The Monte Carlo driven and Machine Learning enhanced Process Simulator

This study presents a methodology with tools integration to apply advanced uncertainty propagation and sensitivity analysis in connection with commercial process simulation software. The methodology was applied to two processes: a heat pump system and a molecular distillation process. The input parameters of the selected thermodynamic model, namely critical temperature, critical pressure and acentric factor, were considered as a source of uncertainty and analyzed using Monte Carlo sampling techniques. This enabled the process model output uncertainty to be described as an empirical distribution function with a 95% confidence interval. Variance-based decomposition such as the Sobol method or standard regression were used to analyse the sensitivity of the respective properties. We also show that machine learning methods such as polynomial chaos expansion (PCE) can be applied to reduce the number of necessary process simulations and obtained equivalent results in comparison with the more costly full Monte Carlo based procedure.

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