

515a A Numerical Method for the Accurate Simulation of Fast Cyclic Adsorption Processes

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In the simulation of fast cyclic adsorption processes, to apply the Fickian diffusion model it is necessary to include an increasing number of numerical discretization points as the cycle time is reduced in comparison to the characteristic diffusional time constant. We propose a new numerical method based on the definition of two distinct regions within an adsorbent particle: an outer layer where the concentration varies significantly with large internal gradients leading to enhanced mass fluxes, and an internal region where the concentration profile is virtually flat. The proposed method leads to the automated generation of a numerical grid that has a constant number of elements independent of the process cycle time. The procedure is demonstrated on a model for the simulation of a heatless dryer pressure swing adsorption process.