# Rapid Screening of Solvents for Post-Combustion $CO_2$ Capture Processes

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The capture of $CO_2$ from the industrial emissions has been the prime focus of research. Absorption-based processes are well-established and has been applied at an industrial scale using MEA 30 wt.%. Yet, the energy penalty of such process is hefty due to the high energy demand of the solvent regeneration. Improvements to the conventional process can take multiple forms including the employment of novel solvents and the modification of the process configuration. The evaluation of candidate solvents and process modifications is usually bided by key performance indicators such as the net power of regeneration, capture cost per tonne of $CO_2$, CAPEX, and OPEX. This work presents a decision-matrix tool developed to choose the best solvent for the capture plant. The thermophysical properties of the solvents impose varying effects on the economics of the process. It has been obtained that along with the absorption capacity and reaction rate, the heat of absorption, and the viscosity of the liquid phase have the greatest effect on CAPEX. Several solvents are predicted to have superior performance to MEA including 2ADP, AEEA, MAPA, TEA, and PZ. Another element of the study was to develop an enhancement factor index that does not depend on the kinetics of the process, which serves as a short-cut to estimate the size of the absorber and subsequently the CAPEX for the whole plant. The newly developed index is mainly dependent on the chemical potential of the species in physisorption and chemisorption settings. This factor aids in the screening of candidate solvents without the need to go through rigorous calculations. The study sets a methodological approach towards solvent screening, which is needed in the light of increasing discovery and the need to attain comparisons in a practical manner.

This work has been financially supported by Khalifa University through project RC2-2019-007.