COMPUTATIONAL IDENTIFICATION OF ADSORPTION AND DESORPTION PARAMETERS FOR PORE SCALE TRANSPORT IN PERIODIC POROUS MEDIA

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Computational identification of unknown adsorption and desorption rates is discussed in conjunction with reactive flow considered at pore scale. Measured concentration of the specie at the outlet of the domain has to be provided to carry out the identification procedure. The reactive transport is governed by incompressible Navier-Stokes equations, coupled with convection-diffusion equation for species transport. The surface reactions, namely adsorption and desorption, are accounted via Robin boundary conditions. Henry and Langmuir isotherms are considered. The computational modeling is performed for a 2D periodic porous media. Finite element approximation in space and implicit time discretization are exploited. Deterministic and stojastic parameter identification approaches are considered. The influence of the noise in the measurements on the accuracy of the identified parameters is discussed. Multistage identification procedure is suggested for the considered class of problems. Computational results demonstrating the potential of the considered parameter identification approaches are presented.