Abstract

Pyrolysis of methane is carried out at 1 atm pressure, in the presence of Sodium catalyst at 973 K temperature. Partial pressure of methane and argon gases is 0.45 atm, and for sodium it is 0.45 atm. Based upon the reaction kinetics and mechanisms, a data of concentration of CH4 vs time is plotted.

Sensitivity Analysis using Degree of Reaction Control

A method of sensitivity analysis, called Degree of Reaction Control (DRC) is used here to determine the rate-limiting steps from the number of reaction steps. Following is the equation to calculate DRC:

$$X_i = \left(\frac{k_i}{r} * \frac{\partial r}{\partial k_i}\right)_{k_{i\neq j}, K_j} = \left(\frac{\partial [ln(r)]}{\partial [ln(k_i)]}\right)_{k_{i\neq j}, K_j}$$

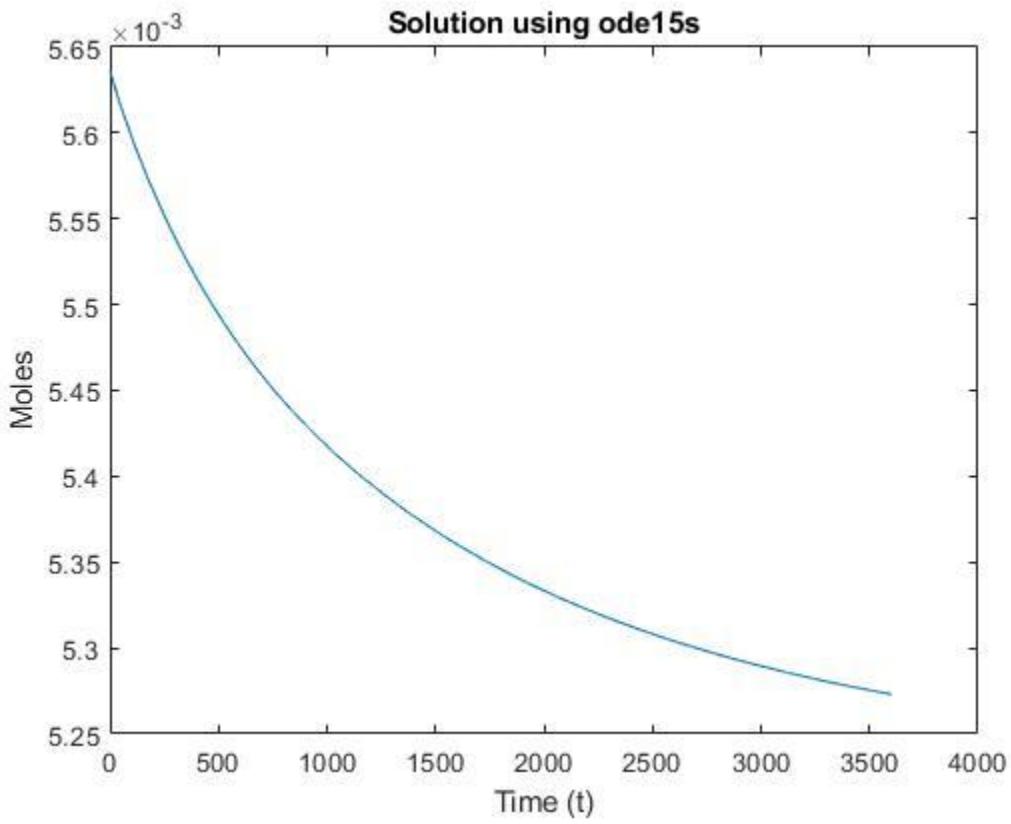
Where,
K_i = Equilibrium constant for i^{th} reaction
r = Rate of reaction
X_i = DRC Parameter
k_i = Rate constant for i^{th} reaction

Rate Equation

$$Rate = \frac{1}{V}\frac{dN}{dt} = -\sum_{j=1}^{m} k_j \prod_{i=1}^{n} \left(\frac{N_i}{V}\right)^{|\nu_{ij}|} + \sum_{j=1}^{m} k_{-j} \prod_{i=1}^{n} \left(\frac{N_i}{V}\right)^{|\nu_{ij}|}$$

Where,
V = Volume of the reaction mixture
N_i = Moles of species i
k_j = Forward reaction rate constant
k_{-j} = Backward reaction rate constant
ν_{ij} = Stoichiometric coefficient

Result Plot


Solution using ode15s
×10^-3
5.65
5.6
5.55
5.5
5.45
5.4
5.35
5.3
5.25
Moles
0
500
1000
1500
2000
2500
3000
3500
4000
Time (t)