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# ACCEPTED MANUSCRIPT

### Pressure-swing-adsorption of gaseous mixture in isotropic porous medium: Transient 3D modeling and validation

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#### Abstract

A 3D Computational Fluid Dynamics (CFD) model is developed, applied and validated for a 4-steps PSA cycle operating for  $CO_2/CH_4$  separation by using Carbon Molecular Sieves (CMS). The computational results are addressed and found to be in good agreement with experimental data. The Linear Driving Force (LDF) model is employed in the present 3D CFD approach to compute the adsorption/desorption rates in the packed bed. The physical parameters which are crucial for better predicting the behavior of a PSA cycle at different operating conditions are identified. The present developed 3D CFD model of PSA processes will serve as a powerful optimization tool in CFD to enhance and create future optimal designs of gas separation systems operating simultaneously in both temperature and pressure swing.

*Keywords:* adsorption modeling, gas separation process, PSA cycle, isotropic porous media, heat and mass transfer in porous material

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