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Computational Fluid Dynamics Modeling of Physical Mass Transfer of CO_2 by N_2O Analogy Using One Fluid Formulation in OpenFOAM

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Abstract : Removal of CO_2 by MEA (monoethanolamine) in structured packing columns depends highly on the gas-liquid interfacial area and film thickness (liquid load). CFD (computational fluid dynamics) is used to find the interfacial area, film thickness and their impact on mass transfer in gas-liquid flow effectively in any column geometry. In general modeling approaches used in CFD derive mass transfer parameters from standard correlations based on penetration or surface renewal theories. In order to avoid the effect of assumptions involved in deriving the correlations and model the mass transfer based solely on fluid properties, state of art approaches like one fluid formulation is useful. In this work, the one fluid formulation was implemented and evaluated for modeling the physical mass transfer of CO_2 by N_2O analogy in OpenFOAM CFD software. N_2O analogy avoids the effect of chemical reactions on absorption and allows studying the amount of CO_2 physical mass transfer possible in a given geometry. The computational domain in the current study was a flat plate with gas and liquid flowing in the countercurrent direction. The effect of operating parameters such as flow rate, the concentration of MEA and angle of inclination on the physical mass transfer is studied in detail. Liquid side mass transfer coefficients obtained by simulations are compared to the correlations available in the literature and it was found that the one fluid formulation was effectively capturing the effects of interface surface instabilities on mass transfer coefficient with higher accuracy. The high mesh refinement near the interface region was found as a limiting reason for utilizing this approach on large-scale simulations. Overall, the one fluid formulation is found more promising for CFD studies involving the CO_2 mass transfer.

Keywords : one fluid formulation, CO_2 absorption, liquid mass transfer coefficient, OpenFOAM, N_2O analogy
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