

CO₂ REMOVAL BY ABSORPTION, CHALLENGES IN MODELLING

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Abstract. The traditional method for large scale CO₂ removal is by absorption in a mixture of an amine and water. MEA (monoethanol amine) is the most actual amine for CO₂ removal at atmospheric conditions. The tasks of modelling this process can be divided in detailed description of absorption and reaction kinetics, gas/liquid equilibrium, gas and liquid flows, pressure drop, energy consumption, mechanical equipment dimensioning and economical optimization of the process. Process simulation tools containing models for most of these tasks are commercially available. A process model in the program Aspen HYSYS is used as an example. Other process models have been made with e.g. Fortran code and Matlab. Calculation convergence of the models is important, especially the column convergence is critical. For some simplified conditions, e.g. by using MEA under traditional conditions, calculation of stage efficiencies can give a satisfactory description of the absorption process. Especially when using mixtures of amines, a more rigorous description of the interactions between mass transfer and reaction kinetics is necessary. CFD (Computational Fluid Mechanics) is an efficient tool for calculating flow conditions, pressure drop and temperature profiles, especially for one fluid phase. An unsolved problem when using CFD for gas/liquid processes, is the description of the gas/liquid interface area, and especially combined with absorption. A major challenge is the combination of models. An improvement in one specific model must be available to other tools to be utilized.

1 Introduction

CO₂ has been removed from industrial streams since about 1930. The most important removal processes have been from natural gas and in the production of synthesis gas for ammonia and methanol production. The main process is absorption in a mixture of an amine and water. Other solvents like carbonate salt solutions have also been used. An overview over processes can be found in Kohl and Nielsen, [31].

CO₂ removal from exhaust gases has got much interest due to the environmental need for reducing CO₂ emissions to the atmosphere. Many processes for removal of CO₂ from power plant processes have been suggested. The emphasis is here put on post combustion absorption in an amine based solvent. This is the most actual method for gas based power plants for the nearest future. Absorption is traditionally performed in a column with plates, random packing or structured packing. CO₂ containing gas flows upwards and the absorption liquid flows downwards. The absorbed CO₂ is regenerated in a desorption column, and the solvent is recirculated to the absorption column. A removal process consisting of absorption, desorption, heat exchangers and auxiliary equipment is shown in Figure 1.

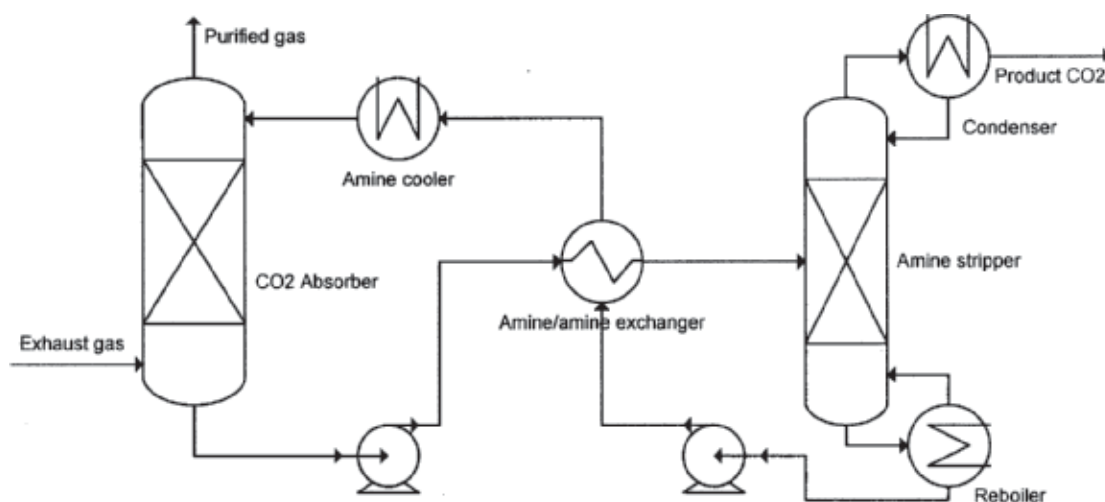
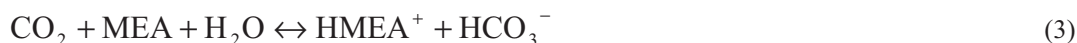
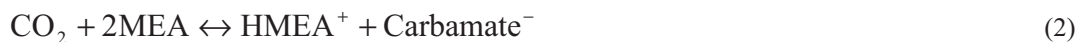


Figure 1. A general CO₂ absorption and desorption process

The absorption of CO₂ in an amine solution like MEA (monoethanol amine, H₂NC₂H₄OH) can be described by the following equations. Equation (1) describes the transfer of CO₂ from gas to liquid, and equation (2) describes the reaction to a protonated amine ion and a carbamate ion. Bicarbonate formation according to equation (3) is also occurring. In the case of other amines than MEA, a reaction equivalent to equation (3) can be more important than reaction (2).



In CO₂ absorption and desorption, the modelling challenges can be divided into the following tasks:

- Absorption and reaction kinetics
- Gas/liquid equilibrium
- Gas and liquid flows
- Pressure drop
- Heat and energy consumption
- Mechanical equipment dimensioning
- Cost estimation and economical optimization

Calculation methods for most of these tasks have been available for a long time. Danckwerts and Sharma, [16], wrote a review as early as in 1966. When computers were introduced for chemical engineering calculations, computer programs were made to perform these calculations.

Commercial process simulation programs have models available to calculate specifically on this system. Examples of such programs are Aspen HYSYS, Aspen Plus, Pro/II and ProMax. These programs have built-in models especially for vapour/liquid equilibrium and column solving. Some of them also have kinetic models available. Most of the tasks in the list above can be handled in a process simulation program.

CFD (Computational Fluid Dynamics) modelling can be used to calculate the flow phenomena in absorption and desorption columns. This can then be used to calculate liquid hold-up, pressure drop and capacity. Fluent and CFX are examples of commercial CFD programs. An optimistic aim for CFD modelling of absorption and desorption is to contribute to a complete, detailed and quantitative description of the absorption/desorption process.

The models for solving specific tasks of the CO₂ absorption process differ in accuracy, complexity and robustness. The main purpose of this paper is to pinpoint areas where further modelling can lead to important improvements. One main challenge is how to combine different models in existing tools.

2 Modelling of CO₂ removal using process simulation tools

2.1 Use of process simulation programs for absorption and desorption

Process simulation programs as Aspen Hysys, Aspen Plus, Pro/II and ProMax have been used to calculate the absorption and stripping column in CO₂ removal. The main advantage of these process simulation tools is that a large number of models for vapour/liquid equilibrium and unit operations are available.

Simulation of CO₂ removal from flue gas in a MEA/water system has been performed by Desideri and Paolucci, [21], and by Alie et al., [2]. Both have used the simulation program Aspen Plus with the MEA property insert, which is based on the Chen/Austgen electrolyte-NRTL equilibrium model, [13][6]. Desideri and Paolucci used a specified number of theoretical stages in the absorption and stripping column. Tobiesen et al., [53], and Aroonwilas et al., [4] have made Fortran programs to perform similar calculations. At Telemark University College, Matlab has also been used to model CO₂ absorption and desorption processes.

An important feature of the commercial process simulation programs is the available convergence methods for the process flowsheet. For flowsheet convergence, the programs can make use of recycle blocks, nested or simultaneous calculation sequences and different acceleration methods like Wegstein or dominant eigenvalue methods. Convergence of the columns is especially important, and was the core technology in the early process simulation programs. Column solver methods available in the Aspen HYSYS program are:

- Modified Hysim Inside-Out
- Newton Raphson Inside-Out
- Sparse Continuation Solver
- Simultaneous Correction
- OLI Solver
- Fixed or adaptive damping factor

Because the CO₂/amine/water system is highly non-ideal, the need for efficient and robust column solvers is of major importance.

Figure 2 shows an Aspen HYSYS model from Øi, [59].

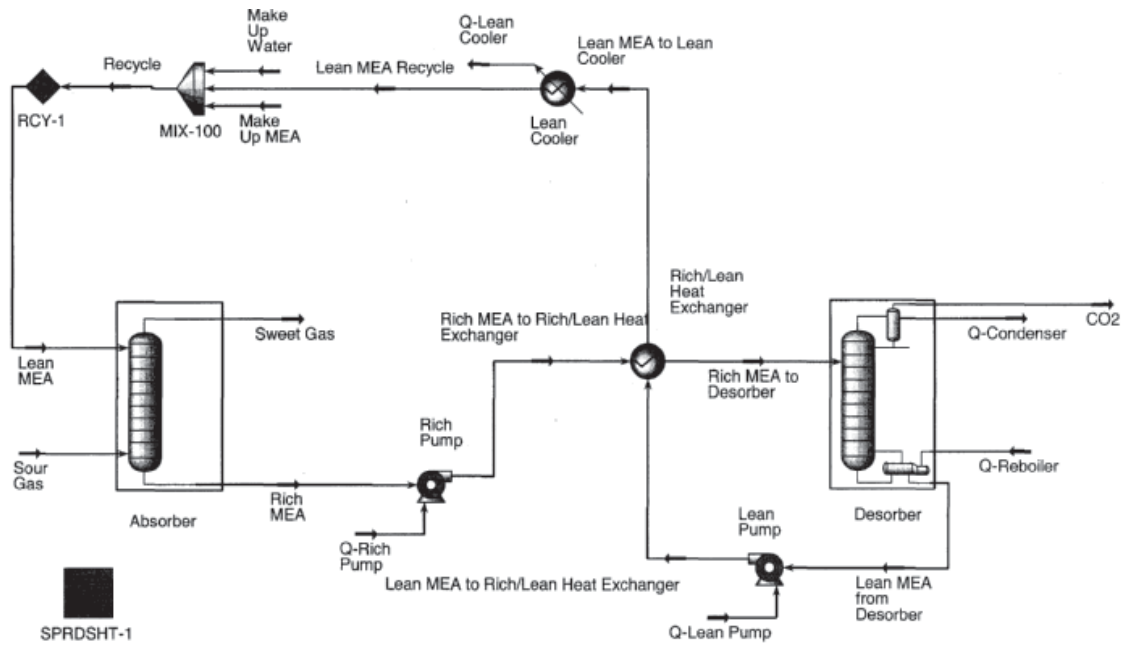


Figure 2. Aspen Hysys model of a CO₂ removal process (from Øi, [59])

Figure 3 shows the calculated CO₂ removal efficiency and heat consumption when the amine circulation rate is varied in the Aspen HYSYS model. 10 stages with 0.25 Murphree efficiency were used, and the Aspen HYSYS version of the Kent Eisenberg equilibrium model, [29], was used. The calculation shows a minimum heat consumption at a certain circulation rate.

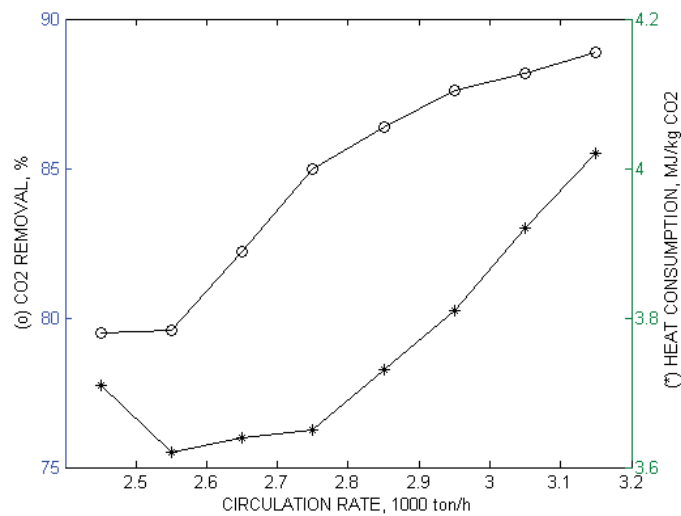


Figure 3. CO₂ removal grade and heat consumption as a function of amine circulation rate (from Øi, [59])

Most of the process simulation calculations of CO₂ removal from atmospheric exhaust in the open literature are simplified processes at steady state. One challenge is to include the simulation of a water wash section above the amine absorption. Another challenge is to simulate the process at dynamic conditions.

2.2 Rigorous simulation in process simulation programs

Most of the column models in commercial process simulation programs are based on equilibrium stages or stages with a stage efficiency (an approach to equilibrium). More rigorous column models, which include kinetic expressions, are available. Some of these are able to calculate the concentration profiles of all the diffusing components through the liquid film near the gas/liquid surface. This kind of approach is based on the solving of the differential equations describing the diffusion and chemical kinetics in the liquid film. An approach for rigorous modelling with resulting differential equations is presented in chapter 5.

The program Aspen Plus has possibilities to include such calculations. Al-Baghli et al., [1], has made a rate-based model for the design of gas absorbers for the removal of CO₂ and H₂S using aqueous solutions of MEA and DEA. Freguia and Rochelle, [23], used a Fortran subroutine integrated in Aspen Plus to perform a rate-based calculation of CO₂ absorption into MEA. Kucka et al., [32], have used the Aspen Custom Modeler tool in Aspen Plus to model the liquid film by dividing the film into a number of segments.

3 Chemistry of CO₂ removal with amines

3.1 Reaction kinetics for MEA (and other primary and secondary amines) with CO₂

The detailed reaction kinetics for the reaction between even simple amines and CO₂ are quite complicated. However, for the simple amines, e.g. MEA, the kinetics are now regarded as well-known. Overviews can be found in the review articles by Danckwerts and Sharma, [16], and Versteeg et al., [57]. The mass transfer kinetics of MEA absorption in laboratory absorption equipment under controlled conditions can be explained by traditional mass transfer models, [57].

It has been known for a long time that the main reaction described by equation (2) of primary amines like MEA and CO₂ is a 2nd order reaction under normal conditions:

$$(-r_{\text{CO}_2}) = k \cdot C_{\text{CO}_2} \cdot C_{\text{MEA}} \quad (4)$$

In equation (4), $(-r_{\text{CO}_2})$ is the reaction rate (pr. volume), k is the reaction rate constant, and C_{CO_2} and C_{MEA} are the liquid concentrations of CO₂ and MEA in molecular form. Versteeg et al., [57], give temperature dependent values for the reaction rate constant. Caplow, [11], gave a detailed description of the reaction kinetics, introducing the zwitterion mechanism. This has later been generally accepted as the actual mechanism, [57]. The mechanism is similar for simple primary and secondary amines.

3.2 Kinetics for MDEA (and other tertiary amines) and sterically hindered amines with CO₂

MDEA (N-methyldiethanolamine) is a tertiary amine and does not react with CO₂ according to the carbamate formation reaction. In a tertiary amine, the central nitrogen atom is connected to three organic groups, and this makes the amine less reactive. The absorption of CO₂ is in this case rather followed by an acid/base reaction as in equation (3). The reaction is described in Blauwhoff et al., [8], and Rinker et al., [46]. The mechanism is similar for many of the tertiary amines.

Not all primary and secondary amines react with CO₂ to form carbamate. Due to bulky groups close to the nitrogen atom in the amine group, some primary and secondary (alkanol) amines do not react with CO₂. These are called sterically hindered amines. One example is AMP (2-amino-2-methyl-1-propanol). The sterically hindered amines perform in contact with water and CO₂ in many ways like tertiary amines. They are less reactive and have a low desorption energy. The idea of using sterically hindered amines is described by Sartori and Savage, [49]. The solvent KS-1 (which is based on sterically hindered amines) is used by Mitsubishi Heavy Industries in their commercial process for CO₂ removal from flue gases. The KS-1 process is claimed to have much lower energy consumption than an MEA based process, [38].

3.3 Reaction kinetics of mixtures of amines with CO₂

Using mixtures of amines for CO₂ removal is first described by Chakrawarty et al., [12]. One idea is to combine the reactivity of one amine (e.g. MEA) with the low desorption energy of another amine (e.g. MDEA). The reaction kinetics can normally be described by the kinetics of the single amines. The combination of reaction kinetics with mass transfer will however be much more complicated in the case of mixed amines. The challenge of combining reaction kinetics, diffusion and equilibrium is treated in more detail in chapter 5.

4 Equilibrium description of mixtures of water, CO₂ and amines

4.1 General equilibrium models

The equilibrium conditions are of course important to describe the reaction and absorption in mixtures of water, amines and dissolved CO₂. The water, CO₂, bicarbonate and carbonate system is a widely studied and well described system, [16]. Amine systems may be described by the connection between partial pressures of CO₂ above a specified solution at equilibrium. In equation (5), the total CO₂ is the sum of CO₂ as molecular CO₂, carbonate ion, bicarbonate ion and carbamate ion:

$$p_{\text{CO}_2} = f(C_{\text{CO}_2, \text{TOT}}) \quad (5)$$

Kent and Eisenberg, [29], gave a description based on known equilibrium constants (Henry's constants) for the physical solution of CO₂ and the equilibrium constants for the water, carbonate and bicarbonate system. Then the equilibrium constants for the amine/carbamate equilibrium and the amine/protonated amine were fitted to experimental data. A modified version of this model is used by the process simulation program Aspen HYSYS.

4.2 Activity based equations/electrolyte models

A more detailed description can be done by expressing the activities (or chemical potentials) of all the ionic and molecular components as a function of liquid concentration and temperature. The Chen/Austgen model, [6], for simple amine systems, is based on the general electrolyte-NRTL model of Chen and Evans, [13]. This model is available in the simulation program Aspen Plus. This is a rigorous model, and has a high complexity and accuracy. Liu et al., [36], have adjusted the parameters for the MEA/water system from the Chen/Austgen model to make the heat of vaporization to be more accurate. Li Mather, [35], is a similar model available in Aspen HYSYS, using an electrolyte-Margules model. Kaewsichan et al., [28], gave an overview of equilibrium models in amine systems, and also presented a model based on an electrolyte-UNIQUAC model.

The accuracy of models for amine mixtures is often limited by the accuracy in the available equilibrium data. Equilibrium models often have a trade-off between a complex model with high accuracy and a simpler model with less accuracy, which is often easier to converge. There is a challenge to find equilibrium models that are simple, accurate and easy to converge.

4.3 Gas phase non-idealities

Under atmospheric conditions, gas non-idealities are normally negligible, and the ideal gas law is sufficient to describe the gas phase. An equation of state like Peng Robinson, [43], can also be used to take care of the minor gas non-idealities.

5 Models for absorption followed by chemical reaction

5.1 Process description

The total CO₂ removal process consists of absorption, desorption, heat exchange and auxiliary equipment. A schematic overview of the concentration profiles at a certain column height in the absorber is given in Figure 4.

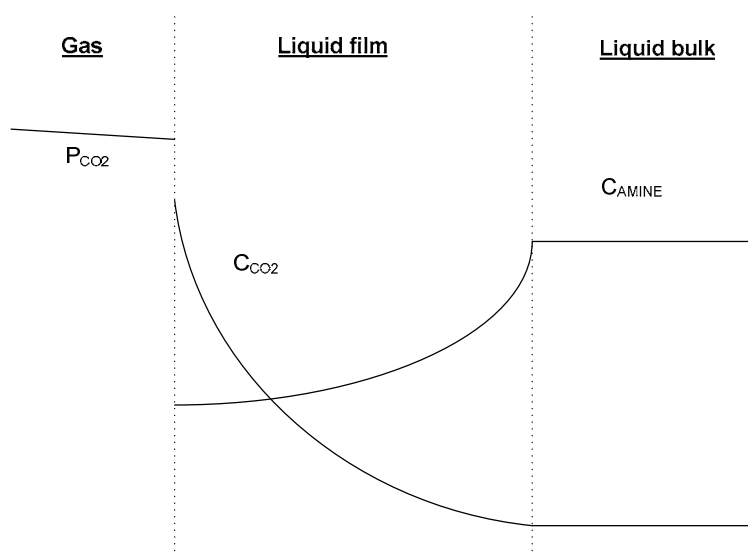


Figure 4. Concentration profiles in liquid film with absorption and chemical reaction

CO₂ is transported from the bulk gas to the gas/liquid interface. Gas/liquid equilibrium is assumed at the interface. After absorption, CO₂ can either react directly in the liquid close to the interface, or it can be transported into the bulk liquid. In the bulk liquid, CO₂ or other species can react further, limited either by equilibrium or chemical kinetics.

5.2 Mass transfer models

Popular models are the two-film theory by Lewis and Whitman, [34], and the penetration model or surface renewal model developed by Higbie, [27], and Danckwerts, [15]. The two-film model is based on the concept of thin gas and liquid films with a constant thickness, and transport rate based on molecular diffusion. This model results in mass transfer proportional to diffusivity. The penetration and the surface renewal models are regarded to be more realistic models for the liquid film. They are based on the idea of continuous transport of volume elements from the interface to the liquid bulk. The difference is that the penetration model assumes a constant contact time for the elements, while the surface renewal model assumes a distribution. Both of these models result in mass transfer proportional to the square root of the diffusivity. Boundary layer theory has also been used to calculate mass transfer from basic laws of fluid dynamics, mainly for simple geometries.

A mass transfer number for the liquid film, k_L , can be defined by equation (6). The gas/liquid interface area per volume has symbol a , and the interface and bulk positions are shown in Figure 4.

$$(-r_{CO_2}) = k_L \cdot a \cdot (C_{CO_2,INTERFACE} - C_{CO_2,BULK}) \quad (6)$$

The gas transport of CO₂ to the interface is normally not rate-limiting, [16]. The gas side mass transfer can often be neglected or it can be described by a simple empirical correlation.

5.3 Simplified models for absorption followed by chemical reaction

This kind of processes has been treated by e.g. Van Krevelen and Hofstijzer, [56]. They use an enhancement factor which is the ratio of the actual absorption rate divided by the absorption rate by purely mass transfer based absorption:

$$Enh = k_L / k_{L,WITHOUT_REACTION} \quad (7)$$

In the case where the amine concentration can be assumed to be constant through the liquid film, the pseudo first order conditions occur. In that case, the rate expression becomes

$$(-r_{CO_2}) = C_{CO_2,INTERFACE} \cdot a \cdot \sqrt{k \cdot D_{CO_2} \cdot C_{MEA}} \quad (8)$$

D_{CO_2} is the molecular diffusivity of CO₂ in the liquid. In case of this rate expressions, it is possible to calculate a Murphree efficiency for a tray or a packed section at the given flow conditions. Murphree efficiency for a tray or a packing section can be defined as shown in Figure 5.

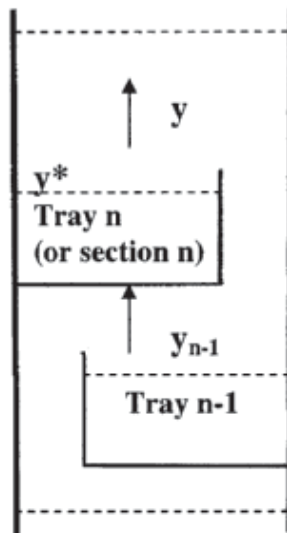


Figure 5. Definition of Murphree efficiency, $E_{MURPHREE} = (y - y_{n-1}) / (y^* - y_{n-1})$, where y is mole fraction (CO₂) in the gas phase leaving tray (or section) n , and y^* is in equilibrium with the liquid on tray (or section) n .

Aspen HYSYS has a model for calculating Murphree efficiencies in plate columns based on a pseudo first order expression. This model is based on the work by Tomkej et al., [54].

There has been much work on calculation methods for enhancement factors, and evaluations of the conditions for when to use approximate expressions. DeCoursey, [18], developed an explicit approximate expression for the case of absorption followed by a second order irreversible reaction. Later, this was extended to reversible reactions, [19], like CO₂ absorption in an amine solution. For the case of CO₂ absorption into MEA solutions at atmospheric conditions, it is not clear whether the pseudo first order approximation is valid under all conditions.

5.4 Models for CO₂ absorption into mixed amines

In the case of mixed amines, the combined reaction and mass transfer kinetics might be quite complicated. One model is the shuttle mechanism from Astarita et al., [5], which tries to model absorption into a mixture of a reactive amine (e.g. MEA) in small amounts and a less reactive amine (e.g. MDEA) in larger amounts. The idea is that CO₂ first reacts with MEA in the film close to the surface and is transferred into the bulk liquid. In the bulk liquid, CO₂ is released from MEA and reacts with MDEA, so that the MEA can be shuttled back to the liquid film. Hagewiesche et al., [26], have modelled absorption into blends of MEA and MDEA. The absorption mechanism was shown to follow the shuttle mechanism proposed by Astarita.

5.5 Rigorous simulation

There have been several attempts to calculate the concentration profiles through the liquid films based on available mass transfer and kinetic models. De Leye and Froment, [20], Al-Baghli et al., [1], and Kucka et al., [32], are examples. Equations (9) and (10) are from DeCoursey, [18], for the case of a second order irreversible reaction between an absorbed component A (e.g. CO₂) and a liquid component B (e.g. MEA). Mass transfer is based on a surface renewal model, [15]. The equations represent a time-dependent material balance for CO₂ and MEA.

$$D_A \frac{\partial^2 C_A}{\partial x^2} - \frac{\partial C_A}{\partial t} - k \cdot C_A \cdot C_B = 0 \quad (9)$$

$$D_B \frac{\partial^2 C_B}{\partial x^2} - \frac{\partial C_B}{\partial t} - 2 \cdot k \cdot C_A \cdot C_B = 0 \quad (10)$$

The boundary conditions are that for $t = 0$ and $x > 0$ and for $t > 0$ and $x = \infty$, C_A and C_B are equal to the bulk concentrations, and for $t > 0$ and $x = 0$, C_A is the interface concentration and $\partial C_B / \partial x = 0$. The solution of these equations gives the concentration profiles through the liquid film. The accuracy is of course limited to the accuracy of the data used and the assumptions taken.

Reversible reactions add complexity especially by making equilibrium calculations necessary. It is a challenge to combine such complex models with accurate gas/liquid equilibrium models and with optimizing tools.

6 Pressure drop, interfacial area, mass transfer, gas and liquid distribution in columns

6.1 Traditional design methods for random and structured packing

Design of packed columns is generally based on empirical correlations for liquid hold-up, pressure drop, gas/liquid interface area and mass transfer. The resistance to absorption is often divided into gas side and liquid side resistance. These methods are described in e.g. Kohl and Nielsen, [31].



Figure 6. Absorption column with structured packing and internals (from www.sulzerchemtech)

Structured packed columns will probably be the primary choice in case of a large scale CO₂ removal process from atmospheric exhaust. Structured packing is very effective and gives a very low pressure drop. Plate columns will probably not be practical for columns with large diameters (more than 15 m). Random packing will have lower investment than structured packing, and might be an economical alternative.

To calculate flooding (capacity) and pressure drop in random packing, empirical charts or equations as in Sherwood et al., [50], and Eckert, [22], are traditional. They are based on correlations from dimensional analysis which are fitted to performance data. The empirical Onda, [42], and Bravo and Fair, [9], correlations are standard methods to calculate mass transfer in random packing. They have different correlations for calculating the gas side and liquid side mass transfer.

Design methods for structured packing are based on the same type of correlations as for random packing, e.g. Rocha et al., [47][48], Billet and Schultes, [7], and De Brito et al., [17]. Most of these methods are limited to the flow regime below the loading point. Droplet formation (which occurs above the loading point) and its influence on interface area and mass transfer is difficult to predict. Review articles for mass transfer in structured packing are written by Brunazzi et al., [10], Valluri et al., [55] and Wang, [58].

The semi-empirical calculation methods for mass transfer are traditionally based on the following calculation steps, [10]:

- liquid hold-up
- gas/liquid interface area
- mass transfer coefficient for gas side
- mass transfer coefficient for liquid side

The scatter between the estimation methods is especially large for the calculated effective interface area. This is an important parameter because the absorption rate is normally proportional to this entity. The potential in improving the estimation methods for the effective interfacial area is large.

6.2 Non-empirical modelling of absorption in structured packing

In their review, Valluri et al., [55], have one section for non-empirical modelling of the design parameters. They refer to Shetti and Cerro, [51], as the first complete model of this kind. One of their aims was to estimate design parameters in structured packing without any adjustable parameters. An idea is to establish the equations for the fluid flow pattern and mass transfer through the films, and then solve the equations to achieve the design parameters for heat and mass transfer. The equations to be solved are typically a set of algebraic and differential equations. Another early presentation of a mechanistic model for mass transfer in structured packing is by Nawrocki et al., [39].

At Delft University, they have studied models for columns with structured packing. Olujić et al., [40][41], distinguish between modelling at a geometric macro level (channel dimensions) and micro level (film and surface texture dimensions). Models for film flow, gas side mass transfer and liquid side mass transfer are suggested. Their prediction method does not require packing specific constants. It is stated that a reliable prediction of the effective surface area is the key to the success of a prediction method.

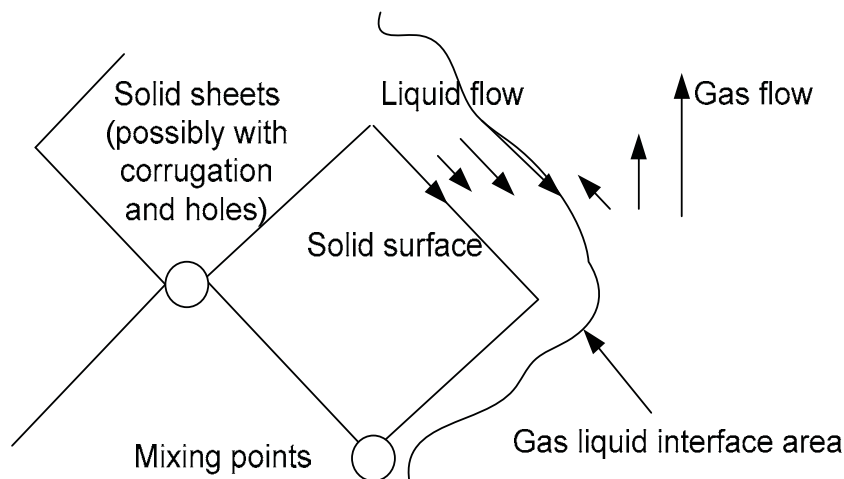


Figure 7. Modelling flow in structured packing

Shilkin and Kenig, [52], from the University of Dortmund, have made a model for structured packing columns giving a set of differential equations. The concept is based on two phases which are totally mixed at regular intervals. The equations are solved numerically. The results are the velocity profiles, the concentration profiles and the temperature profiles through the column.

Iliuta and Larachi, [24], at the Laval University in Quebec, have made a mechanistic model for structured packing columns, calculating pressure drop, liquid hold-up, and wetted area. The model is based on a double-slit mechanistic approach. In a channel, the liquid film flows downwards in one slit, and the gas upwards in another slit. The resulting model gives three coupled algebraic equations to be solved. The model requires no adjustable parameters. Their work has been developed further into CFD modelling.

6.3 CFD modelling of separation columns with structured packing

A CFD (Computational Fluid Dynamics) program divides a fluid flow geometry into a grid of small volumes, and then solves the fundamental equations for mass, energy and momentum conservation for each volume. Modelling of turbulence is an important part of a CFD program. Equations for chemical kinetics and equilibrium can be included. Because a CFD simulation consists of an enormous amount of equations, CFD simulation consumes much computer space and time. Fluent and CFX are commercial CFD programs.

Valluri et al., [55], state that very few publications have been presented in the field of using CFD for structured packings. Most of them are about catalytic reactors. However, mass transfer both in gas and liquid in structured packing was also covered. Klöcker et al., [30], have tried to integrate CFD and process simulation for reactive distillation in structured packing.

Petre et al., [44], from the Laval group in Quebec, calculate dry pressure drop in structured packing for large scale absorption with 3-D CFD. The CFD program Fluent was used with the RNG k - ϵ turbulence model. Larachi et al., [33] and Iliuta et al., [25], calculated the pressure drop for two-phase flow using CFD. The types of structured packing studied were MellaPak, GemPak, Sulzer BX and Montz-Pak.

Raynal et al., [45], wrote an article called "Liquid Holdup and Pressure Drop Determination in Structured Packing with CFD Simulations". Dry pressure drop was calculated in 3-D CFD using Fluent with the k - ϵ turbulence model and the RNG k - ϵ model. Hold-up was calculated using a 2-D laminar model. The calculations were compared with experiments from an air/water system.

CFD modelling of packed columns may be used for the calculation of total pressure drop, and for the modelling of different mechanisms resulting in pressure drop. This may be used for predicting performance and for optimizing operation conditions. The information gained can also be used for improving the packing. CFD is obviously suitable for simulating flow distribution and calculating pressure drop in auxiliary column equipment like liquid and gas distributors.

There seems to be no attempts in the literature to simulate an overall model for an absorption process with CFD. A major challenge is how to model the gas/liquid interface.

7 Combination of models

7.1 Process simulation programs and Cape-Open

Process simulation programs are specialized in combining many types of models like equilibrium models and models for columns and other unit operations. The objective of the projects Cape-Open from 1997 to 1999 and Global Cape-Open from 1999 to 2001 was to define standard interfaces between the major components of a process simulation program. The contributors to these projects were mainly vendors of major process simulator programs and major chemical companies. One result of these programs was a set of interface standards between models and programs. The organization Cape-Open Laboratory Network (www.colan.org) is now maintaining the Cape-Open interface standards.

7.2 Cost estimation of CO₂ removal from flue gas with amines

Most cost estimation work is made within commercial companies and is not published. Mariz, [37], has given some background for cost estimation of an Econamine process (MEA based process from Fluor Daniel) for CO₂ removal from flue gas. In the CO₂ Capture Project (CPP), Choi et al., [14], performed a study with title: "CO₂ Removal from Power Plant Flue Gas – Cost Efficient Design and Integration Study".

In several student projects at Telemark University College, Aspen HYSYS has been used for process simulation of a CO₂ removal process followed by mechanical equipment dimensioning, cost estimation of the equipment and the entire plant, and energy cost as the most important operation cost. Parameter variation makes it possible to find the most economical temperatures, circulation rates and column heights, [3].

If the aim is to cost optimize a CO₂ removal process, it is an obvious challenge to combine process calculation tools with cost estimation tools.

8 Summary

There is serious scatter in different estimation methods for mass transfer in structured packing. The scatter is especially large for the different prediction methods for effective gas/liquid area.

There is still a challenge to search for improved vapour/liquid equilibrium models. There is need for improved accuracy, and the models should be easy to converge and to use in combination with kinetic models.

CFD (Computational Fluid Mechanics) is an efficient tool for calculating flow conditions, pressure drop and temperature profiles, especially for one fluid phase. CFD is obviously suitable for simulating flow distribution and for calculating pressure drop in auxiliary equipment like liquid and gas distributors. It is a challenge to make use of CFD for gas/liquid processes. An unsolved problem is the description of the gas/liquid interface area, and especially combined with absorption.

There is a traditional trade-off between complex and accurate models compared to simpler and more robust models. Under some conditions, a non-rigorous model is accurately enough. There is a challenge to find out under which conditions a simplified method is satisfactory.

A major challenge is the combination of models. In the case of process simulation programs, Cape-Open is an example of a standard interface for introducing a new model into an existing program package. An improvement in one specific model must be available to other tools to be utilized.

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