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PARABOLIC SYSTEMS IN CATALYTIC REACTOR MODELING

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Abstract. Several numerical properties associated to the modeling of chemical reactors as sets of parabolic problems with nonlinear boundary conditions of Robin type are studied. The main issue in the modelisation and solution procedure is the nonlinearity and presence of boundary singularities that are essential to these systems and their relationship with the error estimations for adaptivity. The focus of this work is, in consequence, to assess different types of error estimators associated to linearization based in a Picard-like scheme. A system of parabolic (non-stationary) reaction-advection-diffusion equations with boundary conditions of numerically demanding singular nonlinear Robin type is posed and algorithms for their numerical solution are proposed. The models are stated and solved in the adaptive finite element software environment ALBERTA. The numerical examples are associated to problems drawn from Chemical Engineering (Simplified Catalytic Reactors) with the aim of providing approximate solutions and sound `a posteriori' error estimates oriented to the adaptation of meshes and timesteps. The schematic and simplified modeling and simulation of the reactor is a critical issue in this article, due to the characteristics of the original problem. In this sense the justification of the simplifications that are necessary in order to obtain reasonable numerical approximations is treated.