SIMULATION-BASED QUALIFICATION AND VERIFICATION OF CO_2 CAPTURE PROCESSES

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Introduction

This work presents 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. The objective is to provide well-established simulation platforms for independent assessment of CO_2 capture processes, either as part of risk-based qualification [1] and verification services [2], or to be used as part of separate assessments. The specific focus of this work is to establish reference models for independent simulation-based technology assessment within chemical absorption, oxy-fuel combustion, and chemical conversion processes relevant to pre-combustion CO_2 capture, such as hydrocarbon reforming and shift reactors. The use of process modelling and simulation in integrated design of full-scale CO_2 capture systems and the use of such tools for proving that a CO_2 capture process or system work as intended according to specified requirements are discussed.

Methodology

For developing simulation-based qualification or verification, there is a need for a structured approach and to establish validated and verified simulation platforms. DNV has previously presented development of general qualification procedures for CO_2 capture processes [3, 4] and this is thus not shown here. The present work expands upon this recommended practice and constitutes the overall framework for the development of the simulation platforms. Three reference modelling cases are presented: Chemical absorption, oxy-fuel combustion, and pre-combustion capture chemical processes. Simulation and validation results are presented and discussed in relation to risk-based qualification and verification of the respective processes.

Development of simulation platforms

Chemical absorption

In the modelling and simulation of CO_2 absorption systems there are two general pathways, 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 predicting power of equilibrium based models can be improved by incorporating tray efficiencies, but in new design tray efficiencies may be error-prone, since these are based on historical plant data which may have restricted validity. For the rate-based approach, the reactions and transport phenomena are accounted for in contactor model equations. The model equations thus will be more challenging to treat numerically, but since the model in a more direct way account for the phenomena occurring in the system it can

be applied to any contactor without relying on plant data such as tray efficiencies. In this work issues with respect to the two different modelling strategies will be highlighted and simulator performance will be addressed in terms of a comparison with pilot plant data.

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 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. As part of this work the predictions of different sub-models will be analyzed and compared with experimental data from the literature.

Oxy-fuel combustion
A semi-closed oxy-combustion combined cycle is modelled. The simulation model includes an oxy-fuel combustor, a gas turbine, a heat recovery steam generator, a 3-stage steam turbine cycle and an exhaust gas recycle compressor. The main focus of this work is to study uncertainties in the modelling of the combustion conditions within the novel oxy-fuel combustor, such as flame temperature and emissions, and the effects this have on the overall cycle. The simulation tool used for the approach is Aspen HYSYS. Simulation tools such as HYSYS use chemical equilibrium models, or simple reactor models. Such simplified modelling of the complex combustion reactions that occur within the combustor does not take into account aspects such as detailed chemical reactions, complex turbulent flow, and detailed modelling of radiative fluxes. The effect these uncertainties have on turbine inlet temperature and combustor exit emissions, such as NO_x and CO levels are investigated and its further effect on the total system is explored.

Pre-combustion capture chemical processes
In this case, the aim is to develop a simulation platform for chemical processes involved in a pre-combustion CO_2 capture cycle utilizing different natural gas reforming technologies (e.g. methane steam reforming or auto thermal reforming) or coal gasification units followed by water-gas shift reactors. This could then be further coupled to a standard amine absorption process for CO_2 separation. Development of the plant concept, optimization of the CO-shift conversion and analysis of the plant efficiency will be included in this task. The developed simulation platform will be verified using available data in the literature.

References

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