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Pressure swing adsorption (PSA) and vacuum swing adsorption (VSA) are gas separation processes which have attracted increasing interest because of their low energy requirements as well as low capital investment costs in comparison to the traditional separation processes. Hence, the development of optimization strategies for the design and operation of simple and complex PSA/VSA processes are of great importance in improving process performance.

A modelling framework for the separation of gas mixtures using multibed PSA/VSA flowsheets has been developed. The core of the framework represents a detailed adsorbent bed model relying on a coupled set of mixed algebraic and partial differential equations for mass, heat and momentum balance at both bulk gas and particle level, equilibrium isotherm equations and boundary conditions according to the operating steps. The adsorbent bed model provides the basis for building a PSA/VSA flowsheet with all feasible bed interconnections. The modelling framework provides a comprehensive qualitative and quantitative insight into phenomena that take place in the process. The modelling equations have been implemented in the gPROMS modelling environment.

We present the development of a modelling framework for efficient simulation and optimization strategies for the design of PSA/VSA processes with detailed adsorption and transport models. The modelling framework has been applied on the capture of post-combustion carbon dioxide (CO_2) from dry flue gas by PSA/VSA process. We also present an extension of the modelling framework with other types of adsorbents such as zeolites, activated carbon and Metal Organic Frameworks (MOFs). A detailed comparison reveals the most promising adsorbents under specified process constraints and capital cost limitations. Finally we present the optimization of the PSA/VSA process concerning the separation of CO_2 from dry flue gas using zeolite 13X as an adsorbent in order to maximize CO_2 purity and minimize power consumption of the process.