



Review

Simulation based improvement techniques for acid gases sweetening by chemical absorption: A review

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Abbreviations:

VLE, vapor–liquid equilibrium

FEED, front-end-engineering design

CO₂, carbon dioxideH₂S, hydrogen sulphideNH₃, ammonia

MEA, monoethanolamine

DEA, diethanolamine

TEA, triethanolamine

MDEA, methyldiethanolamine

PZ, piperazine

QSAR, quantitative structure–activity relationships

CFD, computational fluid dynamics

AMP, amino-methyl propanol

HETP, height equivalent to theoretical plates

SVM, support vector machine

COSMO-RS, conductor like screening model for real solvents

OPLS, optimized potentials for liquid simulations

DFT, density function theory

ABSTRACT

There are various theoretical approaches to design, improve and optimize CO₂ capture from natural gas sweetening units through chemical absorption. The aim objective of the present review is to explore various theoretical approaches developed by process and research engineers to improve the design and operation of chemical absorption sweetening units. Therefore, this review is divided into four parts. The first part discusses the basic thermodynamic and kinetic principles that represent the main core of any process simulation research. The second part is devoted to designing and improving the main columns i.e., the absorber and the stripper. The third part reviews previous research aiming at designing or optimizing the whole sweetening unit. The last part briefly discusses computational chemistry techniques used by chemists and chemical engineers to design novel solvents at the molecular level. The review ends with conclusions and a brief discussion about future perspectives to improve the process and areas that require further research effort.

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