Computational Assignment

Here we are doing the pyrolysis of methane at a temperature of 973K in the presence of sodium (Na) as a gas phase catalyst.

To investigate the temporal change in moles of methane with time, **Micro-Kinetic Modelling** is carried out.

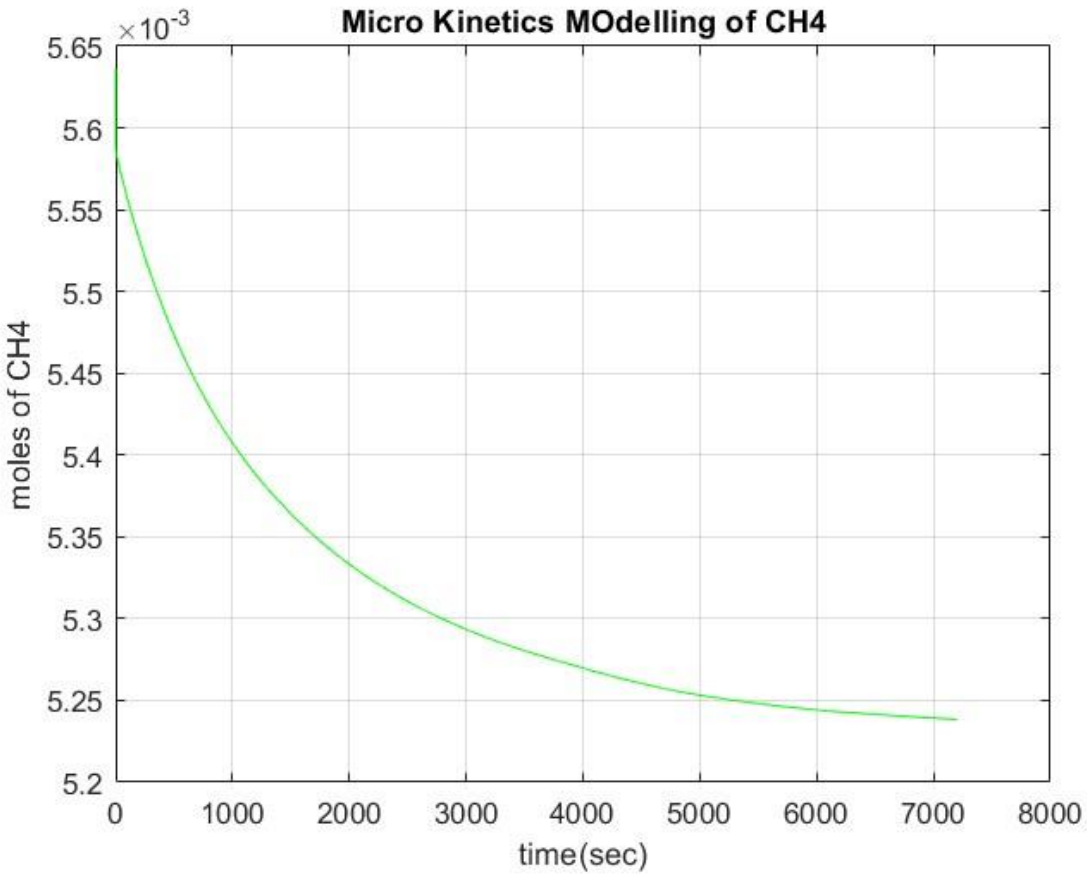
Microkinetic Modelling

Microkinetic modelling is used to determine critical reaction intermediates and rate-determining elementary reactions, thereby provides crucial information to design an improved catalyst.

Assumptions are: -

1. As methane is pyrolyzed at very high temperature, we can take ideal gas assumptions here. So, we have calculated the moles using ideal gas law.
2. Here we have assumed that each globule behaves as batch reactor.

MATLAB result of Micro Kinetic Modelling is:-



From the graph we get to know that moles of CH4 decreases exponentially with time and after 7200 s it will be constant.

Sensitivity Analysis

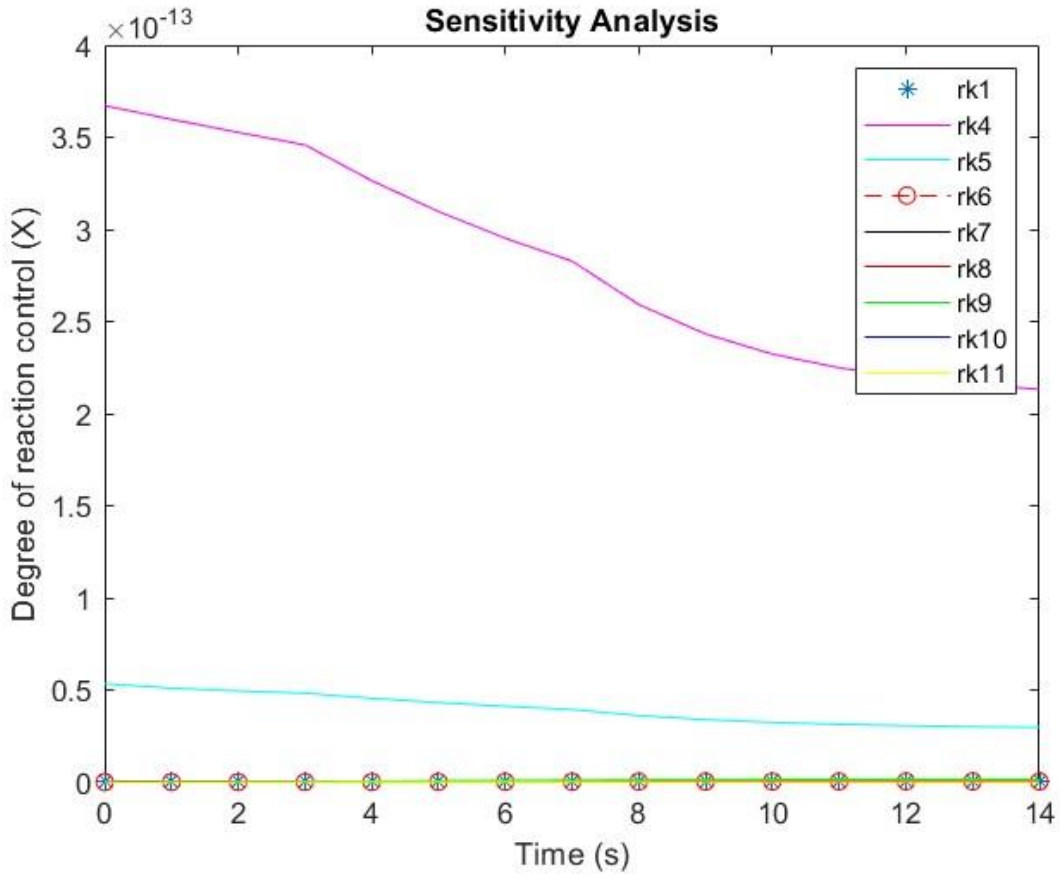
- The basis of sensitivity analysis is the level of rate control. The purpose of this analysis is to identify the reaction that influences the total rate of reaction.

- We alter the forward reaction rate coefficient in this analysis while maintaining the equilibrium rate coefficient constant to observe the impact on each reaction.
- The reactions that have the biggest effects on the overall reaction rate are those that are more impacted.

Degree of Rate control is given by :-

$$\chi = \frac{k_i}{r}\left(\frac{\partial r}{\partial k_i}\right)_{k_{j\neq i}, k_i}$$

MATLAB Result :-



From these graph, it can be observed that the two reactions mainly are the rate limiting steps. That is kinetic parameters of these reactions

contribute to the overall rate of methane pyrolysis and rest reactions degree of reaction control is ZERO.