Supplementary Materials: Monolithic Stirrer Reactors for the Sustainable Production of Dihydroxybenzenes over 3D Printed Fe/γ-Al_2O_3 Monoliths: Kinetic Modeling and CFD Simulation

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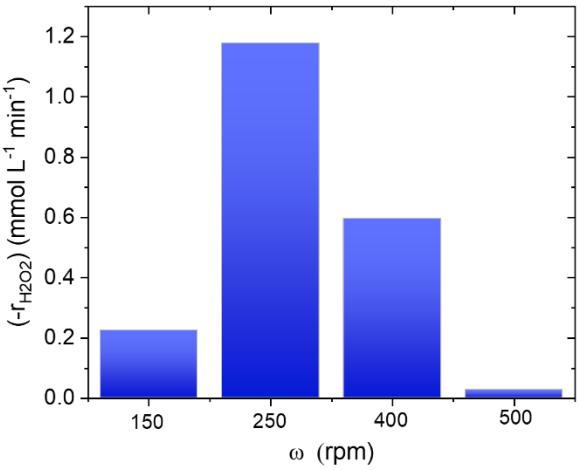


Figure S1. Effect of the stirring speed on the initial reaction rate of the H_2O_2 decomposition in the Fenton reaction. Operating conditions: $C_{H2O2,0}$ = 14.7 mM, $C_{Fe^{2+}}$ = 0.178 mM (from $FeCl_2$ salt), T = 25 °C and pH_0 = 3 (adjusted with HCl). Further details of this reaction is provided in Section 3.3 of Materials and Methods.

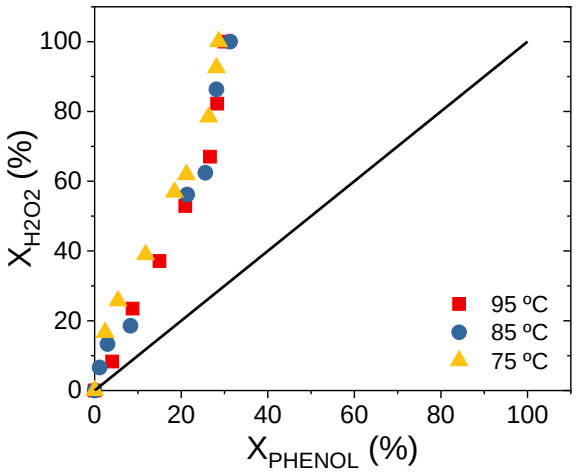


Figure S2. Efficiency in the consumption of H_2O_2 in the hydroxylation of phenol by H_2O_2 over 3D Fe/Al_2O_3 catalysts.

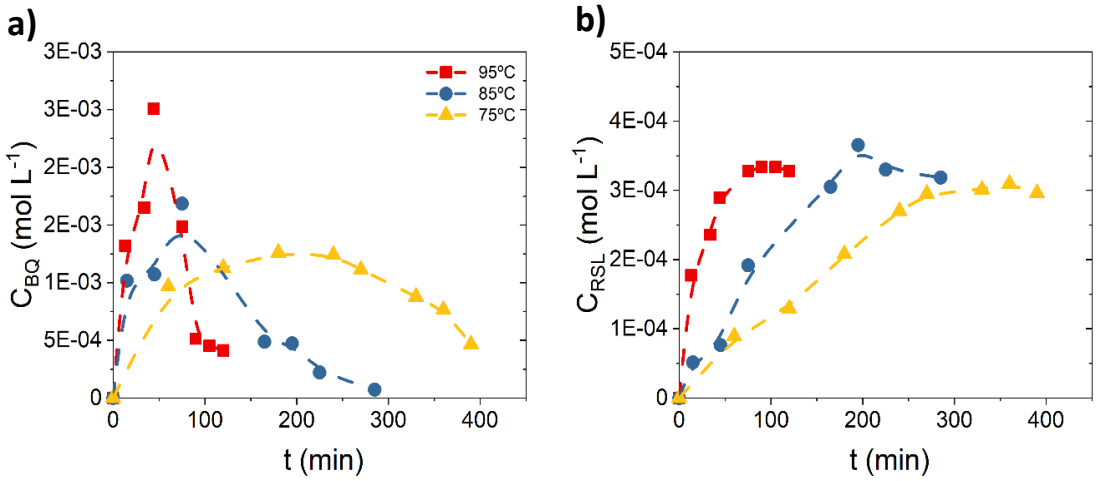


Figure S3. Experimental concentration profiles of (a) BQ and (b) RSL at different temperatures. Operating conditions: $C_{PHENOL,0}$ = $C_{H2O2,0}$ = 0.33 M, W_{CAT} = 1.1 g_{CAT} and T = 85–95 °C.

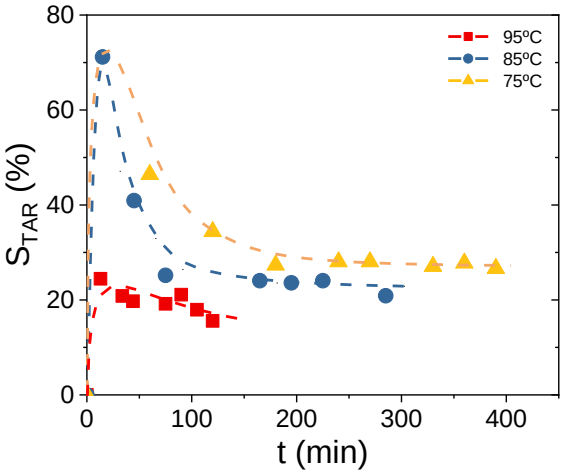


Figure S4. Experimental concentration profiles of tar at different temperatures. Operating conditions: $C_{PHENOL,0}$ = $C_{H2O2,0}$ = 0.33 M, W_{CAT} = 1.1 g_{CAT} and T = 85–95 °C.

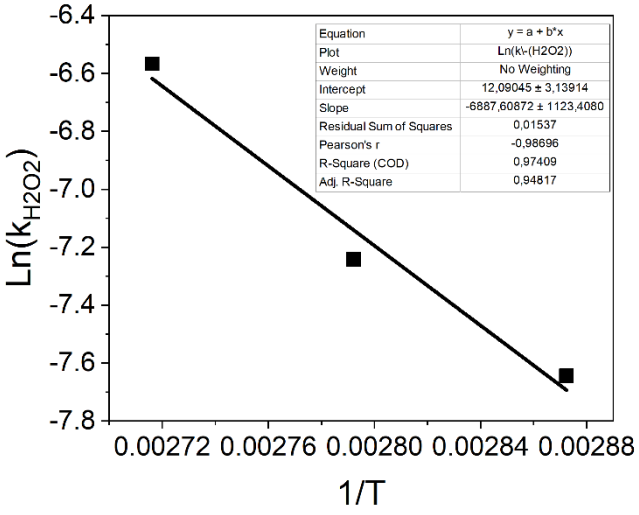


Figure S5. Dependence of k_{H2O2} with the reaction temperature.

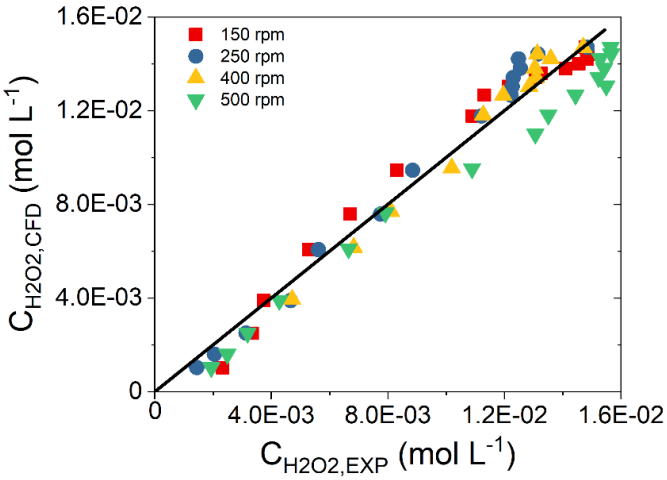
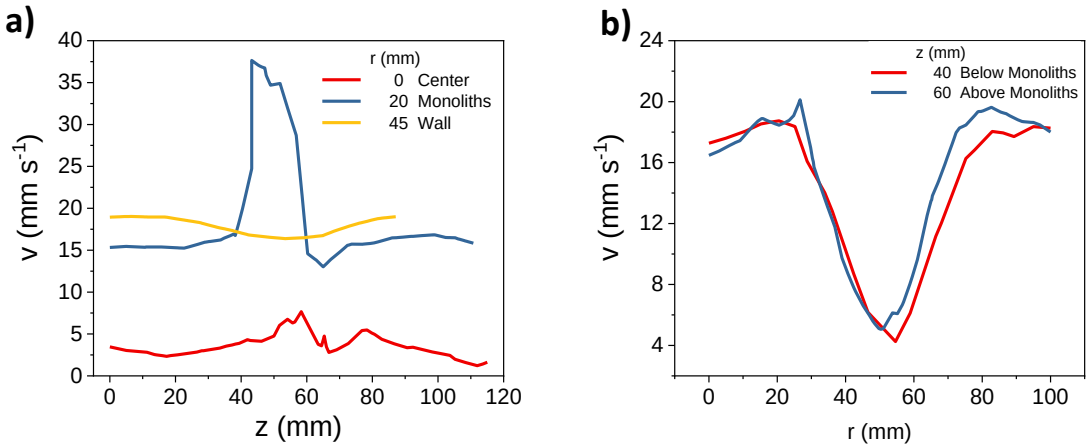


Figure S6. Parity plot of experimental and calculated concentrations by CFD assuming laminar flow for the Fenton reaction carried out at different stirring speed.



Figures S7. (a) Axial and (b) radial velocity profiles at different radios and axial positions, respectively, at ω =250 rpm and T = 85 ºC

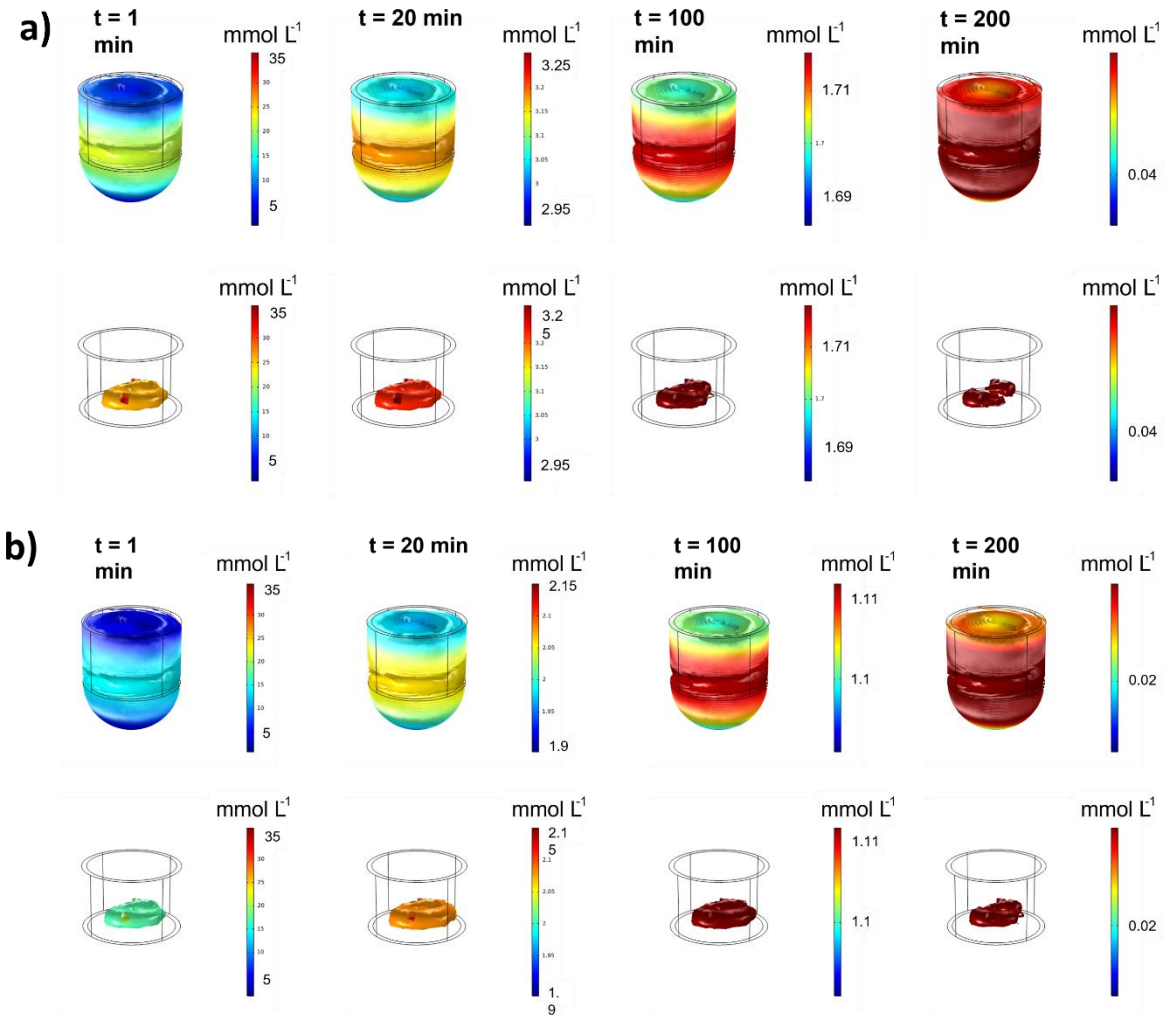


Figure S8. Three-dimensional profiles of the concentration isosurface of (a) CTL and (b) HQ during the hydroxylation of phenol by H_2O_2 at ω =250 rpm and 85 ºC.

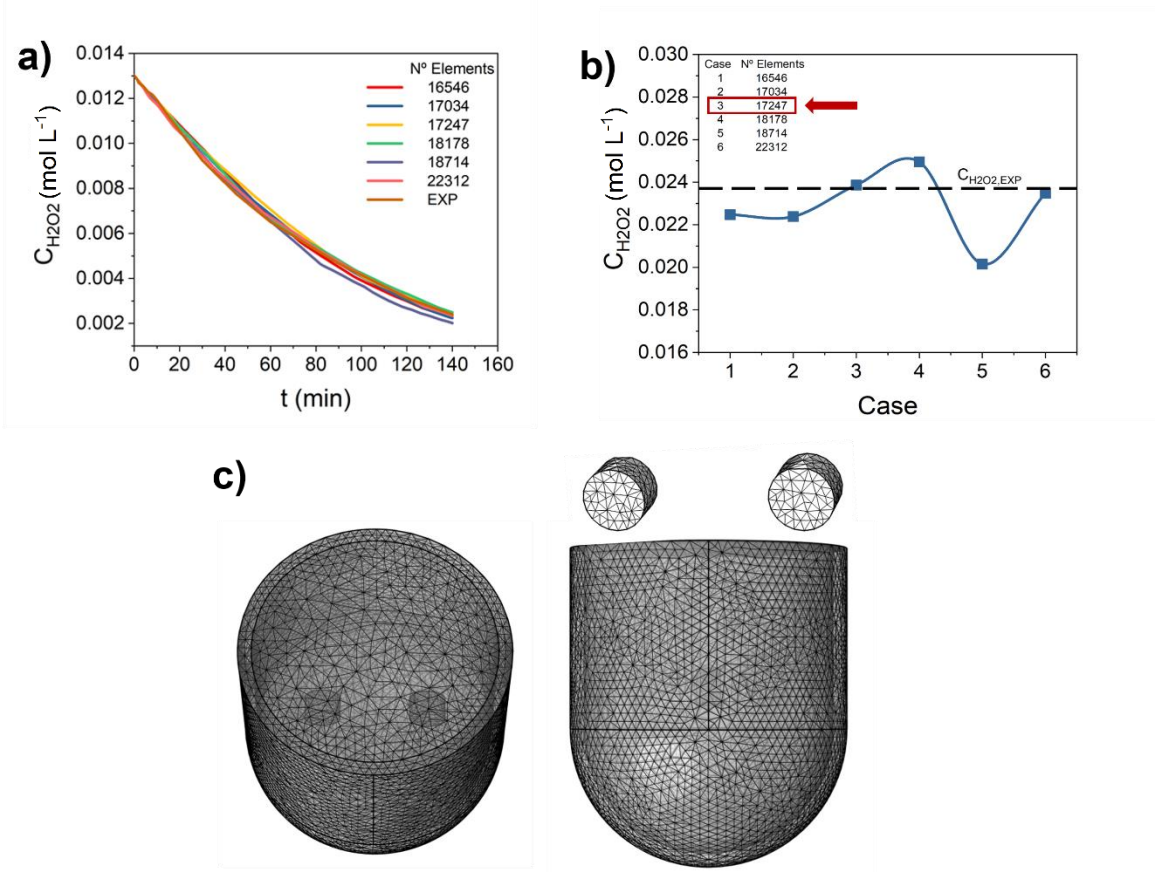


Figure S9. Mesh sensitivity analysis in COMSOL Multiphysics® for the SMR: (a) comparison between experimental and CFD concentration for then Fenton reaction at different grid meshes, (b) selection of the Normal grid mesh and (c) appearance of the selected grid mesh. Operating conditions: $C_{H2O2,0}$ = 13 mM, $C_{Fe^{2+}}$ = 0.178 mM (from $FeCl_2$ salt), T = 25 °C, pH_0 = 3 and ω = 250 rpm.