

Numerical Study of the Self-ignition of Tetrafluoroethylene in a 100-dm³-reactor

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Abstract

The self-ignition of tetrafluoroethylene (TFE) caused by contact with hot surfaces has been analyzed with the help of simulations performed with COMSOL Multiphysics®.

The current study focuses on large-scale heated reactors for the industrial production of polytetrafluoroethylene (PTFE) from TFE at high pressures. Under undesired circumstances (e.g. wrong filling, failure of temperature control) gaseous TFE in contact with the hot walls may start to dimerize exothermically into octafluorocyclobutane (OFCB). Possibly, the energy released can heat up the gas phase to a temperature at which TFE decomposes in carbon black (soot) and tetrafluoromethane. The decomposition, once triggered, runs explosively and can result in the vessel rupture with consequent economical and eventually human losses.

Simulations of the self-heating and consequent self-ignition of TFE in a 100-dm³-reactor were carried out. The model solved three application modes of the Chemical Reaction Engineering Module of COMSOL Multiphysics®:

- the non-isothermal flow mode was used to describe the free convection caused by the volume forces generated by different densities due to the exothermic dimerization reaction. This model solved the impulse equation and the corresponding continuity equation;
- the convection and conduction mode was used to model the heat transfer resulting from the extended reaction net. Beside the exothermic dimerization reaction of TFE into OFCB and the endothermic back reaction, five additional reactions were considered, as shown in Figure 1. The dimerization reaction is the main responsible for the initial self-heating of TFE and has to experience a runaway, in order for decomposition reaction to be triggered. Due to lacking kinetic data, the decomposition itself is not included in the model, but this is not necessary to assess if the system will undergo an ignition;
- the convection and diffusion mode was used to model the mass balance by linking the reaction kinetics.

The results of the computations performed were compared with experimental data for the model validation. As shown in Figure 2, a good agreement was observed, since ignition temperatures of TFE (MITD) are well predicted.

Figures used in the abstract

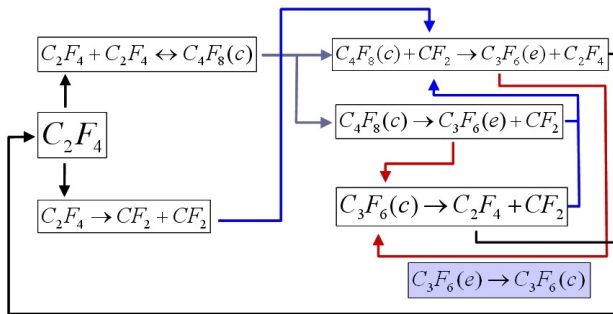


Figure 1: Reaction net used in the simulations.

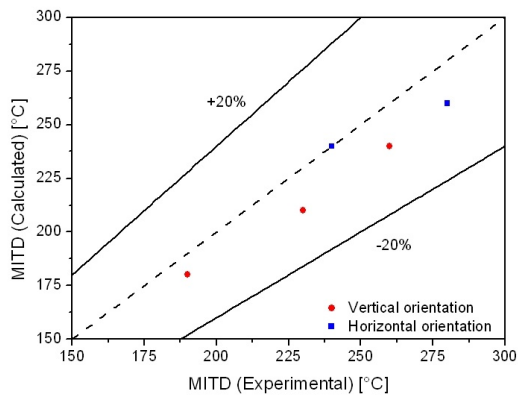


Figure 2: Accuracy of the predictions of the ignition temperatures of TFE.