### Title:

Kinetic and dynamic analysis of ozonolysis pre-treatment of empty fruit bunch in a well-mixed reactor for sugar production

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## Abstract:

Pre-treatment is the key step in biorefinery for enhancing cellulose accessibility from lignocellulosic biomass (LB) such as empty fruit bunch (EFB), which contains highly valuable cellulose. Ozonolysis pre-treatment appears as a promising green alternative for isolation of EFB to cellulose. This study develops the diffusion-reaction model of EFB ozonolysis inside a wellmixed novel OzBiONY® ozonolysis reactor at lab scale production. The mathematical model is numerically solved using COMSOL Multiphysics® software. Kinetic reaction parameters are computationally estimated via gradient-based Sparse Nonlinear Optimizer (SNOPT) method with sequential quadratic programming (SQP) algorithm. The evolution of ozone velocity and concentration profiles inside the reactor are simulated by computational fluid dynamics (CFD) method to study the effect of biomass particle sizes. The larger particle size consumes higher ozone ( $k_1 = 2.23 \text{ m}^3/\text{mol} \cdot \text{s}$ ) compared to the smaller particle size ( $k_{1=} 0.09 \text{ m}^3/\text{mol} \cdot \text{s}$ ). This reveals that larger biomass particle confers faster delignification rate and a much higher degradation of insoluble lignin. The simulation results demonstrate ozone velocity at the surface of larger particle is lower, but the surface concentration of ozone is higher. The diffusion-reaction model of EFB ozonolysis elucidates the plausible reaction pathway of lignin degradation via ozonolysis pretreatment with minimum objective function (Z) of  $1.41 \times 10^{-3}$ . From experimental results, the highest lignin degradation is 78 wt.% and the highest glucose yield is 12 wt.%. The outcomes of this research will contribute to the development of smart biorefinery technology and systems for sugar production in a sustainable and circular economy.