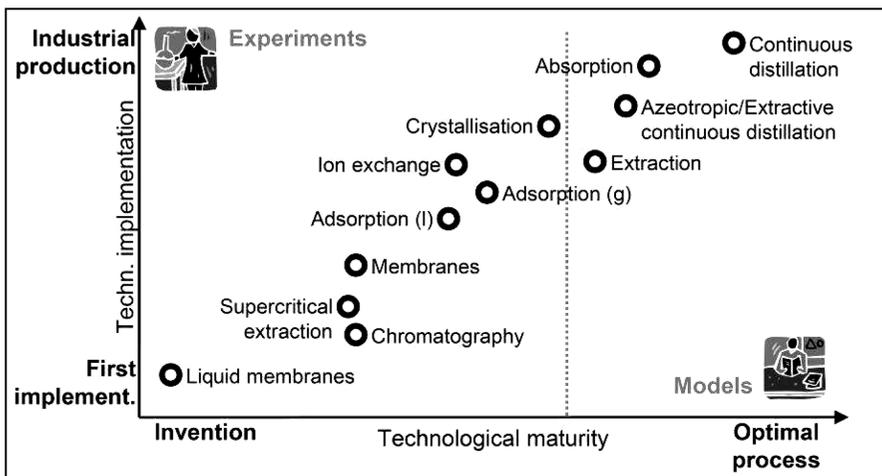


Figure 1. Applications of fluid separation processes in chemical and petrochemical industries after Górak and Schoenmakers [6]

Examples from other industries in comparable scales and economical requirements are available, e.g.

- Gas sweetening of natural gas and LPG sweetening in petrochemical industry [4], [9]
- Coke oven gas treatment [11]
- Flue gas desulphurisation [12]

The economical interests concerning absorption are quite different regarding the various players in the market: For chemical and process industry absorption has to be the most cost effective separation technology compared with alternative pathways and compared with competitor's technologies. In modern process design tools absorption units are regarded, like other units, as knots in optimizing mass, heat and "money flows" [13].

Following time to market aspects for chemical products simultaneous engineering is also nowadays standard way during detailed synthesis and design of absorption processes. Choice of the solvent, property evaluation and modeling, if necessary miniplant testing, selection of apparatus and its internals, detailed process simulation and mechanical engineering have to be done simultaneously but always with respect to short start-up times and dedicated design of the process.

To identify economic relevance, absorption tasks can be classified into two groups: On one hand, process integrated absorption is often economically dominant for total process costs and therefore regarded with detailed modeling. Extended capital investment

and high operational costs are based on large vapour loads and often strong separation efficiencies (Figure 2). On the other hand, end off pipe absorption is usually common business with low economical attractiveness but following conservative design criteria [14].

Manufacturers of column internals estimate the current global absorption market to have a value of 90 Mio.\$/a, whereas 50% are related to absorption systems with chemical reactions [15]. This market is dominated by random packings (50%), whereas structured

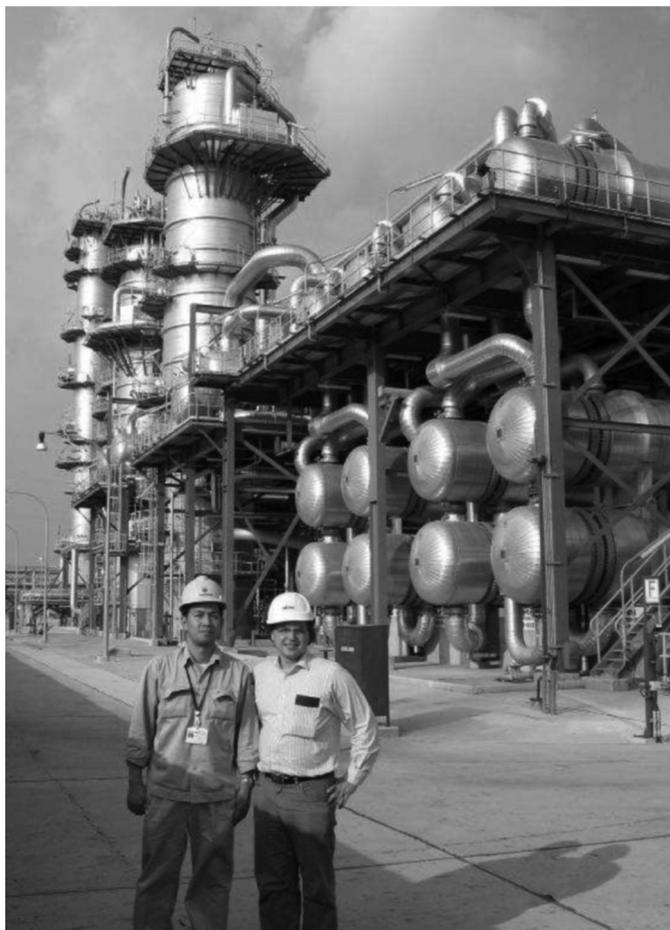


Figure 2. Natural gas separation plant of PTT public company Ltd., Thailand using BASF's aMDEA-technology for CO₂-removal (capacity 590.000 Nm³/h)

packings (25%) and trays (25%) are comparable in market size. Currently high material prices for metal dominate the equipment market. By the development of high capacity internals with reduced material consumption, the manufacturers reduce operational and investment costs for the equipment users and improve their own competitiveness.

Like in other classical unit operations, absorption is technically, theoretically and economically well developed. Therefore the market attractiveness of absorption for universities, scientific institutes and young researchers is still decreasing. This includes the risk of competence loss and a decreasing number of well educated employees. A permanent performance improvement, the integration of hybrid separations and new applications in various process industries (e.g. biotechnology, biorefining) are highlighted as guidelines to overcome this lack [6].

Absorption applications will increase with the market growth of the related process industries. Possible future applications, like CO₂-capture from flue gases may enhance this growth [16].

TECHNICAL ASPECTS

Industrial absorption is still carried out in conventional **apparatus**' like packed columns, tray columns, bubble columns or spray absorbers in co- or countercurrent flow [17]. The dimension of this equipment is in the range of 100 mm for very small applications up to several meters for high vapour loads. Packed absorbers of up to 7 m in diameter and operating pressure of 68 bar have been reported [18]. For spray absorbers diameters of up to 15 m are realized [19]. The size of that columns is nowadays often not limited by principle design criteria but by construction and transportation facilities. The complexity of such columns can be very high, e.g. absorption towers for 1500 tons per day concentrated nitric acid with diameter of 6 m, 40 cooled sieve trays and 75 m total height [23].

New types of apparatus for absorption have been developed that intend to intensify mass transfer by using non classical conditions [20], [21] or combine absorption with another unit operation in one unit [22]. Following the current trend of micro reaction process engineering only a few attempts have been described for 'micro-absorption' devices so far. These may be favourable in systems with extended heats of absorption or toxic substances, but are limited strictly by effects like foaming, fouling or solids in the treated gas stream.

More work has been done on the development of new **column internals**. As the basic fluid dynamic and mass transfer behaviour of classical packings [24], [25] and trays for absorption [26] have been investigated in the 1980–1990's, the actual focus is given on high high capacity random packing, e.g. Raschig-Super-ring [27], IMTP-ring [28] or structured packing. e.g. Sulzer MellapakPlus[®], Montz-Pak Type M[®] or Koch-Glitsch Flexipac[®]HC[®]. Lower Pressure drop and up to 45% higher capacity than conventional structured packing are significant for these new types. Figure 3 shows some examples of modern random packing types and a high capacity structured packing that are used in absorption applications. Less work is done for further tray development in absorption systems.

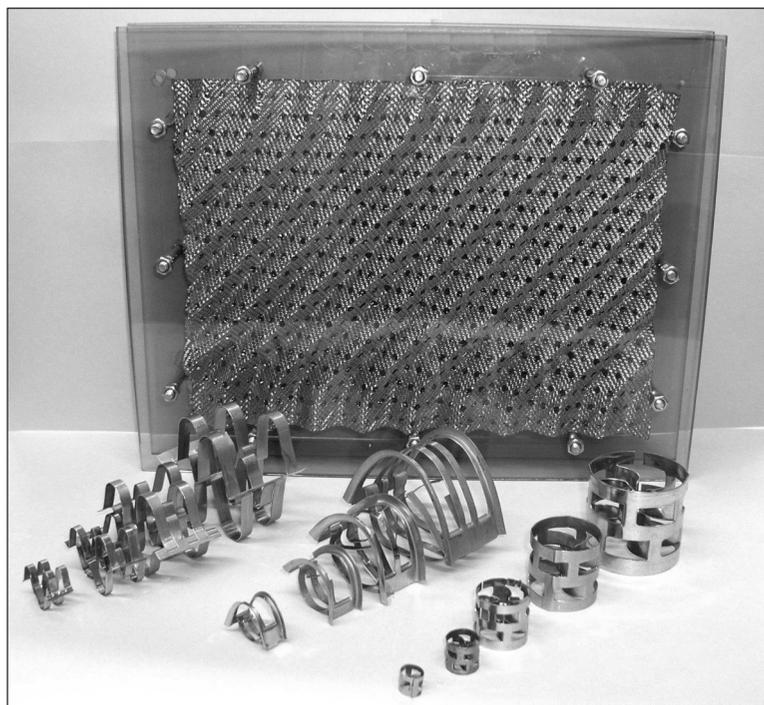


Figure 3. Modern types of random and structured packing typed together with classical pall rings

The aim of all current developments is to maximize separation efficiency at optimized pressure drop. In times of still increasing material prices, especially for metals, the economic issue is also to minimize the mass of metal [in kg] per volume of the column [in m³] to achieve a desired separation efficiency (e.g. HTU_{OG}).

The key issue for industrial application of new types of internals is not only an optimized performance, shown in lab or technical scale tests, but also in providing the users with accurate test data concerning fluid dynamics and mass transfer capacity. These data have to be available in a wide range of vapour and liquid loads under real but also comparable conditions. Whereas hydrodynamic measurements of internals can be used both for distillation and absorption, the derivation of mass transfer data needed for absorption design (HTU , k_g , k_l , a_{eff}) from HETP normally fails. Recently, a method to standardize mass transfer measurements for absorption systems is suggested. The aim is to achieve comparability and to develop or improve reliable mass transfer correlations [29].

Several publications can be found concerning the measurement of **mass transfer coefficients** of different packing types [30], [31]. Some of these papers compare different types of packing with the same nominal geometric data and give an idea of the favourable type. But a strict economic comparison of different types of mass transfer internals is still missing. This comparison should be the basis for an “expert system” to choose the best mass transfer device [15] for a given separation task.

Based on mass transfer measurements a lot of **mass transfer correlations** have been published [32]. These mass transfer correlations are the most important toolkit for the design of absorption columns, as modern computer rate-based models are available in common flowsheet simulators (e.g. ASPEN RATESEP[®], ChemSep[™] by Kooijman and Taylor, SimSci-Esscor Pro/II RATEFRAC[®], Chemstations CHEMCad SCDS-Column, gProms RateBased-Modul). Most mass transfer correlations have been developed for random packing [31], [33], [34], but the correlations show significant differences comparing their results [14], [34]. Normally packing specific parameters from experiments are needed [31]. Only a few correlations have been derived for structured packing [35], [36], but the accuracy of various published correlations does not allow a safe design of absorption columns [15]. The issue for both types of internals is to regard the different shapes of the internals in a common correlation. For tray absorbers only a very small data basis is available.

With the development of modern column packing types also further development of “non-separating internals” like distributors, redistributors and support grids is needed. Maldistribution in absorbers equipped with modern types of internals is important because the self-redistribution of the packing is minimized in order to enhance fluid dynamic loads [37], [38], [39]. Also, a lot of work on column troubleshooting is done on maldistribution effects [40], [41]. However, it has to be noted that maldistribution affects more desorption than absorption [1], leading to a less regenerated solution coming from the desorber which leads then to a higher outlet gas concentration at the top of the absorber in combined systems.

Standard **absorption systems** e.g. HCl-water, NO_x-water, NH₃-acids are well established technology concerning basic thermodynamic data as well as operability and materials for construction. Thermodynamic models even for complex systems have been developed (see Chapter 4). New possible applications of absorption regarding the gas side will be described in Chapter 5.

For given gaseous components (normally the separation task is fixed) a large potential for process optimization is given by the right choice of the solvent. Nowadays modern quantum chemistry methods can be used for physical **solvent** screening [42]. By combining quantum chemical calculations and exact statistical thermodynamics information is provided that is necessary for evaluation of molecular interactions. Gas-liquid equilibria even in the diluted range of Henry’s law can be predicted a priori and can therefore be used for solvent selection. But a suitable program for selecting technical solvents should also include other relevant parameters like viscosity, vapour pressure, toxics or corrosion effects. More difficulties occur in screening selective and chemical absorbents [43].

In conclusion it can be derived that the technical aspects of industrial absorption are highly developed. Only slight increase and innovations are expected regarding the long time from first technical idea towards technical use with references needed for acceptance of the market. Significant innovations are possible in the solvent market.

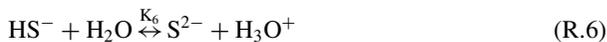
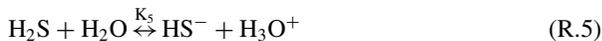
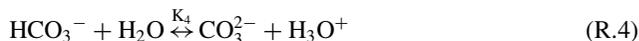
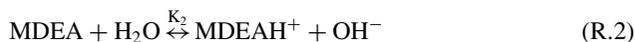
FUNDAMENTAL ASPECTS

Absorption is often carried out with the aid of chemical reactions in the liquid phase in order to increase absorbent capacity and solubility. In contrary, to typical distillation or physical absorption processes, these cases require the consideration of the occurring chemical reactions. The thermodynamic and mathematical description of such a system is similar to non-electrolyte systems. It only requires the inclusion of all chemical reactions, their equilibria, and the activity coefficients of all species. The complexity of such a system and the mathematical problems to solve the underlying equations is not only a result of the increased number of components but also due to the highly non-linear linkage between the relationships for chemical equilibria and activity coefficients of the different species [44]. Complexity increases when ionic compounds are involved and specific models for electrolyte thermodynamics have to be regarded.

COMPLEX CHEMICAL AND PHASE EQUILIBRIUM

As an example for the complex behaviour and equations to be solved in chemical absorption with electrolytes the absorption of CO₂ and H₂S in a mixed amine system is described below. The reactions to be considered are:

Instantaneous reversible reactions:



Kinetically controlled reactions:



The existence of additional electrolytes e.g. NaOH or Na₂CO₃, KOH or K₂CO₃ can be considered by:



The also occurring reaction $\text{CO}_2 + 2\text{H}_2\text{O} \leftrightarrow \text{HCO}_3^- + \text{H}_3\text{O}^+$ is very slow compared to (R.7) especially in alkaline solutions. Its contribution to the overall rate of reaction is therefore small and can be neglected. Reactions involving protonation or hydrolysis can be considered as instantaneous compared to the diffusion process. Eigen gives reaction rates for different reactions in aqueous systems [45].

To calculate the exact concentrations of molecular and ionic species in solution the chemical equilibria are expressed with their dissociation constants K_j , which should be based on activities taking non-idealities into account:

$$K_j = \prod_{i=1}^{nc} a_i^{v_{ij}} = \prod_{i=1}^{nc} m_i^{v_{ij}} \gamma_i^{v_{ij}} \quad (1)$$

To complete the set of equations the chemical equilibrium and the concentrations of species in solution, the total mass balances for each apparent component and a charge balance (electro neutrality) for the solution have to be added to the set of equations.

$$\text{e.g. } m_{\text{CO}_2}^{\text{tot}} = m_{\text{CO}_2} + m_{\text{CO}_3^-} + m_{\text{CO}_3^{2-}} + m_{\text{MEACOO}^-} \quad (2) \dots (7)$$

electro-neutrality condition:

$$\sum_i^{nc} m_i z_i = 0 \quad (8)$$

This results in 17 equations for 17 species presuming knowledge of the 6 total molalities for apparent components. Total mass and concentration of the molecular species water are constant since the concentration measure is molality in mol per kg of solvent (H₂O).

If equilibrium exists at the interface the chemical potentials of the molecular components in both phases has to be equal.

$$y_i \cdot \varphi_i \cdot P = x_i \cdot \gamma_i \cdot H_{i,\text{H}_2\text{O}}(T, p) \quad (9)$$

The Henry coefficient $H_{i,\text{H}_2\text{O}}$ of the component i in water for dissolved diluted gases is used for the standard-state fugacity, the fugacity coefficient φ_i considers the non-ideality

of the gas phase. The activity coefficient γ_i has to be calculated by using an adapted electrolyte model, e.g. the Pitzer- or Electrolyte-NRTL-model [47].

Combining chemistry and thermodynamics, it is important to consider a consistent set of activities. The data calculated on the basis of activity coefficients have to fit the vapour-liquid data as well as the kinetics and chemical equilibria [46].

Unfortunately, considering all these details is often the only way to describe those systems with an accuracy needed in industry. These data also have to be combined with the complex equations describing heat and mass transfer that are described below.

MASS TRANSFER FUNDAMENTALS

For a non-equilibrium model the column is divided into stages. In each segment the vapour and the liquid phase is considered separately regarding balances for mass, components and enthalpy. Mass transfer between both phases over the interfacial area is evaluated with the film theory, which assumes onedimensional diffusion in the film and a completely mixed bulk phase.

The diffusion in multicomponent systems is often described by the General-Maxwell-Stefan (GMS) approach derived from the kinetic gas theory taking intermolecular friction into account [3]. All simplified models (e.g. Fick's law) can be derived from General-Stefan-Maxwell.

The driving force d_i in terms of diffusion fluxes j in GMS is given by:

$$d_i = \sum_{j=1}^{nc} \frac{x_i j_j - x_j j_i}{c_t D_{i,j}} \quad (10)$$

Assuming electro-neutrality of the entire solution and a constant pressure, the generalised driving force in electrolyte systems is given in [3] and adapted to the one-dimensional case by:

$$d_i = \frac{x_i}{RT} \frac{d\mu_i}{dy} + x_i z_i \frac{F}{RT} \frac{d\phi}{dy} \quad (11)$$

To calculate the diffusion in the film, equations 10 and 11 have to be combined.

In electrolyte solutions different diffusivities of ions cause small charge separations leading to electric forces between ions of opposite charge. The diffusivities of hydrogen and hydroxyl ions occurring in the aqueous solution are considerably higher than those of other species [48].

The mass transfer rate N_i can then be calculated taking into account convection:

$$N_i = J_i + x_i \sum_{j=1}^{nc} N_j, \quad (12)$$

and that:

$$0 = \sum_{i=1}^{nc} J_i \quad (13)$$

The solution of the equation system consisting of equations. (10), (11), (12) and (13) can lead to the so-called cross-effects, such as the “diffusion barrier”, “counter diffusion” or “osmotic diffusion”, e.g. zero diffusion despite a concentration gradient or diffusion of one component against its own concentration gradient or without a gradient. These effects cannot be predicted by the normal Fick’s law.

However, these effects occur only in concentrated solutions and can often be neglected in diluted systems [49], as they occur typically in absorption processes. Higher concentrations in the vapour phase at the top of desorber might introduce a small influence of these effects.

MASS TRANSFER MODELS

For the calculation of mass transfer between two phases in an absorption process several models exist, such as the film theory, penetration theory or surface renewal theory. All of these models simplify the hydrodynamic behaviour significantly and require a decisive parameter. For the film theory this parameter is the thickness of the boundary layer δ , which can also be expressed in a mass transfer coefficient β :

$$\beta = \frac{D}{\delta} \quad (14)$$

Specific accuracy is needed when mass transfer coefficients from classical correlations [33] are combined with diffusion coefficients that have been calculated from binary diffusion coefficient [51].

These parameters have either to be determined from laborious experiments and adapted to the particular problem or might also be predicted. Newer approaches use hydrodynamic analogies or CFD calculations [50].

In most chemical absorption problems the chemical reactions are fast enough to influence the mass transfer in the film. Thus, mass transport and reactions occur simultaneously leading to changes in concentration gradients and therefore an enhancement of mass transfer. Several models exist for the consideration of these effects (Figure 4).

The reactions can either be considered as instantaneous and thus equilibrium can be assumed, or can be incorporated into the model using detailed reaction kinetics for both the film and the bulk phase or just for the film assuming that equilibrium of the reaction is achieved in the bulk phase.

The simplest modelling approach, the equilibrium model, usually fails to predict chemical absorption processes. The deviation from the assumption that equilibrium

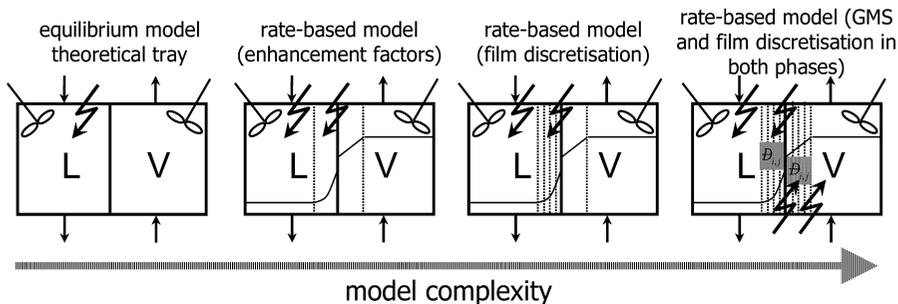


Figure 4. Different modelling approaches for one segment

exists at the exit of a theoretical stage can be accounted for by Murphree or vaporisation efficiencies. These efficiencies cannot be reliably predicted, since they depend on the component, the geometry, process parameters, the type of absorbent, its concentration and loading.

A better predictivity provides a rate-based approach with the before mentioned equations for mass transfer. The influence of the chemical reaction on mass transfer can be accounted for by enhancement factors in a simple way.

Enhancement factors can be found in the literature for different types of reactions, reaction orders and reaction pathways based on the film theory, penetration theory or surface renewal theory. They are either derived analytical by solving the governing differential equations with a reaction rate term in the film or approximate solutions are given.

For complex reaction systems no reliable enhancement factors might be available. In those cases the modelling approach has to divide the film in radial segments. The reactions are then incorporated by adding reaction rate terms into the component balances for each film segment. Regarding Figure 4 this approach has the highest complexity, does not require enhancement factors and can handle many different reactions. However, the computational effort compared to the enhancement factor approach rises significantly, since all equations for mass and heat transport, chemical reactions and thermodynamic properties have to be calculated for each film element. A typical number of film elements is between 6 and 40 for an accurate calculation of the profiles in the film [51].

Several commercially available simulators have already been mentioned in Chapter 3. The report of Asprion [51] shows that also the film discretisation approach (the two most advanced approaches in Figure 4) is already applied in industry and can be regarded as state-of-the-art modelling [14]. The requirements of these models, regarding accuracy of the parameters needed, are high, in order to justify the substantial efforts on modelling and the high computational efforts. If the knowledge of a system is low and thus the availability of parameters and their accuracy is also low, simplified modelling approaches are normally used. Common rules for the right choice of the adapted model complexity have been not published yet.

The consideration of the full General-Maxwell-Stefan Theory (GMS, compare Figure 4) is often done in available simulators. However, the increase in predictivity for absorption systems is low or even questionable. Other effects like maldistribution and the development of rivulets and droplets in aqueous systems might affect mass transfer by a much higher degree than the cross-effects within the GMS approach. Furthermore, the prediction of the required parameters by standard prediction methods, for e.g. binary diffusion coefficients $D_{i,j}$, of an ion i in an ion j , can hardly be experimentally validated and are thus not feasible.

MODEL SIMPLIFICATION

The choice for one of the different models should be based on the individual requirements, the knowledge about the process, the availability of properties and parameters for the system and the time allowed for setting up the simulation and the simulation time.

Increasing modelling complexity requires an increasing number of model parameters and physical properties. To justify the increased modelling efforts these parameters have to be of high accuracy. The relationship between model complexity and costs and efforts for parameter determination, modelling and costs due to inaccuracy are shown in Figure 5 (taken from [52]).

Many different parameters are required for the above mentioned different models: parameters for a g^E -modell to calculate activity coefficients, Henry coefficients, an equation-of-state to calculate fugacity to coefficients, reaction rates, densities, enthalpies, diffusivities in electrolyte solutions, viscosities, surface tension, interfacial areas, mass-transfer coefficient correlations, thermal conductivities, heat-transfer coefficients.

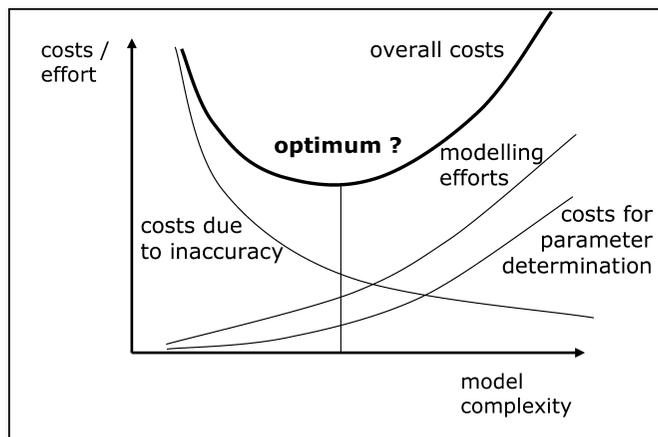


Figure 5. Model complexity vs. costs after Górak [52]

Correlations for all of these parameters are subject to error, they might not be available for the given problem and have to be extrapolated to the process parameter range used, leading to large errors. If no accurate measurement method is available, they have to be estimated.

Another method is the parameter estimation from existing experiments or plant data. Using mathematical methods to solve large-scale non-linear problems these parameters can be adapted using a rigorous rate-based model and several sets of experimental data [53], [54].

All rate-based approaches require correlations for mass-transfer coefficients and effective surface areas. Thus, when new packings are developed, these parameters have to be provided by either the manufacturers or determined by an independent research institution, in order to evaluate their performance regarding a specific absorption task. These parameters are usually given with an accuracy of $\pm 20\text{--}40\%$, showing again the difficulty in obtaining accurate parameters for a rate-based simulation.

FUTURE ASPECTS

Several new **applications** of absorption will occur with increasing importance of gas-based techniques and environmental demands. A promising example, as already mentioned, is the CO₂-capture from conventional power plants. Since these power plants contribute to the global anthropogenic CO₂ emissions to a very large extent, the associated flue gas flows from these plants are large and the heat requirements for regeneration of today's available solvents are high, this problem can be considered as one of the most challenging tasks in chemical engineering in this century. Due to the low available partial pressure of CO₂, chemical absorption has to be favoured for this task. Using a typical MEA-solvent a loss of 10% efficiency for the power plant is still too high to be commercially feasible [55]. Thus, one of the future aspects is the search for a new solvent. In industrial practice these solvents should possess for CO₂-capture the following attributes:

- Low evaporation and reaction enthalpy to reduce steam requirements for regeneration
- Low vapour pressure to reduce solvent losses
- Fast reaction with CO₂
- Low toxicity
- Little degradation with O₂, NO_x, SO₂
- No corrosion
- No foam

An overview of possible solvents is given in [16]. Tailor made amine solutions can be an attractive alternative [55]. In this context the design of Ionic Liquids (IL) for this specific task is currently carried out [16]. IL's can also be used for gas absorption of other components [57]. Due to their major advantages (no vapour pressure, possibility for tailor made design) they may become once standard absorbents, if availability and prices in 100 tons scale fit industrial requirements.

Concerning the **mass transfer** aspects of absorption, extensive CFD calculations are carried out [58] to improve modelling of a structured packing and to receive parameters for rate-based models easily without experiments. The idea is to develop mass transfer correlations based on computer experiments.

Figure 6 shows the geometry of a structured packing (Mellapak) with two corrugated sheets and a liquid flowing in a channel between two sheets. The pictures show the development of rivulets and droplets with the metal sheets not being completely wetted. From these extensive computations the hydrodynamic behaviour and, in the future, parameters like surface area and mass transfer coefficients can be predicted. Similar research is also being done on the example of another structured packing KÜHNI Rombopak [59].

With respect to industrial applications the development of extended mass transfer correlations should be an issue. Examples are:

- Total absorption of components from streams without inert gas
- Absorption at very low gas velocities
- Absorption of non-moving gas in column

Leaving the world of the classical film model new approaches are made to describe mass transfer phenomena in fluid separations [50]. A good example is given by the hydrodynamic analogy developed for structured packings. This method is based on an analogy between the complex behaviour in separation processes and the phenomena in simplified film flow. The basic partial differential equations for convective transport are used for mass transfer modelling.

To improve **fundamental** knowledge and **thermodynamics** in complex or reactive absorption systems a dynamic analysis of vapour-liquid equilibria and detailed species

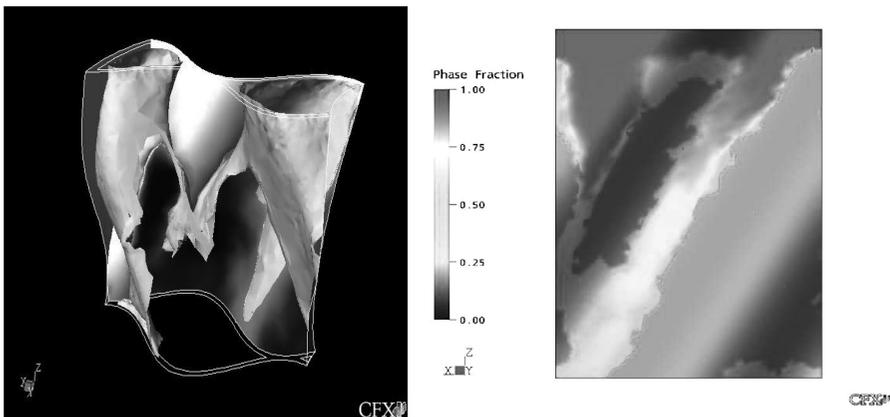


Figure 6. CFD-Simulation of film-flow in a structured packing, development of rivulets and droplets [58]

behaviour by using NMR-technology can be used [60], [61]. With this technique kinetic reactions and intermediates can be measured in small time scales leading to improved thermodynamic models.

CONCLUSIONS

Regarding its complexity today's industrial absorption is a well developed and established unit operation. Commercially absorption is often the 'cash cow' of processes where it is used as a main process step and not only for off-gas treatment. New and exciting challenges especially concerning new applications occur for absorption. Several lacks in the existing models and data basis have to be clarified.

All this work can only be done by a fundamental understanding of this unit operation. A problem-to-problem based strategy fails because of the extensive physical, chemical and mass transfer phenomena and parameters involved in absorption.

NOMENCLATURE

VARIABLES

a_{eff}	effective surface area	m^2/m^3
a_i	activity of component i	-
c	concentration	kmol/m^3
d	driving force in GMS	$1/\text{m}$
D	diffusion coefficient	m^2/s
E	enhancement factor	-
F	Faradays constant	C/mol
H	Henry coefficient	Pa
j	diffusion flux density	$\text{kmol}/\text{m}^2\text{s}$
J	diffusion flux	kmol/s
k	mass transfer coefficient	m/s
N	molar flow	kmol/s
nc	number of components	-
p	pressure	Pa
R	universal gas constant	$\text{J}/\text{mol K}$
T	temperature	K
β	mass transfer coefficient	m/s
δ	thickness of the film	m
γ	activity coefficient	-
ϕ	electrical potential	V
φ	fugacity coefficient	-
ρ	density	kg/m^3
x	liquid phase mole fraction	-
y	vapour phase mole fraction	-
μ	chemical potential	-

SUB- AND SUPERSCRIPTS

<i>chem</i>	chemical
<i>eff</i>	effective
<i>g</i>	gas phase
<i>l</i>	liquid phase
<i>i</i>	component <i>i</i>
<i>j</i>	component <i>j</i>

REFERENCES

1. P.V. Danckwerts, *Gas-Liquid Reactions*, New-York, McGraw-Hill, 1970.
2. Astarita, G., Savage, D., Bisio, A., *Gas Treating with Chemical Solvents*, New York, John Wiley & Sons, 1983.
3. Taylor, R., Krishna, R., *Multicomponent mass transfer*, New York, John Wiley & Sons, 1993.
4. Kohl, A.L., Nielsen, R., *Gas Purification - 5th edition*, Houston, Gulf Publishing Company, 1997.
5. Gödecke, R., *Fluidverfahrenstechnik*, Weinheim, Wiley-VCH, 2006.
6. Górak, A., Schoenmakers, H., *Quo vadis Fluid Separation Processes – a German perspective*, Oral Presentation, EFCE Working Party on Distillation, Absorption and Extraction, September 16, 2004, Huelva-E.
7. PERP Report 03/04s10, *Advances in LNG Technologies*, New York, Nextant Chem Systems, October 2004.
8. U.S. Department of Energy, *Gasification Technology R&D*, <http://www.fossil.energy.gov/programs/powersystems/gasification/>.
9. Maddox, R., Morgan, D., *Gas Conditioning and Processing, Vol. 4: Gas Treating and Sulfur Recovery*, 4th edition, Norman, Campbell Petroleum Series, 1998.
10. 2006 Gas Processes Handbook, Hydrocarbon Processing **85** (2006) CD-Rom.
11. Brettschneider, O., Thiele, R., Faber, R., Thielert, H., Wozny, G., Experimental Investigation and Simulation of the Chemical Absorption in a Packed Column for the System NH₃-CO₂-H₂S-NaOH/H₂O, *Separation and Purification Technology* 39 (2004) p. 139–159.
12. Singer, J.G. (editor), *Combustion fossil power. A reference book on fuel burning and steam generation*, Windsor, Connecticut, 1991.
13. O'Driscoll, C., *Creative cost-cutting*, *European Chemical News* (2005) September, p. 34–35.
14. Brettschneider, O., Clausen, I., Lichtfers, U., Löning, J.-M., *Anforderung an die Modellierungssystematik von Absorptionsprozessen*, Plenary Lecture, GVC-Fachausschussitzung Fluidverfahrenstechnik, April 1, 2004, Leipzig, Germany.
15. Duss, M., *Absorption Column Design: Industrial Challenges and Research Questions*, OPTABSOWorkshop: October 7–8, 2004, Delft-NL.
16. Rolker, J., Arlt, W., *Abtrennung von Kohlendioxid aus Rauchgasen mittels Absorption - Capture of CO₂ from Flue Gases using Absorption*, *Chem. Ing. Tech.* **78** (2006), p. 416–424.

17. Benitez, J., *Principles and modern applications of mass transfer operations*, New York, J. Wiley, 2002.
18. http://www.lurgi.de/lurgi_headoffice_kopie/english/nbsp/menu/products/gas_production_and_purification/natural_gas_treatment/markets/index.html.
19. *Toughness test for 700 tons of metal*, PROCESS Worldwide-01-2005.
20. Trent, D.L., Chemical processing in high - gravity fields in Stankiewicz, A.; Moulijn, J. A. (Eds.) *Re – engineering the chemical processing plant - Process intensification*, MARCEL DEKKER, INC., New York Basel, 2004.
21. Ramshaw, C., Mallinson, R.H., *Mass Transfer Process*, U.S. Patent, 4,283,255 (1981).
22. Kumar, P.S., Hogendoorn, J.A., Feron, P.H.M., Versteeg, G.F., *New absorption liquids for the removal of CO₂ from dilute gas streams using membrane contactors*, Chem. Eng. Sci. **57** (2002) 1639–1651.
23. More, A., *Raring to go*, Nitrogen&Methanol (2003) March–April, p. 35–40.
24. Billet, R., *Packed Towers*, Weinheim, VCH, 1995.
25. Mackowiak, J., *Fluiddynamik von Füllkörpern und Packungen*, Berlin, Springer, 2003.
26. Stichlmair, J., *Grundlagen der Dimensionierung des Gas/Flüssig-Kontaktapparates Bodenkolonnen*, Weinheim, VCH, 1978.
27. Schultes, M., *RASCHIG SUPER-RING - A New Fourth Generation Packing Offers New Advantages*, Chem. Eng. Res. Des. **81** (2003), p. 48–57.
28. Moucha, T., Linek, V., Prokopova, E., *Effect Of Packing Geometrical Details - Influence of Free Tips on Volumetric Mass Transfer Coefficients of Intalox Saddles*, Chem. Eng. Res. Des. **83** (2005), p. 88–92.
29. Hüpen, B., Hoffmann, A., Górak, A., Löning, J.-M., Haas, M., Runowski, T., Hallenberger, K., *Standardisation of mass transfer measurements – A basis for the description of absorption processes*, accepted lecture for Distillation&Absorption 2006, London, UK, 2006.
30. Kolev, N., Nakov, S., Ljutzkanov, L., Kolev, D., *Effective area of a highly efficient random packing*, Chem. Eng. Proc. **45** (2006), p. 429–436.
31. Billet, R., Schultes, M., *Prediction Of Mass Transfer Columns With Dumped And Arranged Packings - Updated Summary of the Calculation Method of Billet and Schultes*, Chem. Eng. Res. Des. **77** (1999), p. 498–504.
32. Wang, G.Q. Yuan, X.G., Yu, K.T., *Review of Mass-Transfer Correlations for Packed Columns*, Ind. Eng. Chem. Res. **44** (2005), p. 8715–8729.
33. Onda, K., Takeuchi, H., Okumoto, Y., *Mass Transfer Coefficients between Gas and Liquid Phases in Packed Columns*, J. Chem. Eng. Jpn. **1** (1968), p. 56–62.
34. Kolev, N., *Operational Parameters of Randomly Packed Columns*, Chem. Ing. Tech. **48** (1976), p. 1105.
35. Rocha, J.A., Bravo, J.L., Fair, J.R., *Distillation Columns Containing Structured Packings: A Comprehensive Model for Their Performance. 2. Mass-Transfer Models*, Ind. Eng. Chem. Res. **35** (1996), pp. 1660.
36. Brunazzi, E., Paglianti, A., *Liquid-Film Mass-Transfer Coefficient in a Column Equipped with Structured Packings*, Ind. Eng. Chem. Res. **36** (1997), pp. 3792.
37. Stichlmair, J., Stemmer, A., *Influence of Maldistribution on Mass Transfer in Packed Columns*, I. Chem. E. Symp. Series **104** (1987) 2, B213–B224.

38. Darakchiev, R., Petrova, T., Darakchiev, S., *Gas distribution in columns with packing Raschig Super-Ring*, Chemical Engineering and Processing **44** (2005), p. 827–833.
39. Darakchiev, R., Petrova, T., Darakchiev, S., *Gas distribution in packed-bed columns with IMTP-ring and RALU-flow*, Chemical and Biochemical Engineering Quarterly **19** (2005), p. 147–152.
40. Kister, H., *Distillation Troubleshooting*, New York, John Wiley & Sons, 2006.
41. Thiele, R., Brettschneider, O., Repke, J.-U., Thielert, H., Wozny, G., *Experimental Investigations of Foaming in a Packed Tower for Sour Water Stripping*, Ind. Eng. Chem. Res. **42** (2003), p. 1426–1432.
42. Eckert, F., Klamt, A., *Fast solvent screening via quantum chemistry: COSMO-RS approach*, AIChE J. **48** (2004), p. 369–385.
43. Son, S.J., Choi, H. W., Choi, D.K., Lee, S.D., Kim, H.S., Kim, S.W., *Selective Absorption of Isoprene from C5 Mixtures by δ -Complexation with Cu(I)*, Ind. Eng. Chem. Res. **44** (2005), p. 4717–4720.
44. Luckas, M., Krissmann, J., *Thermodynamik der Elektrolytlösungen – Thermodynamics of electrolyte systems*, Springer-Verlag, Berlin, 2001.
45. Eigen, M., *Protonenübertragung, Säure-Base-Katalyse und enzymatische Hydrolyse. Teil I: Elementarvorgänge – Proton transfer, acid-base catalysis and enzymatical hydrolysis. Part I: Elementary processes*, Angewandte Chemie **75** (1963), p. 489–508.
46. Haubrock, J., Hogendoorn, Versteeg, G.F., *The Applicability of Activities in kinetic expressions: a more fundamental approach to represent kinetics of the System CO₂-OH in terms of activities*, Int.l J. Chem. Reactor Eng. (2005), article A40.
47. Austgen, D.M., Rochelle, G.T., Peng, X., Chen, C.C., *Model of Vapor-Liquid Equilibria for Aqueous Acid Gas-Alkanolamine Systems Using the Electrolyte-NRTL Equation*, Ind. Eng. Chem. Res. **28** (1989) p. 1060–1073.
48. Wesselingh, J.A., Krishna, R., *Mass Transfer in Multicomponent Mixtures*, Delft, Delft University Press, 2000.
49. Cussler, E., *Diffusion, mass transfer in fluid systems - 2nd ed.*, Cambridge University Press, Cambridge, 1997.
50. Shilkin, A., Kenig, E.Y., *A new approach to fluid separation modelling in the columns equipped with structured packings*, Chem. Eng. Journ. **110** (2005) p. 87–100.
51. Asprión, N., *Nonequilibrium Rate-Based Simulation of Reactive Systems: Simulation Model, Heat Transfer, and Influence of Film Discretization*, Ind. Eng. Chem. Res. **45** (2006), p. 2054–2069.
52. Górák, A., *Reactive Separations: Simulation and Experimental Verification*, Camure-5 & ISMR-4 Portorose, Slovenien (2005).
53. Faber, R., Li, P., Wozny, G., *Sequential Parameter Estimation for Large-Scale Systems with Multiple Data Sets. I: Computational Framework*, Ind. Eng. Chem. Res. **42** (2003), p. 5850 – 5860.
54. Faber, R., Li, P., Wozny, G., *Sequential Parameter Estimation for Large-Scale Systems with Multiple Data Sets. 2. Application to an Industrial Coke-Oven-Gas Purification Process*, Industrial & Engineering Chemistry Research **43** (2004), p. 4350–4362.
55. SRI-PEP-Report 180A, CO₂-Capture, SRI-Consulting 2004.

56. <http://www.co2castor.com/>.
57. Authony, J.L., Maginn, E.J., Brennecke, J.F., *Gas Solubilities in 1-n-Butyl-3-methylimidazolium Hexafluorophosphate*, in Rogers, R.D., Seddon, K.R. (eds.), *Ionic Liquids – Industrial Applications for Green Chemistry*, ACS Symposium Series 818, Oxford U. Press (2003), p. 260–269.
58. Ausner, I., Hoffmann, A., Repke, J.-U., Wozny, G., *Multiphase film flow investigations on inclined plates*, 3rd International Berlin Workshop on Transport Phenomena with Moving Boundaries (IBW3), 6th-7th October 2005, Berlin – Germany.
59. Ataki, A., Bart, H.-J., *Experimental and CFD Simulation Study for the Wetting of a Structured Packing Element with Liquids*, Chem. Eng. Tech. **29** (2006), p. 336–347.
60. Cullinane, J.T., Rochelle, G.T., *Thermodynamics of aqueous potassium carbonate, piperazine, and carbon dioxide*, *Fluid Phase Equilibria* **227** (2005), p. 197–213.
61. Albert, M., Hasse, H., Kuhnert, C., Maurer, G., *New experimental results for the vapor-liquid equilibrium of the binary system (trioxane + water) and the ternary system (formaldehyde + trioxane + water)*, J. Chem. Eng. Data **50** (2005) 1218–1223.