Indoor Air Quality Improvement Applying Photocatalytic Oxidation: a Computational Fluid Dynamics Modelling Approach

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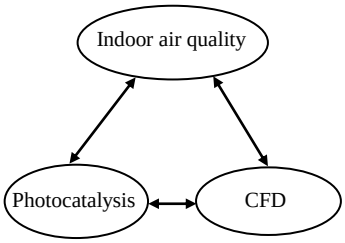

The present study addresses the indoor air quality improvement applying heterogeneous photocatalytic oxidation technology. A developed novel indoor wall covering with the air purifying function by a modified TiO_2 coated layer is applied to study the indoor air pollutants removal ability using computational fluid dynamics (CFD) approach.
A CFD model is developed in FLUENT to the reactor employed in the present study and to the photocatalytic removal of the pollutants in the reactor. The developed model is validated against the performed experiments. The effect of the experimental conditions on the pollutants removal efficiency is studied. Furthermore, the hydrodynamics of the reactor is analyzed.

1. Introduction

Heterogeneous photocatalytic oxidation (PCO) has shown to be a successful technology for water or air purification in outdoor conditions and to date the photocatalytic oxidation has been investigated intensively [2]. The PCO experiments performed under different indoor air conditions and results presented in the previous chapter prove that the PCO is also suitable for the indoor air quality improvement [1].

Computational Fluid Dynamics (CFD), a branch of fluid mechanics, uses numerical methods and algorithms to solve and analyze problems that involve fluid flows. It is widely applied to different fields such as combustion, airplane design, submarines etc. By far CFD has been also applied to reactor modelling in chemical engineering field [3,4]. But no research has yet been reported on the application of CFD on the photocatalytic oxidation of indoor air pollutants.

Employing nitric oxide (NO) as target pollutant, this article addresses its photocatalytic removal process under indoor air conditions using modelling approach. A reactor model is built applying CFD commercial software, using a kinetic model derived elsewhere [5]. The built reactor model is validated against the experimental data, in which the PCO tests were performed to a newly developed photocatalytic wall covering under a typical indoor air condition [1]. The good agreement between the predicted values and the experimental results indicates its validity. Furthermore, the influence of the experimental conditions such as the NO inlet concentration, the volumetric flow rate of the NO, the relative humidity, the irradiance, the dosage of the photocatalyst, together as well the effect of the intermediate product NO_2 is investigated.

2. Reactor modelling

The reactor model is built in 2-dimensional structure because the reactor is completely symmetrical [1]. The 2-D model provides a simpler and less time-consuming approach than the 3-D version. The geometry of the reactor, along with its boundaries, is shown in Figure 1.

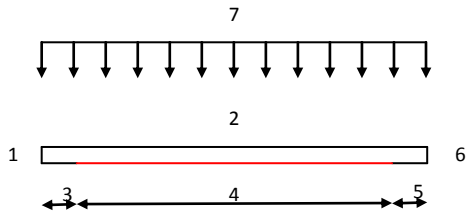

Figure 1. Geometry of the reactor model (1. Inlet; 2. Glass cover; 3. Regular surface; 4. Photocatalytically active surface; 5. Regular surface; 6. Outlet; 7. Light source).

The first step towards the CFD modelling is the creation of a mesh. Employing the software Gambit, a mesh is developed to provide the sufficient control volumes (CVs) for the CFD simulation in Fluent. Horizontally, the CVs are spaced proportionally every 2 mm, yielding 110 cells through the reactor length; while vertically, the CVs are spaced with an exponential space factor of 0.75, which results in that more CVs are

generated near the lower wall (surface 4, see Figure 1) where bigger variable gradients are expected. The performed grid independence test shows the validity of the created mesh. The second step in building the reactor model is the definition of the boundary conditions, as listed in Table 1. Here the name of each boundary is the same as defined in geometry of the reactor model, see Figure 1.

Table 1. Gambit boundary conditions.

Name	Boundary conditions
Inlet	Mass-Velocity inlet
Glass	Wall
Regular surface	Wall
Active surface	Wall
Regular surface	Wall
Outlet	Outflow

The area inside of the reactor is defined as two different zones. The first zone consists of a narrow group of cells adjacent to the active surface to simulate the surface reaction of PCO of NO_x. This region, covers 30 μm vertically (1% of the height of the reactor) and the whole length of the active surface horizontally along the reactor, is the space where the photocatalytic reactions take place. The rest of the reactor is defined as the second zone. The applied height of the photocatalytic zone is checked by performing the grid independence test and the results indicate its validity.

The conservation equations for mass and momentum of the flow in the reactor are solved in FLUENT. The flow in the reactor is assumed to be incompressible because of the ambient test conditions and the gas does not undergo any significant compression or expansion. The reactor is assumed to be isothermal because it always works under room temperature. The conservation equations for turbulent modeling are not needed because the flow in the reactor is laminar [1]. Here in the species transport equations, the used reaction rates of the reactants (NO_x) are derived from previous work [5], and the PCO reaction rates are introduced to the FLUENT solver by a user-defined function. A detailed description of all the governing equations is presented in [6].

3. Modelling results and validation

The developed reactor model is validated against the experimental data presented in [1,6]. The influence of experimental conditions such as the pollutant initial concentration, the volumetric flow rate, the relative humidity, the irradiance and the dosage of the photocatalyst on the PCO efficiency is analyzed, and the results also confirm the validity of the developed CFD model.

Throughout the whole experiments, the inlet concentrations of NO_2 are set to zero. Figure 2 shows the CFD model predictions when varying the inlet concentrations of NO. The outlet concentrations of both nitrogen oxides are correctly predicted by the CFD model in the test range, with the maximum divergence at the lowest inlet concentration.

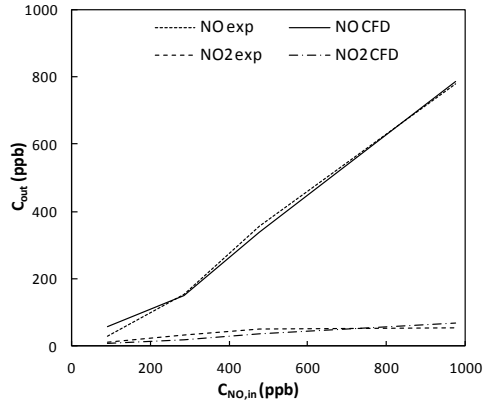

Figure 2. CFD model predictions versus the experimental results (effect of the initial NO concentration) (Q = 3 L min^{-1}; RH = 50%; I = 10 W m^{-2}).

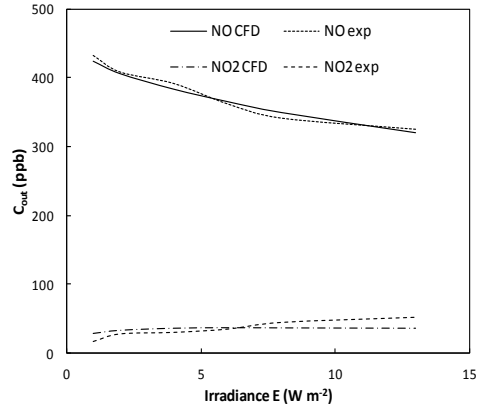

Figure 3. CFD model predictions versus the experimental results (effect of the irradiance) ($C_{NO,in}$ = 0.5 ppm; Q = 3 L min^{-1}; RH = 50%).

Figure 3 shows the CFD simulation results contrasted with the experimental data when varying the irradiance. The irradiance is varied between 1 and 13 W m^{-2} and the model performed accurately throughout the whole range when simulating the NO outlet concentrations. The concentration of NO_2 is overpredicted at 1 W m^{-2}, and underpredicted at irradiance values higher than 6 W m^{-2}.

It can be well stated that the CFD reactor model is a fair predictor through the ranges of experimental conditions, although there is still room for improvement.

4. Hydrodynamics

Figure 4 shows the velocity development of the flow at the entrance of the reactor with an inlet flow of 0.167 m s^{-1} (3 L min^{-1}). It shows that it takes only several millimeters to develop a steady-stable laminar flow, which indicates the usefulness of the added extra length at the entrance of the reactor. The maximum x-velocity is 0.247 m s^{-1} at the center of the reactor.

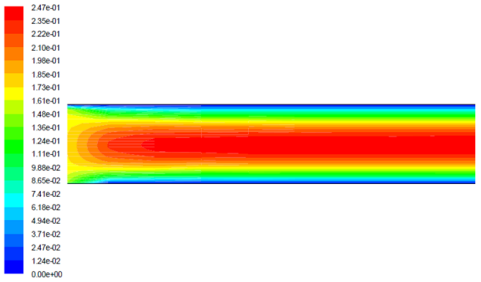

Figure 4. Contour plot of velocity magnitude (m/s) at the entrance of the reactor (first 18 mm).

Figure 5 shows the contours of static pressure. It can be seen that the pressure gradient occurs only in the horizontal direction, and a pressure drop of 0.821 Pa along the reactor is resulted.

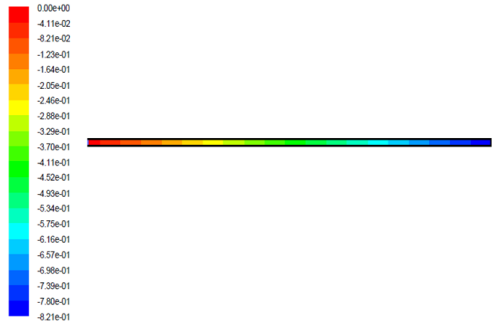

Figure 5. Contours of static pressure (Pa) along the reactor.

5. Summary

The present article addresses the indoor air quality improvement applying the heterogeneous photocatalytic oxidation technology, from a CFD modelling approach. A reactor, employed in the present study, model is developed employing a CFD software FLUENT. The photocatalytic removal of a model indoor air pollutant (NO) is investigated using a novel developed wall covering and the influential factors such as initial pollutant concentration and irradiance on the PCO effenciency are analyzed. The present results show a promising way to further study the indoor air quality improvement combining photocatalytic oxidation and computational dynamics fluid.

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