REPORT ON COMPUTATIONAL ASSIGNMENT

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Aim- Plotting temporal variation of methane pyrolysis by initial decomposition pathways by MATLAB. And also using degree of rate control method finding the rate determining step (RDC).

Theory- Micro-Kinetic Model is a method that helps to develop a feasible reaction scheme. By this method we get a kinetic parameter of all steps.

Degree of rate control (DRC):

$$\chi i = (ki/r) * (\partial r/\partial k)_{kj \neq i}$$

$$x_i^+ = \frac{ki}{r}(\partial r/\partial ki) kj \neq i, k_{-j}$$

$$x_i^- = k_{-i}/r \left(\frac{\partial r}{\partial k_{-i}}\right)_{kj \neq i, kj}$$

$X_i = X_i^+ + X_i^-$

Where,

ki= forward reaction rate constant

k-i= backward reaction rate constant

r = overall rate of reaction (mols/m3 sec)

x = degree of rate control

Result:

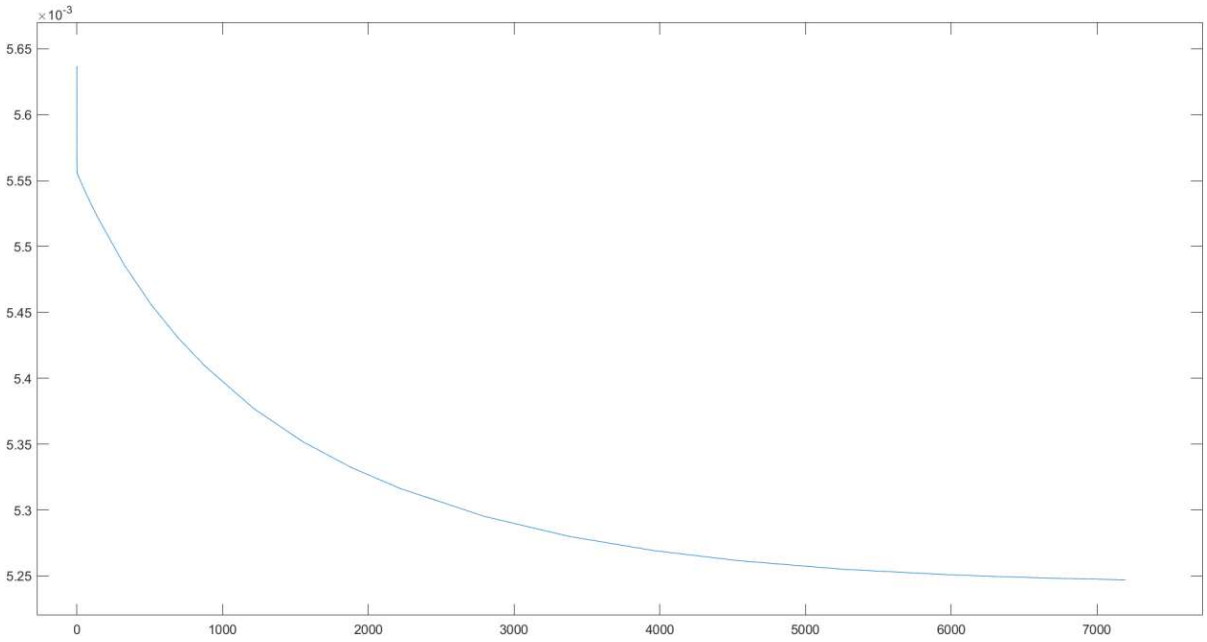
Initially at higher value of concentration there is negligible variation in time. But as time increases the moles decreases asymptotically and then remains constant.

Sensitivity analysis:

Sensitivity analysis is done to simplify the reaction network using degree of rate control

$Xi = (ki/r) * (\partial r/\partial ki) \,|kj \neq i$ (Where Xi is the degree of rate control);

If Xi = 0 then the reaction is insensitive and overall rate will not depend on that i^th reaction.



TIME (IN SEC.)

RDS BY SENSITIVITY ANALYSIS