A Study of the \( \text{C} + \text{H}_2 \) Reaction, Taking into Account \( \text{H}_2 \) Chemisorption

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Introduction

In previous communications we reported the mathematical models for the \( \text{C} + \text{H}_2\text{O} \) and \( \text{C} + \text{O}_2 \) reactions. We showed that the rate-controlling steps of the above-mentioned reactions were chemisorption of \( \text{H}_2\text{O} \) and disintegration of oxygen surface complexes respectively. In this paper we report a mathematical model for the \( \text{C} + \text{H}_2 \) reaction, taking into account \( \text{H}_2 \) chemisorption.

Theoretical Analysis

The apparent rate of the \( \text{C} + \text{H}_2 \) reaction is determined in the kinetic area, taking account of the variation in the gas volume:

\[
-P \frac{dx}{dt} = kF_k P_{H_2} \tag{1}
\]

where \( P \) is the total pressure in the system, \( x \) is the proportion by volume of unconverted \( \text{H}_2 \), \( K \) is the experimental rate constant, \( F_k \) is the external specific surface of the carbon \( (m^2/m^3) \) and \( P_{H_2} \) is the partial pressure of \( \text{H}_2 \).

If chemisorption of \( \text{H}_2\text{O} \) is taken into account, the apparent rate of reaction is given by

\[
-P \frac{dx}{dt} = K' F_k \frac{b P_{H_2}}{1 + b P_{H_2}} \tag{2}
\]

where \( K' \) is the theoretical rate constant and \( \theta \) is the fraction of the carbon surface occupied by \( \text{H}_2 \), given by the Langmuir Equation

\[
\theta = \frac{b P_{H_2}}{K_a P_{H_2} + K_d} \tag{3}
\]

where \( K_a, K_d \) are rates of chemisorption and desorption of \( \text{H}_2 \) respectively, \( b = K/K_d \).

Using proposed mathematical model and experimental data following kinetic parameters of the \( \text{C} + \text{H}_2 \) reaction were obtained.
<table>
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<th>T°K</th>
<th>K'</th>
<th>K_a</th>
<th>K_d</th>
<th>K_d'</th>
<th>b</th>
<th>b_1</th>
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</tbody>
</table>

P = 0.13 Mpa

|     |      |      |      |      |      |      |
| 1133| 1.06 10^{-3} | 2.14 10^{-5} | 4.25 10^{-3} | 3.19 10^{-3} | 5.00 10^{-7} | 6.70 10^{-7} |
| 1173| 2.07 10^{-3} | 3.69 10^{-5} | 8.49 10^{-3} | 3.40 10^{-3} | 4.20 10^{-7} | 6.03 10^{-7} |
| 1213| 3.13 10^{-3} | 4.10 10^{-4} | 9.34 10^{-3} | 6.22 10^{-3} | 3.05 10^{-4} | 4.59 10^{-4} |

P = 2.00 Mpa

References


469