Simulation of Aerosol formation in Post Combustion CO_2 Capture (PCCC) Plants

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Keywords: Post combustion CO_2 plant, aerosol, modelling, reactive absorption
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Over the past years, CO_2 emission reducing technologies were widely investigated due to alarming climate change, particularly, global warming. International energy agency states that one third of all CO_2 emissions are due to the combustion of anthropogenic fossil fuels, and forecasts that transport and power generation sectors will be responsible for 70% of CO_2 emission increase to 2030 (IEA, 2008). One of the most promising and perspective methods for capturing CO_2 is applying Carbon Capture and Storage (CCS) of flue gases using reactive absorption based Post Combustion CO_2 Plants (CESAR, 2011) using a 30 wt.% aqueous solution of the monoethanolamine (MEA); however, high energy consumption of this process results in the decline of the overall plant efficiency. Apart from mechanical losses, solvent loss due to evaporation and aerosol particulate phase emissions result in the increase in total operational cost and environmental impact (IEAGHG, 2010). Solvent loss due to mechanical entrainment and vapour emissions have been well investigated. On the other hand, experimental studies on particulate matter (PM) measurements in PCCC columns are scarce in the literature necessitating developments of simulation and modelling studies in this field. Nonetheless, prediction of PM formation in PCCC columns is a complex task requiring modelling of several steps including gas-phase supersaturation, PM formation (nucleation) and PM dynamics (growth and loss). Pre-existing PM into PCCC columns facilitates formation of new particles as a result of gas phase supersaturation. Hence, developing a simulation tool to understand the key parameters impacting the supersaturation of the gas phase in PCCC columns is of paramount importance. Few attempts were made to setup a simulation tool using Aspen Plus simulator to predict supersaturation of gas streams in PCCC columns in the absence of particulate phase, and in the presence of the flue gas PM. However, such simulation models still need to be improved to better understand the interactions between the particulate phase and other phases inside the column. The true mass and heat transfer between the particulate phase and gas phase needs to be determined using a nonequilibrium (rate-based) model. The first objective of this study is to firstly set up a simulation model to predict gas phase supersaturation inside PCCC columns. Under this objective, the influences of two separation modelling approach (equilibrium vs. nonequilibrium) on the level of gas phase supersaturation, mass transfer from gas to PM phase and MEA loss through the particulate phase were investigated. Hence, two models were created: (1) first model assumes equilibrium between gas and PM phases, and (2) the second model, (the rate based model) calculates true mass and heat transfer between the gas and PM phases using theoretical mass transfer correlations and estimated interfacial area.

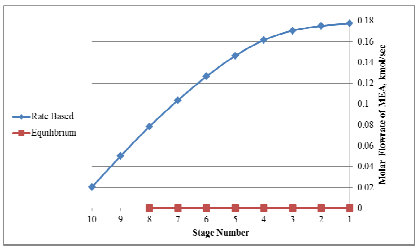

Figure1. The MEA loss in aerosol stream via gas-aerosol interaction

It can be observed from Figure1 that the MEA content of PM phase representing MEA (solvent) loss in absorber stream, increases from bottom (stage 10) to the top (stage 1) of the absorber column. In addition, it is shown that the change in the molar flowrate of MEA is very negligible in the equilibrium based model compared to rate-based model.

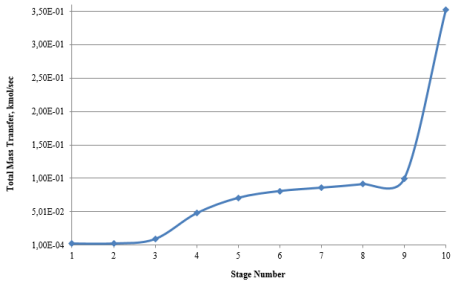

Figure 2. Estimated nucleation rate

Figure 2 shows the estimated nucleation rate on each stage which is found to be higher at lower section of the column. The second objective of this study is to find more accurate values for nucleation rate using molecular dynamics simulation. Finally, this study is aimed to model PM dynamics along the column.

1- IEAGHG, 2010. *Environmental Impacts of Amine Emissions During Post Combustion Capture*, Rep. No 201011 2010.

2- International Energy Agency (IEA), 2008. World Energy Outlook 2008, OECD/IEA. CESAR, 2011. *EU-Project, CO2 Enhanced Separation and Recovery (CESAR): Integrated Research Project Partially Funded by the European Commission Under the 7th Frame Work Program*, Grant Agreement Number 213569