

## عنوان مقاله:

Thermodynamic Analysis of Direct Partial Oxidation of Methane to Benzene

## محل انتشار:

ششمین کنگره بین المللی مهندسی شیمی (سال: 1388)

تعداد صفحات اصل مقاله: 6

## نویسندگان:

Mohammad Haghighi - *Reactor and Catalysis Research Center, Chemical Engineering Faculty, Sahand University of Technology, Tabriz, Iran*

Mozaffar Abdollahifar - *Reactor and Catalysis Research Center, Chemical Engineering Faculty, Sahand University of Technology, Tabriz, Iran*

Dang-ke Zhang - *Centre for Fuels and Energy, Curtin University of Technology, Western Australia*

## خلاصه مقاله:

Recent reports on methane aromatisation have shown that the partial oxidation of methane to benzene can be made to proceed at about 1000 K, but it is limited by thermodynamic equilibrium and the eventual deactivation of any catalyst by coking. In order to identify the most favourable operating conditions for the direct partial oxidation of methane to benzene thermodynamic aspects of the reaction system have been analysed. The present contribution examines the equilibrium compositions of products from direct partial oxidation of methane to benzene. The study was conducted over a temperature range of 500-1500K, pressure range of 0.1-5 MPa, CH<sub>4</sub>/O<sub>2</sub> ratio of 2-20. CHEMKIN software is used for thermodynamic equilibrium calculations using the Gibbs free energy minimisation method. It has been found that from the thermodynamic viewpoint the reforming products, H<sub>2</sub>, H<sub>2</sub>O, CO and CO<sub>2</sub>, are the major compounds at temperatures around 1000 K, while benzene is produced mostly at temperatures above 1200 K. It is shown that pressure inhibits methane conversion, benzene selectivity and the molar ratio of C<sub>6</sub>H<sub>6</sub>/(C<sub>2</sub>+C<sub>3</sub>) at equilibrium. The feed CH<sub>4</sub>/O<sub>2</sub> ratio has an important role in the conversion of methane to hydrocarbons, C<sub>6</sub>H<sub>6</sub>, C<sub>2</sub> and C<sub>3</sub>. While methane conversion decreases with increasing CH<sub>4</sub>/O<sub>2</sub> ratio, benzene selectivity and the C<sub>6</sub>H<sub>6</sub>/(C<sub>2</sub>+C<sub>3</sub>) equilibrium molar ratio are enhanced.

## کلمات کلیدی:

Direct Partial Oxidation, Methane, Benzene, Thermodynamic, Equilibrium

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