

### Computational Simulation methods for gas separation processes

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Gas separation processes are currently designed based on knowledge of the process and subsequent predictions of the separation equipment performance at various different conditions. For this purpose models are typically constructed and simulated using computers programs to calculate solutions giving high separation efficiency while satisfying all the relevant mass and energy balances. For the development of gas separation processes we demonstrate how modelling equations can be formulated as computer models and numerical methods and strategies for their solution. The numerical methods under consideration include both dynamic/relaxation and steady-state approaches. Example calculations for different configurations of membrane separation systems show their computational stability and efficiency when using different numerical solution strategies. Hence, the most efficient and stable methods can be considered for use in future process design and optimization studies.

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