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P4.182 Simulating gas adsorption processes via kinetic modeling

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Gas adsorption processes are widely used in industrial applications including vacuum pumping in fusion reactors (getters and cryogenic pumps). In gas adsorption flows mass transfer occurs coupled with heat transfer. Modeling of such flows must be based on kinetic theory by applying the Boltzmann equation (BE) or kinetic model equations or alternatively the Direct Simulation Monte Carlo Method (DSMC). The latter approach has been successfully applied in several works to simulate gas adsorption at the ITER cryopumps, while more recently, there has been one attempt to introduce kinetic modeling based on the BGK kinetic model equation to investigate the effect of partial thermal accommodation on the sticking coefficient in half-space adsorption [1]. Here, this work is extended to model more general multidimensional gas flows, based on advanced kinetic model equations including the BE. More specifically, the fully-developed flow of monatomic and polyatomic gases through and above long plates is investigated based on the Shakhov and Holway kinetic models with adsorption and injection at the walls. The differences between the various kinetic models as well as between monatomic and polyatomic gases are identified. A comparison with corresponding results obtained by the BE is performed. Furthermore, a two-dimensional gas flow configuration similar to the one in cryogenic pumps is simulated obtaining the adsorption flux in terms of the sticking and the inflow conditions for various gases including hydrogen isotopes. Comparisons with corresponding DSMC results are performed. Overall, it is demonstrated that kinetic modeling is a reliable computational tool in order to effectively simulate gas adsorption processes.

[1] C. Tantos et al., Vacuum, 125, 65-74, 2016.

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