Supporting Information

A novel numerical method coupling CFD with PSO *vs.* mathematical approach in the modeling of photocatalytic degradation of NO

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The interaction tool in COMSOL Multiphysics, LiveLink™ *for* MATLAB®, allows for the creation of bidirectional integration between COMSOL Multiphysics and MATLAB platforms. The prerequisite for live link is that the COMSOL model can run independently. For the current study, the specific numerical procedures of how CFD computation in COMSOL is live-linked to PSO algorithm in MATLAB are described as follows:

Step 1: Initiate particle swarm. The particle swarm size (N = 20), the dimension of the solution space (d = 2), and the maximum iteration number (n_{max} = 50) are determined.

Step 2: Evaluate the individual fitness function. Enter commands in MATLAB Workspace to set CFD model parameters (k and K), run the CFD model, and extract calculation results. Subsequently, the fitness function value of every particle is calculated according to the extracted model prediction results and experimental results.

Step 3: Update individual extreme value and global extreme value.

Step 4: Check termination condition. Output the optimal results when the maximum iteration is reached. Otherwise, loop to Step 2 and conduct the next iteration calculation.

Step 5: Update the locations and velocities of particles.

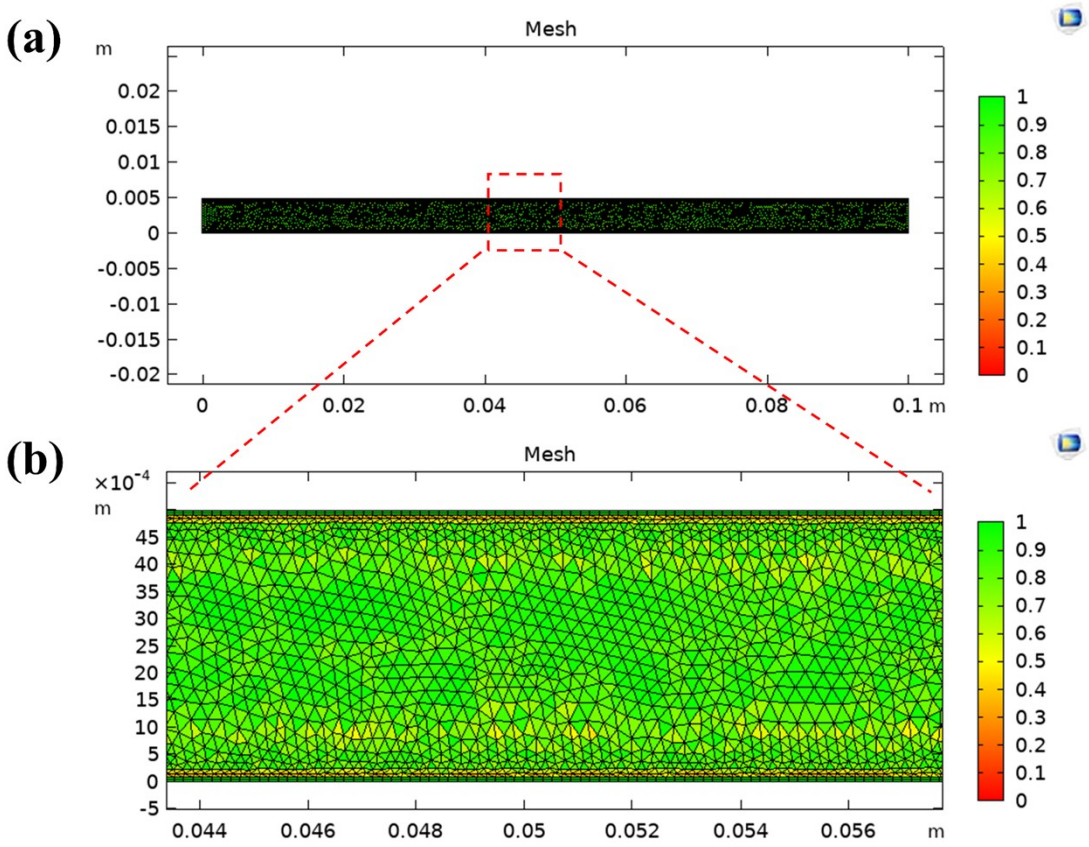

Fig.S1 Meshes for the 2D geometry (with the distribution of mesh element quality).

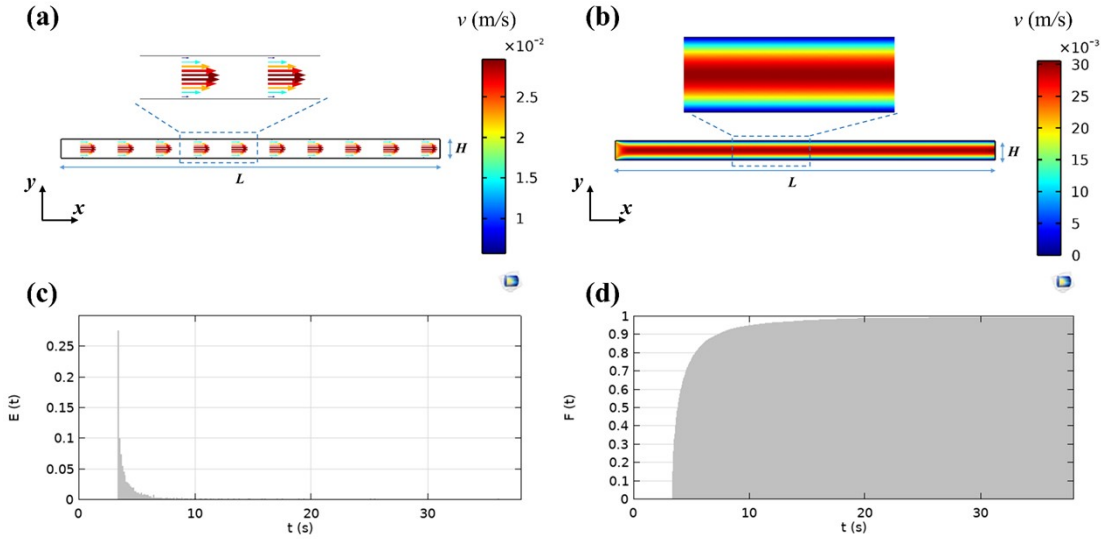

Fig.S2 The simulation results of velocity field and residence time at the flow rate of 300 mL·min^{-1}. (a)Velocity vector in the reactor, (b) velocity contour in the reactor, (c) residence time distribution, and (d) cumulative distribution function.