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PII: S1004-9541(17)30496-2
DOI: doi:10.1016/j.cjche.2017.06.024
Reference: CJCHE 868

To appear in:

Received date: 26 April 2017
Revised date: 2 June 2017
Accepted date: 20 June 2017

Please cite this article as: Cong Zhou, Yuanyi Yang, Wei Li, Ying Shi, Li Jin, Zhaobin Zhang, Guoqing Wang, Free radical reaction model for *n*-pentane pyrolysis, (2017), doi:10.1016/j.cjche.2017.06.024

Catalysis, Kinetics and Reaction Engineering

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Abstract A mathematical mechanism of the *n*-pentane pyrolysis process based on free radical reaction model was presented. The kinetic parameters of n-pentane pyrolysis are obtained by quantum chemistry and the reaction network is established. The solution of the stiff ordinary differential equations in the *n*-pentane pyrolysis model is completed by semi implicit Eular algorithm. Then the pyrolysis mechanism based on free radical reaction model is built, and the computational efficiency increases 10 times by algorithm optimization. The validity of this model and its solution method is confirmed by the experimental results of n-pentane pyrolysis.

Keywords: pyrolysis, free radical reaction, model

1 INTRODUCTION

Ethylene, propylene, butadiene, and aromatics are the basic chemicals which are mainly produced by steam pyrolysis of petroleum hydrocarbons in the steam crackers. Petroleum hydrocarbons are preheated by superheated steam in the convection section of the furnace, and then the pyrolysis process takes place mainly in the radiant section of the furnace, where tubes are externally heated to 750–900℃. Then the pyrolysis products are separated into hydrogen, ethylene, propylene, butadiene, aromatics and so