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Mathematical modelling and simulation for decomposition of agro-herbicide in accelerated reaction calorimeter to avoid water pollution

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ABSTRACT

Many pesticides, widely used in agriculture, are produced in semi-batch-reactors which involve strong exothermic reactions and show thermal runaway which are difficult to control. In case of failure of cooling systems, the runaway gets triggered. This results in uncontrolled increase in temperature for adiabatic systems with consequent reactor pressurization due to uncontrollable formation of gases. Finally, safety of the reactor becomes questionable with release of hazardous gases to the environment increasing the pollution. Simultaneous decomposition of the product may lead to an accident requiring emergency environmental disaster management plan. In this work, decomposition of 4-chloro-3-nitro benzene tri fluoride in batch reactors is considered. for which a mathematical model has been formulated and is validated. Simulation results comprising of both reactor temperature and pressure profiles are obtained for the effect of cooling failure and other accidental scenarios. This study is helpful to understand possibilities of environmental hazards and increase in the level of air and water pollutions.

Keywords: Agro-herbicide; Semi-batch reactor; Mathematical modelling; Runaway reaction; Water; Pollution

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