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Molecular-level Modeling Investigation of *n*-Decane Pyrolysis at High Temperature

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Research highlights

- A molecular level model was established for *n*-decane pyrolysis under temperatures of (480-720 °C).
- A developed experimental method was used to investigate the cracking of *n*-decane.
- The model consisting of 16 species and 22 reactions performed well even conversions up to 93%.
- The molecular model has better agreement with experiment comparing with other mechanisms.

Abstract: A small-scale molecular reaction model has been established to predict the behavior of thermal cracking *n*-decane based on the experimental study of *n*-decane pyrolysis under supercritical conditions (4 MPa, 480-720 °C). A developed experimental method of electrical heating tube (2 mm inner diameter) was used experimentally to obtain the detailed local chemical compositions and temperatures along the reactor tube. Gas chromatography was used to analysis the pyrolysis products, and the calculated density and corresponding residence times along the

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