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PII: S0040-6031(18)30500-8
DOI: https://doi.org/10.1016/j.tca.2018.09.014
Reference: TCA 78098

To appear in: *Thermochimica Acta*

Received date: 9-7-2018
Revised date: 2-9-2018
Accepted date: 18-9-2018

Please cite this article as: Wang S, Peng X, Li H, Guo Z, Chen L, Chen W, Numerical simulation and experimental study of thermal decomposition of cumene hydroperoxide in closed pressure vessel, *Thermochimica Acta* (2018), https://doi.org/10.1016/j.tca.2018.09.014

# Numerical simulation and experimental study of thermal decomposition of cumene hydroperoxide in closed pressure vessel

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## Highlights

- Incorporation of kinetic model into CFD code for CHP decomposition modelling.
- Study of reaction course of CHP in CPVT through CFD simulation.
- CFD approach is used to visualize the complex phenomena occurred in CHP decomposition.
- CFD approach is proposed for scale-up and reactive hazards assessment in industry.

**Abstract:** Cumene hydroperoxide (CHP) is prone to thermal decomposition in chemical industry, but there are few reports on the related phenomena in the reactor when decomposition occurs. In order to reveal the complex phenomena of fluid-solid coupled heat transfer, two-phase flow and multi-phase chemical reaction in the CHP decomposition, computational fluid dynamics (CFD) approach was applied to simulate the decomposition of CHP with different mass in a closed pressure vessel. Based on a known reaction scheme and the kinetics evaluated from differential scanning calorimeter (DSC) results, a comprehensive CFD model of CHP decomposition was created. As a result, detailed information on the reaction course was obtained, and distribution of temperature, pressure, reaction rate, and