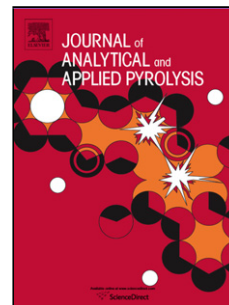


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THERMAL CRACKING OF N-BUTYLBENZENE AT HIGH PRESSURE: EXPERIMENTAL STUDY AND KINETIC MODELLING

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Keywords: pyrolysis, detailed kinetic modelling, alkylbenzene, high pressure, free-radical reactions

Highlights

- Pyrolysis of *n*-butylbenzene at 70 MPa and from 583 K to 623 K was performed in gold sealed tubes.
- The main products are toluene, ethylbenzene, iso-heptyl- and iso-butylbenzene, CH₄ and C₂H₆.
- A detailed kinetic model was constructed and validated over the entire experimental range of conversion (0.7-62%).
- Thermochemical and kinetic parameters of key decomposition routes were computed using theoretical calculations.

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