Despite the efforts and recent advances in renewable energy sources, the energy infrastructure is not yet ready to replace the fossil-fuel fired power plants with renewables. Thermal power plants represent the main energy supply and especially in developing countries, they are expected to dominate the market in the coming decades. However, the growing focus on mitigation of anthropogenic CO$_2$ requires integration of fossil-fuel fired power plant with CO$_2$ capture units. Post-combustion capture is the most mature capture technology and it is suitable for various processes in power plants, steel industry, cement production, and bio-chemical industry. However, to make CO$_2$ capture economically attractive, design of innovative solvents, optimization of operation conditions/process configuration and operational flexibility are of crucial importance.

This thesis aims to contribute to the development of efficient CO$_2$ post-combustion capture technology using alkanolamine solvents. Amine based CO$_2$ post-combustion capture is a reactive absorption process which implies complex mechanism of simultaneously occurring reaction and mass transport phenomena. Accordingly, first a simplified and easy to implement but general valid mass transfer model is developed and applied to single and parallel reactions systems, i.e. MEA, PZ and CA/MDEA. This mass transfer model uses existing correlations for mass and hydraulic characteristic and an enhancement factor to describe the acceleration of the mass transfer rate due to the reaction between CO$_2$ and amines. Afterwards, this sub-model together with the extended UNIQUAC thermodynamic model and correlations for physical properties is incorporated in a rate-based model for CO$_2$ absorption and desorption. The developed model is applied to MEA, PZ, PZ/K$_2$CO$_3$ and CA/MDEA and it is benchmarked against experimental pilot plant data and various models from independent research groups.

The validated steady-state model is used to determine set of optimal operation parameters for CO$_2$ capture post-combustion capture using PZ. This study accounts for the solubility window of PZ when determining the optimal and feasible operating conditions. The results are created in Aspen Plus using the hybrid CAPCO$_2$ rate-based user model. This model considers slurry formation in the calculation of CO$_2$ mass transfer rate. The results show how the capture process needs to be operated up to 14% above the minimum achievable heat duty, to avoid clogging from solid formation. 5 molal PZ is the most promising trade-off between energy efficiency and solid-free operation with a specific reboiler duty of 3.22 GJ/t CO$_2$ at 0.34 lean loading.

Furthermore, this thesis presents a dynamic rate-based model for CO$_2$ absorption and desorption using MEA and PZ as solvent. This dynamic model is an extension of the steady-state model as it uses the same thermodynamic-, mass transfer-, kinetic- and physical property- modules. These modules are implemented in Fortran and interfaced with the dynamic model which is implemented in Matlab. The developed model is used to investigate the transient behavior of a post-combustion plant using MEA and PZ. Moreover, a proportional-integral control structure is developed to investigate the controllability of the PZ based post-combustion plant compared to the MEA plant. The results reveal that PZ may be a better solvent than MEA as it can accommodate disturbances with less variability in the manipulated variables. However, control design alternatives and/or model based control structure should be developed to reduce the long settling time of the PZ plant compared to the MEA plant.