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Bifurcation Analysis of Methane Oxidative Coupling without Catalyst

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Abstract

We present a detailed bifurcation analysis of methane oxidative coupling in the gas phase using a global kinetic model for the various oxidation, reforming and dehydrogenation reactions. The kinetic model satisfies the thermodynamic constraints and is validated with literature data as well as new data obtained under near isothermal conditions. It is used to determine the methane conversion and C_2-products selectivity under various feed and operating conditions in large scale ideal adiabatic reactors. It is found that at higher CH_4/O_2 ratios (e.g. > 4), ignition and extinction points exist only at either high feed temperatures and/or space times, which may not be of practical interest. Autothermal operation on the ignited branch with feed at near ambient conditions ($\sim 300K$ and 1 bar) is feasible for practical range of space times (1 ms to 1 s) only for

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