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材料化学工程与纳米技术

双环戊二烯加压连续聚合制备高能量密度燃料

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摘要

为制备密度大于1 g·ml^{-1} 的高密度燃料母体化合物三环戊二烯（TCPD），研究了双环戊二烯（DCPD）的加压连续聚合反应。分析了聚合反应产物组成和反应途径，研究了反应条件的影响。与常压间歇反应相比，加压连续反应能极大地提高反应转化率和收率，优化产物组成，TCPD中挂式/桥式（exo/endo）比例大大提高，并生成新的产物exo-DCPD。反应途径分析表明，TCPD中exo/endo比例与exo-DCPD选择性呈线性正相关。研究发现，为维持反应进行压力应不低于1.2 MPa，增加温度能提高反应转化率，而TCPD最高收率出现在160℃，TCPD的exo/endo比例随温度增加而降低，反应转化率和收率随停留时间增加而增加，但转化速率降低，缩短停留时间有利于提高TCPD的exo/endo比例，浓度对反应影响不大。在较优条件下，endo-DCPD转化率达82.2%，TCPD收率达41.7%。

关键词 高能量密度燃料 双环戊二烯 环戊二烯三聚物 聚合反应

分类号

Continuous oligomerization of dicyclopentadiene at elevated pressure for synthesis of high energy density fuel

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Abstract

The oligomerization of endo dicyclopentadiene（endo-DCPD）in a continuous flow reactor at elevated pressure was studied to produce tricyclopentadiene（TCPD）that was the precursor of high energy density fuel The composition of the products and possible reaction pathway were analyzed，and the effects of reaction conditions were evaluated Compared with the batchwise reaction at atmospheric pressure，the continuous flow process could significantly enhance the reaction，increase the exo/endo ratio of TCPD，and produce a new product exo-DCPD The exo/endo ratio was linearly dependent on the selectivity of exo-DCPD A high pressure of above 1.2 MPa was necessary to facilitate the reaction The conversion of endo-DCPD increased with the increase of temperature，while the yield of TCPD reached the highest value at 160℃ But the exo/endo ratio decreased with the increase of temperature The conversion of DCPD and the yield of TCPD increased when the residence time was increased，but the reaction rate decreased A short residence time was favorable，because it led to a high exo/endo ratio for TCPD The effect of feed concentration was limited Under the optimal condition，the conversion of endo DCPD was 82.2% and the yield of TCPD was 41.7%.

Key words high energy density fuel dicyclopentadiene tricyclopentadiene oligomerization reaction

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