COMPARISON OF ASPEN HYSYS AND ASPEN PLUS SIMULATION OF CO_2 ABSORPTION INTO MEA FROM ATMOSPHERIC GAS

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The most probable method for CO_2 removal from exhaust gas is by absorption in an amine based solvent like MEA (monoethanolamine) followed by desorption. A CO_2 removal process for 85 % removal based on absorption has been simulated with the process simulation tools Aspen HYSYS and Aspen Plus. The process is based on removing CO_2 from the exhaust from a 400 MW natural gas fired combined cycle power plant.

In the Aspen HYSYS calculations, specified Murphree efficiencies have been used in the absorption column. In the Aspen Plus calculations, both a Murphree efficiency and a rate-based approach were used. Using Murphree efficiencies gives a more realistic description of the concentration and temperature profiles as a function of column height, than using ideal equilibrium stages. When using Murphree efficiencies in these calculations, it is assumed that the temperature is the same in the gas and liquid at a given stage. In a rate-based calculation, the rate of mass and heat transfer between the gas and liquid phases are calculated on each stage.

In the case of a model based on Murphree efficiency, the only needed specifications for an absorption column calculation are the number of stages, the Murphree efficiencies on each stage in addition to the inlet streams and a pressure profile. The Murphree efficiencies for the components except from CO_2 are set to unity. When using rate-based calculations several specifications are necessary. In the calculations in this work, specifications for the structured packing Mellapak 250Y were used. The interfacial area factor was set to 1.0 and the height of one stage was 2.0 meter.

In the Aspen HYSYS calculations, the vapour/liquid equilibrium models Kent-Eisenberg and Li-Mather were used. The equilibrium model used in Aspen Plus was electrolyte NRTL (Non-Random-Two-Liquid) for both types of calculations. When using the electrolyte NRTL model, the parameter set in an example file from Aspentech was used.

Approximately 85 % CO_2 was removed from the exhaust gas in the base case calculations. It was difficult to achieve 85 % removal for the base case conditions using the rate-based model, so the removal grade in the rate-based calculation was slightly less. In the sensitivity calculations, removal grade was calculated as a function of solvent circulation rate, number of column stages and inlet gas and liquid temperature. The temperatures at all stages were also calculated by the simulation programs.

All the calculations using a constant Murphree efficiency of 0.25 for each stage showed similar results. The differences between the equilibrium models and between Aspen HYSYS and Aspen Plus were small. This indicates that there are not important differences in the equilibrium models. The largest deviations when using different equilibrium models was that Aspen Plus with the electrolyte NRTL model calculated higher temperatures in the middle of the column. However, this difference did not result in large differences in CO_2 removal efficiencies.

The rate-based calculations in Aspen Plus were close to similar to the calculations using Murphree efficiencies. The removal grade was calculated slightly lower in the rate-based calculations. The temperature profiles as a function of column height were slightly different. All the calculations showed increasing CO_2 removal grade with increasing circulating rate and number of stages, and decreasing removal grade with increasing temperature. The magnitudes of the effects were slightly different in the calculations using Murphree efficiencies compared to rate-based simulation. The rate-based calculations showed larger effect of solvent circulation rate and less effect of the number of stages and temperature compared to the calculations based on Murphree efficiencies.

A rate-based calculation is in principle predictive when all the details in kinetic data, equilibrium data, mass transfer and interfacial area correlations are specified. It is however normal to utilize e.g. the interfacial area as an adjustable parameter. The Murphree efficiency can be used as an adjustable parameter. The Murphree efficiency for e.g. 1 meter of packing can also be estimated when all the necessary details are known.

The advantages using Murphree efficiencies in CO_2 absorption simulations are that it is simple, and that it can utilize the equilibrium models and robust stage by stage column models already available in commercial process simulation programs. The advantages using rate-based simulations are that it can take into consideration more detailed effects of kinetics and complex mass transfer in combination with equilibrium.

The overall effects of differences in the equilibrium models Kent-Eisenberg, Li-Mather and electrolyte NRTL were very small. There were some differences in the calculation results based on Murphree efficiencies and rate-based calculations. An overall evaluation of the calculations performed in this work, is that all the simulations are close to equivalent if the aim is to calculate CO_2 removal efficiency as a function of e.g. circulation rate, number of column stages and temperature.