Bio-oil resulting from fast pyrolysis of biomass is considered as a valuable resource of chemicals, and process modelling requires to conduct biomass fast pyrolysis under kinetic-controlled regime.  

**Background**

- Chemical reactions:

\[ A \xrightarrow{k_1(t)} B \xrightarrow{k_3(t)} C \xrightarrow{k_6(t)} D \]

\[ T_{up} = 750 \text{ K} \]

**Objectives**

- Study the effect of heat transfer on the distribution of pyrolytic products.
- Model pyrolysis kinetics of a biomass sample arrangement in a reactor by considering the thermal mechanisms of its environment and within it.
- Perform a thermal kinetic coupling in the system (reactor + biomass) through a formulation in path space and as nested expectations, using Monte Carlo simulation.

**Kinetic modeling**

- Degradation pathway: Transcription of a non-linear 1st order ODEs system into an expectation system

\[ \frac{dX_1(t)}{dt} = -k_2(t)X_1(t) \]

\[ \frac{dX_2(t)}{dt} = k_1(t)X_1(t) - (k_3(t) + k_5(t))X_2(t) \]

\[ \frac{dX_3(t)}{dt} = k_4(t)X_2(t) \]

\[ \frac{dX_4(t)}{dt} = k_7(t)X_3(t) \]

Archonius law: \[ k_i(T) = A_i e^{-\frac{E_i}{RT}} \text{ [s}^{-1}] \]

Upper bound of the reaction rate constant, \( k_i \): \( 10^{-5} \text{ [s}^{-1}] \)

**Thermal modeling**

- Heat equation: Thin and non-reactive biomass film

\[ \rho c_p \frac{dT}{dt} = -U_{sec}(T - T_{up})S_b \]

\[ T(t = t_0) = T_0 = 293.15 \text{ K} \]

\[ T_{up} = 750 \text{ K} \]

- Analytical solution:

\[ T(t) \approx T_{up} + \left( T_0 - T_{up} \right) e^{\frac{U_{sec} - c_p}{\rho A}} \]

\[ T \approx 10^{-4} - 10^{-5} \]

**Results and Conclusions**

All calculations were performed with a sample size of \( N = 10^4 \)

- Monte Carlo Integral Formulation can solve a system of non-linear 1st order ODEs and by default a system of linear ODEs.
- It is possible to estimate mass fraction or molar fraction via several independent probe points calculations (Each point showed in the figure above).
- Thermal/kinetic coupling can be treated in the case of prescribed thermal models.