

251d Transversal Hot Zone Formation in Adiabatic Packed Bed Reactors

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We study first the possible formation of a stationary transversal hot zone in an adiabatic packed bed reactor in which a single exothermic chemical reaction occurs. Linearized stability analysis of a pseudo-homogeneous (two variable) model of a shallow bed shows that stable stationary transversal temperature patterns cannot be predicted to form when the reaction rate depends only on the concentration of a limiting reactant and the temperature and the transversal heat dispersion exceeds that of the reactants. Stable stationary temperature patterns may be found only if one makes the unrealistic assumption that the transversal heat dispersion is smaller than that of the limiting reactant. Extensive numerical simulations show that stable stationary transversal hot zone cannot form by a two-phase (four variable) model of either a shallow or a long packed bed reactor. This analysis explains the failure of previous attempts to find via numerical simulations stable, stationary hot zones.

We next show that many different, stable transversal, spatiotemporal temperature patterns can be predicted to form in a shallow adiabatic packed bed reactor used to conduct an exothermic reaction, the isothermal rate of which may be oscillatory. (An established example is the oxidation of CO). The number of possible states increases with increasing reactor diameter. We present a systematic procedure to first bound the operating conditions under which this behavior may occur and then choose initial conditions that lead to the formation of the spatio-temporal state. Principle component analysis of the predicted patterns shows that the spatiotemporal motions have homoclinic features. This explains the long period (order of hours) of the laboratory observed oscillations.