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Process Simulations as a Tool in Risk-Based Verification and Qualification of CO_2 Capture Processes

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1. Introduction

The present work presents and discusses a detailed and structured approach for performing un-biased risk-based qualification and verification of CO_2 capture processes by the use of process modelling and simulation.

As a direct consequence of the increasing attention drawn to climate change and CO_2 capture a large variety of different technologies are emerging. However, for many of these proposed technologies the level of maturity is not adequate and there may be significant challenges tied to scale-up and large scale deployment. As a consequence of this, DNV has previously established a recommended practice for qualification of CO_2 capture technologies [1, 2]. In short terms technology qualification involves a confirmation that the proposed technology meets the specified requirements intended for the process. The main steps in the qualification process are given in Figure 1. In the present work the main focus is to develop a simulation platform for amine based CO_2 capture processes and see this is conjunction with DNV's qualification process. The purpose of the development of the simulation platform is to establish CO_2 absorption reference models for further use within DNV's services for scale-up to large-scale CO_2 capture processes, such as qualification and verification. Further, the work briefly addresses the uncertainties tied to simulations of large scale CO_2 capture processes where there are no commercial scale process data for comparison.

2. Risk assessment

A potential showstopper for a world-wide deployment of Carbon Capture and Storage (CCS) are the costs. As a consequence of this, and the large attention drawn to CCS for the last decades, a large variety of different technologies are emerging. A major challenge for technology developers as well as other stakeholders such as operators, governmental bodies, and investors is to assess that the technologies work as intended within acceptable levels of risk. Large scale post-combustion plants are so large and cost-extensive that failure is not an option, thus

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qualification and verification activities becomes necessary in order to ensure acceptable levels of risk. For post-combustion CO_2 capture processes there are many factors that contribute to the overall risk. Some of these are related to the scale-up from a laboratory or pilot scale to a full commercial scale. In these transitions one may encounter challenges such as fluid by-passing, pressure drop; and flue gas impurities causing solvent degradation or equipment fouling or corrosion. Further, on a large scale, the amount of solvent used in the process will be substantially higher. Thus, it will be important to control e.g. amine slippage through the vented flue gas from the absorber top. Assessing risk, both in general and related to scale-up is a complex process, and it is stressed that this work does not aim at giving a comprehensive and detailed assessment of the field, but rather highlight some challenging features, and see them in conjunction with process simulations and the overall DNV qualification process shown in Figure 1.

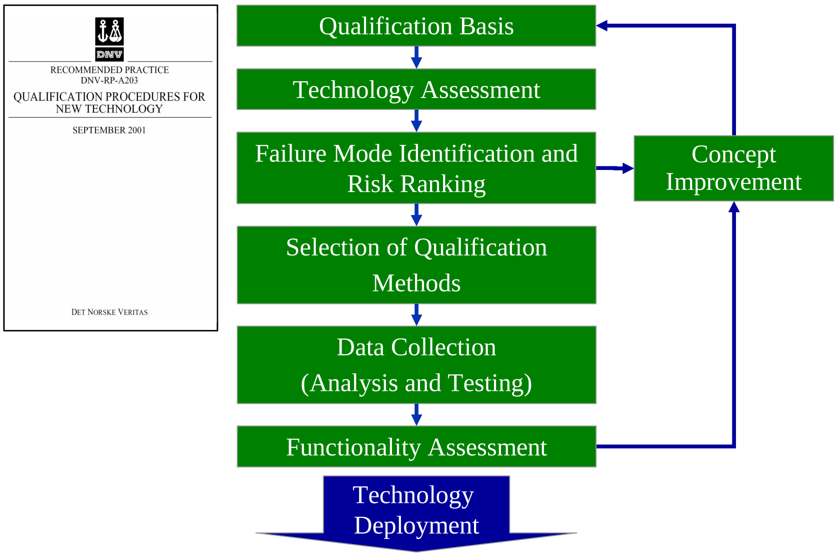

Figure 1: Main steps in the technology qualification process [1]

3. The simulation platform

In the modelling and simulation of CO_2 absorption systems there are two general pathways, namely the equilibrium based approach and the rate-based approach. The former approach is perhaps the most common, but it is also the one that is the least rigorous since it does not explicitly account for mass/heat transfer and chemical reactions at the gas/liquid interface. Instead these models relate the liquid and vapour phase states by assuming physical, chemical and thermal equilibrium between the bulk liquid and vapour phases. The predictability of equilibrium based models can be improved by incorporating tray efficiencies, but when it comes to scale-up the usage of tray efficiencies may be error-prone, since these are based on historical plant data which may not be valid for the new design. For the rate-based approach, the reactions and transport phenomena are accounted for in the contactor model framework. The model equations will thus be more challenging to treat numerically, but since the models in a more direct way accounts for the phenomena occurring in the system, they can be applied to any contactor without relying on plant data such as tray efficiencies. In the present work scale-up issues with respect to these two different modelling strategies will be highlighted.

A mathematical model of the real world – in this case a gas/liquid contactor will never be better than the data provided to the model framework. Rate-based contactor models require sound sub-models for e.g. thermodynamics, kinetics and hydraulics. In terms of verification and validation it is crucial that the user has the possibility of validating these different sub-models/sub-routines against experimental data, and if found necessary, replace or modify them. This is especially important for commercial simulation software where the user has not taken part in the model development. Further, the simulation results can be validated against pilot plant data or commercial scale plant data if available. Sub-models should however not be regressed or tuned to such data, but rather rely solely on describing the physical or chemical phenomena as measured experimentally. Violating this procedure may for example lead to sizing or hydraulic effects being lumped into the kinetics or the thermodynamics, which again may give rise to problems when up-scaling the system at a later stage.

In Figure 2 two different thermodynamic packages are applied in the same absorber model in order to predict the amine partial pressure throughout the column. It is clearly seen that choosing a proper thermodynamic package is of key importance when it comes to addressing the amine partial pressure and thus also the amine slippage from the absorption tower. The amine slippage serves as a good example due to the potential formation of nitrosamines in the atmosphere [3] and thus it constitutes a risk both to the stakeholders and the environment.

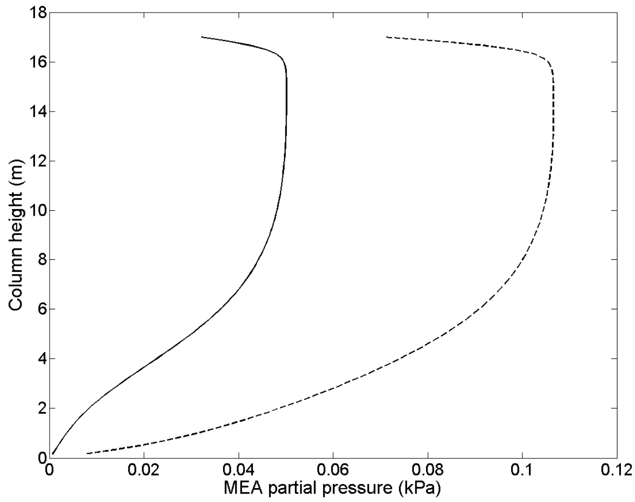

Figure 2: Absorber MEA partial pressure [4]. Solid line: Rigorous model; Dotted line: Simple model

4. Conclusions

In this work a general simulation platform for CO_2 absorption processes is developed seen in conjunction with DNV's services in scaling up CO_2 capture processes, such as qualification and verification. The simulation platform will further be used to assess the impact of the different sub-models on simulator performance, especially with respect to specific scale-up challenges.

References

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