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Review

Simulation based improvement techniques for acid gases sweetening by chemical absorption: A review

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Abbreviations:
VLE, vapor–liquid equilibrium
FEED, front-end-engineering design
CO_2, carbon dioxide
H_2S, hydrogen sulphide
NH3, ammonia
MEA, monoethanolamine
DEA, diethanolamine
TEA, triethanolamine
MDEA, methyldiethanolamine
PZ, piperazine
QSAR, quantitative structure–activity relationships
CFD, computational fluid dynamics
AMP, amino-methyl propoanol
HETP, height equivalent to theoretical plates
SVM, support vector machine
COSMO-RS, conductor like screening model for real solvents
OPLS, optimized potentials for liquid simulations
DFT, density function theory

ABSTRACT

There are various theoretical approaches to design, improve and optimize CO_2 capture from natural gas sweetening units through chemical absorption. The aim objective of the present review is to explore various theoretical approaches developed by process and research engineers to improve the design and operation of chemical absorption sweetening units. Therefore, this review is divided into four parts. The first part discusses the basic thermodynamic and kinetic principles that represent the main core of any process simulation research. The second part is devoted to designing and improving the main columns i.e., the absorber and the stripper. The third part reviews previous research aiming at designing or optimizing the whole sweetening unit. The last part briefly discusses computational chemistry techniques used by chemists and chemical engineers to design novel solvents at the molecular level. The review ends with conclusions and a brief discussion about future perspectives to improve the process and areas that require further research effort.

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1. Introduction

Natural gas (NG) is one of the major types of 'fossil fuels' which could be regarded as a primary energy source for domestic/commercial and as a 'fuel' for power plants to generate electricity. The burning of natural gas further leads to the addition of more CO_2 (a greenhouse gas) emissions to the atmosphere which creates serious environmental concern i.e., global warming. The most widely used technology for CO_2 removal from NG is the chemical absorption with solvents such as alkanolamines. The validation of lab scale experimental solubility data requires a setup of pilot prior to its scale up at industrial scale. To avoid a tedious and lengthy process the simulation techniques are needed in order to improve the reliability and to increase productivity. There are various simulation software tools that can be widely in a power plant integrated with a CO_2 capture plant. However, the potential of software to model and simulate the process correctly, and to generate accurate and reliable results, is of utmost importance.

Front-end-engineering design (FEED) is an essential process design step that any chemical engineering project has to undergo. The FEED depends on simulation and design software to perform material and energy balances, 2D and 3D models, process layout, equipment design and other parameters (Liang, 2011). The computer based simulation techniques are also useful tools for screening alternative design configurations of physical, chemical, and biological processes (Ochieng, 2012). The simulation software plays a key role in studying process alternatives, conducting technical and economic feasibility studies, interpreting pilot-plant data (Solbraa, 2002). The computer-aided process simulation tools are also helpful in determining the optimum operating conditions with a minimum of time, effort, and cost (Sehgal, 2009). Natural gas industry relies heavily on theoretical approaches to design, improve and optimize production and processing units. Several types of software are required for such industry, for instance reservoir simulation, pipeline calculations, modelling of processing units and optimization of operating conditions. During plant commissioning, engineering companies use process simulators to aid in fulfilling their contracts with the gas plant owners. If the performance of the plant is lower than the level specified by the contract at start-up trials, the company has to compensate for such technical gaps (Pellegrini et al., 2011).

The modelling of chemical absorption systems completely relies on comprehensive thermodynamic and kinetic models to accurately represent the composition of each phase at various operating conditions. Based on such models, equilibrium based or rate based models are formulated to simulate the absorber and the distillation towers. Successful representation of the towers allows the simulation to be taken a further step to study the interaction between those towers in the sweetening unit. The modelling software can provide extra tool to evaluate alternative flow sheet configurations, dynamic simulation and economic assessment of the sweetening unit. Moreover, the process simulators that are equipped with thermodynamic and energetic analysis tools could provide more insights about energy conversion and energy destruction through each unit. Nowadays, there is a great interest on relying upon the computational chemistry techniques to design new solvents at the molecular level.

2. Thermodynamic and kinetic models

Thermodynamic models are the backbone of any equipment and process simulation. Before process or equipment simulation, several physical and chemical properties have to be estimated accurately by mathematical models under a wide range of operating conditions for pure and mixed compounds.

2.1. Modelling equilibrium solubility

The most important property to accurately model chemical absorption is the equilibrium solubility of the gaseous solute in the liquid solvent. Accurate estimation of equilibrium solubility is vital for solvent screening, equipment design, alternative process configurations screening and process optimization. A thermodynamic model that can predict equilibrium solubility at different operating conditions of temperature, pressure and compositions of both solvents and solutes is an essential tool for the design engineer. Studying the equilibrium solubility of acid gases in amine solutions is a challenging task. Two types of thermodynamic equilibria have to be accounted for; the chemical equilibrium between the ions and the vapor liquid phase equilibrium. Each of these types are explained in more details in the following sections.

2.1.1. Chemical equilibrium

To study chemical equilibrium, the set of reactions occurring in the liquid phase has to be specified. For instance the main reactions of MEA with CO_2 and H_2S are can be summarized as shown in Table 1 (Kohl and Nielsen, 1997).

As each reaction has equilibrium constant K_j which is defined as the product of the activities of produced molecules or ions divided by that of the reactants. The activity of a molecule or ion is directly proportional to its concentration, with the proportionality constant known as the activity coefficient. However, mathematical representation of activity coefficient is a challenging task and several approximations are used by several groups in the literature.

All models published follow this general mathematical framework while each model uses appropriate simplifications to balance computational effort with simulation accuracy. The mathematical models published in the open literature can be classified into

Table 1
Reactions of MEA with CO_2 and H_2S.

	Reaction	Equation
1.	Water ionization	$H_2O = H^+ + OH^-$
2.	Ionization of dissolved H_2S	$H_2S = H^+ + HS^-$
3.	Hydrolysis and ionization of dissolved CO_2	$CO_2 + H_2O = HCO_3^- + H^+$
4.	Protonation of the primary alkanolamine	$RNH_2 + H^+ = RNH_3^+$
5.	Carbamate formation	$RNH_2 + CO_2 = RNHCOO^- + H^+$

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