PERFORMANCE OF A STOICHIOTO-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:  
Combinaisons of 1+3,  
1+4, 1+2+3,…
What is a Stoichio-kinetics Model?

Example on the modelling of HO° in Fenton Reactions

\[
\frac{d[\text{HO}^\circ]}{dt} = 1*V_1 - 1*V_3 - 1*V_4 - 2*V_{19} = 1k_1[H_2O_2][\text{Fe(II)}] - 1k_3[H_2O_2][\text{HO}^\circ] - 1k_4[\text{Fe(II)}][\text{HO}^\circ] - 2k_{19}[\text{HO}^\circ]^2
\]

→ System of 11 differential equations
  + Arrhenius equation (for temperature effects)
  + \(P_2, P_3\) iron reactivity coefficients

\(K_i, E_{ai}\) coming from literature or identified from dedicated sets of experiments
CONCLUSION

• Stoichio-kinetic 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)