



PERFORMANCE OF A STOICHIOMETRIC-KINETIC MODEL TO PREDICT THE DEGRADATION OF LIGNOCELLULOSE BY REACTIVE OXYGEN SPECIES (ROS) AND THE FORMATION OF MOLECULES OF INTEREST

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Objective: Mathematical model → Understanding & control of the kinetics of the chemical reactions of LC degradation

LC liquid model system:

1/ Cellobiose and cellulose nanocrystals

2/ Coniferyl Alcohol

3/ Fe

4/ Enzyme

Steps:

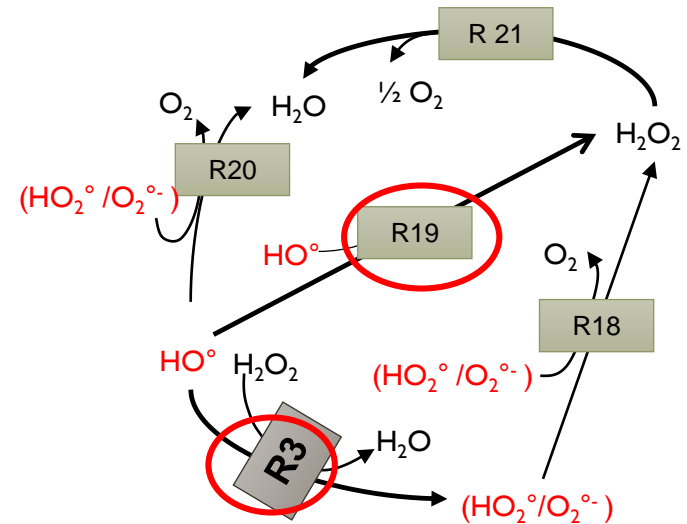
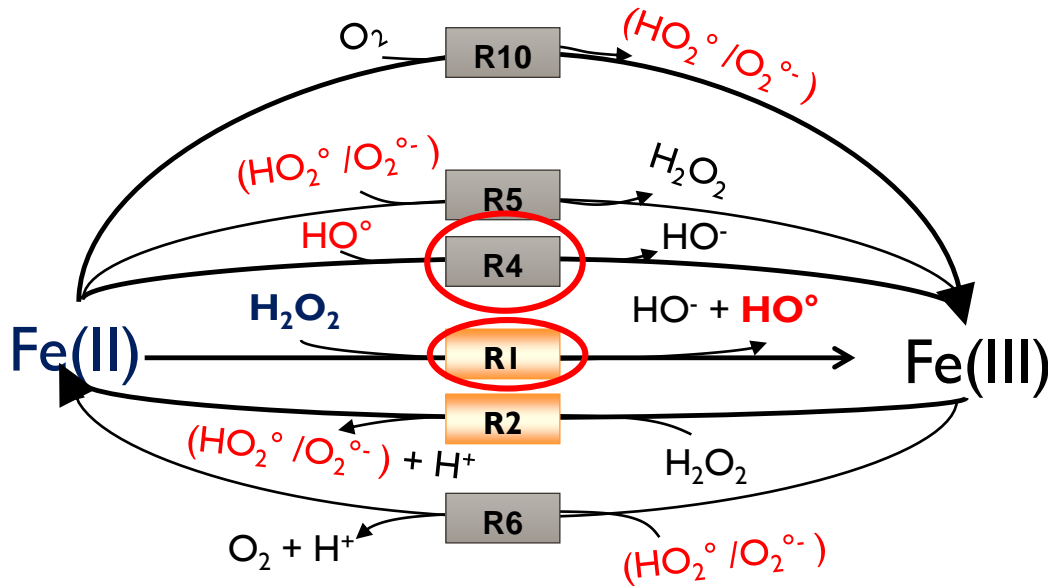
Combinations of 1+3,

1+4, 1+2+3,...



What is a Stoichio-kinetics Model ?

Example on the modelling of HO° in Fenton Reactions

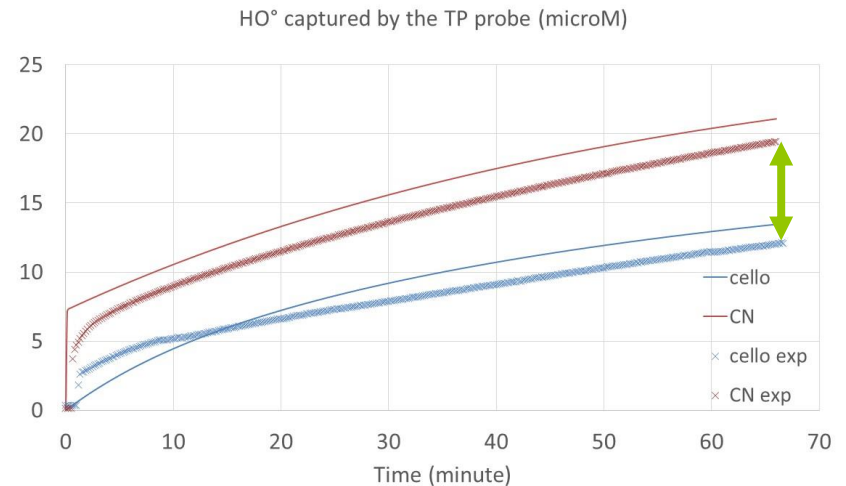
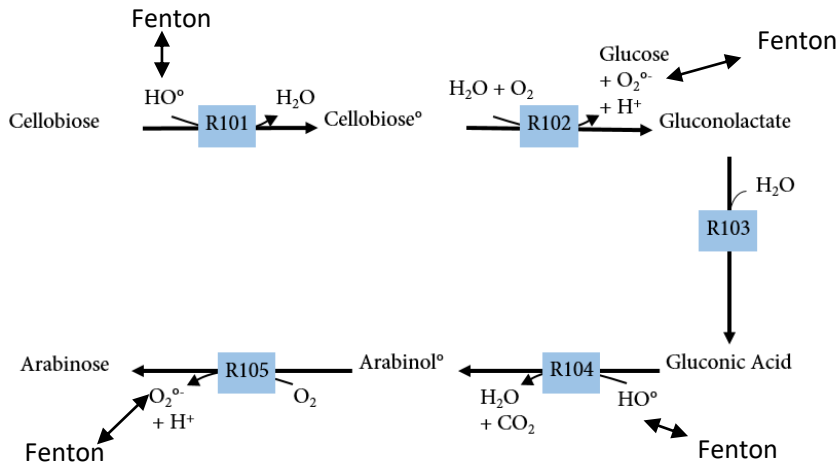


$$\frac{d[\text{HO}^\circ]}{dt} = 1 \cdot V_1 - 1 \cdot V_3 - 1 \cdot V_4 - 2 \cdot V_{19} = 1 k_1 [\text{H}_2\text{O}_2]^1 [\text{FeII}]^1 - 1 k_3 [\text{H}_2\text{O}_2]^1 [\text{HO}^\circ]^1 - 1 k_4 [\text{FeII}]^1 [\text{HO}^\circ]^1 - 2 k_{19} [\text{HO}^\circ]^2$$

- System of 11 differential equations
- + Arrhenius equation (for temperature effects)
- + P₂, P₃ iron reactivity coefficients

K_i, E_{ai} coming from literature or identified from dedicated sets of experiments

Fenton (= Fe) + cellobiose or cellulose nanocrystals



- ⇒ (1) Cellobiose reacts more with HO[•] than CN (less HO[•] are captured by the probe)
- ⇒ (2) Part of Fe is chelated by the nanocrystals leading to a decrease of iron reactivity during CN experiments
- ⇒ **Model suggests that (2) is the most probable interpretation**

CONCLUSION

- Stoichiometric model is an efficient way for understanding the kinetic of complex mixtures of LC.
- Reaction model can be combined with mechanical and convection-diffusion models in solid medium.
- If you have any question, don't hesitate to ask me. (poster 8)