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Preliminary communication

Computational Fluid Dynamics (CFD) Modelling of Annular Reactor for Photocatalytic Degradation of Air Pollutants Using COMSOL Multiphysics Software

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Abstract: An annular reactor is a type of reactor in which chemical reactants move through an annular gap between two concentric cylinders. This type of design is suitable for a variety of chemical processes because it facilitates efficient heat transfer and mixing of reactants. Previous research has shown that this type of reactor shows promising results in the photocatalytic decomposition of pollutants, which is why it is used in air purification tests. This paper presents a model of one such type of air purification reactor modeled in COMSOL Multiphysics simulation software and provides an overview of the steps that need to be taken in order to effectively model the photocatalytic oxidation. The purpose of modelling the reactor is to test its effectiveness in computer simulations of the decomposition of pollutants in the air using the process of photocatalytic oxidation, which is a combination of photooxidation based on the effect of UV radiation and catalytic oxidation. The resulting simulations allow the scaling of the system (its increase or decrease) so that it can be adapted to certain conditions and used in the real world as a method of air purification at the very sources of polluted air.

Keywords: annular reactor; computational fluid dynamics; COMSOL multiphysics; modelling; photocatalysis

1 INTRODUCTION

Photocatalytic oxidation, also known as photocatalysis, is the process of accelerating a photoreaction in the presence of a photocatalytic agent. The method in question employs the synergistic interplay of solar radiation, catalysts, and oxidizing chemicals to degrade contaminants in a fluid (water or air). Photocatalysis development has received a lot of attention in recent years, and the technology is now being employed in a variety of products across a wide range of study disciplines. From today's standpoint, the technology in question has a high economic potential due to its utilization of solar energy. Photocatalytic oxidation can remove the following pollutants: volatile organic compounds (VOC), unpleasant odors, ammonia (NH_3), hydrogen sulfide (H_2S), methane (CH_4), nitrogen oxides (NO_X), sulfur oxides (SO_X), carbon monoxide (CO), and ozone (O_3) [1-3].

Photocatalysis is basically a reaction that requires a catalyst and a radiation source to activate it. Today, titanium dioxide (TiO_2) is the most widely used photocatalyst, and it serves as the foundation for a number of modern composite photoactive materials [4]. The combination of ultraviolet (UV) photons and TiO_2 turns adsorbed water molecules into two highly reactive powerful oxidants: hydroxyl radicals (•OH) and superoxide ions (O_2^-). The •OH radical elements have double the oxidizing power of chlorine (Cl) and breakdown organic compounds (e.g. Non-methane volatile organic compounds - NMVOC) and bacteria into carbon dioxide (CO_2) [5]. Unlike techniques that rely solely on adsorption and result in the transfer of pollutants requiring additional treatments, photocatalytic oxidation completely mineralizes organic pollutants, and operating costs are primarily due to UV lamps and electricity consumption, making it an economically viable solution. In order for photocatalytic oxidation to be effectively used in real systems and not only in laboratory ones, it is necessary to create a reactor that will provide the best possible results. This means that the reactor consistently delivers high pollutant degradation rates, uniformity of the irradiance on the photocatalytic surfaces, maintains performance over time, and operates at maximum efficiency and effectiveness while being cost-effective.

Since photocatalytic oxidation is affected by numerous conditions (such as type of photocatalyst, light source, surface area of photocatalyst, concentration of catalyst, temperature etc.) [6], the reactor itself must be designed in a way so that it can maximize its potential.

Despite a growing number of photocatalysis research and successful applications, there is still a gap between research and commercialization. Often, the processes and materials used in research are not easily scalable to commercial levels. What works in a laboratory setting might not be feasible or economical for mass production. Traditional methods of improving photocatalytic reactors can be time-consuming. Such methods rely on the design, scaling and fabrication of real-life prototype reactors for laboratory testing and are based on empirical methods (e.g. trial and error, direct observation and data collection) and iterative experimentation.

Computer modeling reduces the need for real-life prototypes and thorough testing, lowering the cost and time required to build such a system. The use of Computational Fluid Dynamics (CFD) allows for swift iteration through various designs or scenarios to maximize performance without the requirement for physical prototypes. This results in quicker product development cycles and adaption to real-world systems. By using COMSOL Multiphysics software the goal is to create a set of models which include several modules such as Ray Optics, Chemical Reaction Engineering, CFD. The aforementioned modules will be used for further modelling and optimisation of photocatalytic oxidation.

Given that there are no plentiful published papers on this topic in COMSOL Multiphysics software, this paper presents only an overview of the main physical and chemical phenomena that such model should consider, rather than the experimental results of the model. For a specific case study, the reader is referred to [7] where the first validation is shown, and usefulness of such CFD model is proven and validated.

2 ANNULAR REACTOR

There are several types of photoreactors such as monolith, annular, packed bed and flat plate which are being used and investigated experimentally for air treatment. In general, an efficient reactor requires low air velocity, high surface area and direct light radiation which falls on the reaction surface. It is precisely on this reaction surface that the photocatalytic degradation of pollutants occurs. An annular reactor (AR) is considered as a state-of-the-art reactor for the photocatalytic degradation of pollutants in the air due to uniform light distribution on the catalyst surface, great reactant-catalyst contact and relatively simple construction. Annular reactors are cylindrical in shape to provide uniform flow and made of glass for better light irradiation (Fig. 1). The inner tube separates the lamp as a source of radiation from the glass fiber mesh which serves as the photocatalyst support. The glass fiber mesh is rolled onto the inner tube (attached to the external wall) with a full-spectrum linear fluorescent lamp positioned in the middle of the inner tube (placed on the axis of the reactor). Together, they are simultaneously placed inside the annular reaction space from one side of the reactor [8-10]. AR additionally can have sampling ports which can be connected if needed for direct air quality measurements (temperature, relative humidity, concentrations).

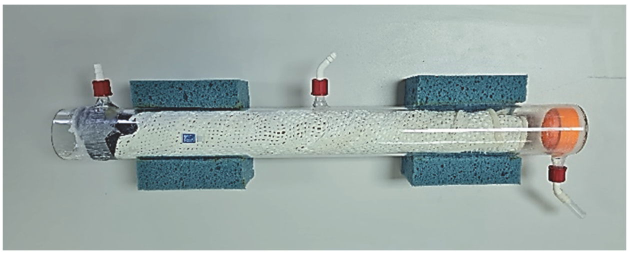

Figure 1 Representation of an annular photocatalytic reactor used in the experiments

The process of scaling up experimental laboratory reactors involves buidling a reactor from small experimental to large industrial-sized setup for the particular practical application while maintaining (or improving) performance, efficiency, and reliability. The experimental models provide an accurate and credible base for the future CFD simulations and validation of photocatalytic degradation [11]. More detailed description of the reactor setup used in the experiments can be found at [2, 12].

3 REACTOR MODELLING

Currently, CFD is a heavily used tool for the modelling of photoreactors.Tools such as this are often of general purpose and are not specifically designed for this application. Therefore, these simulations take a lot of effort and specific knowledge to be implemented in real settings. As photocatalytic oxidation becomes a more widespread technique of breaking down organic pollutants in air and water, it is important to adapt existing computational tools to this method so that they may be utilized more easily and often in today's lab testing. The modeling method for photocatalytic reactors necessitates the creation of mathematical models such as the fluid flow model, lamp emission and radiation model, absorption-scattering model, and kinetic model [13-15]. Integrating these modeling methods allows the development of comprehensive mathematical models that capture the complex interplay between light, mass transfer, reaction kinetics, and fluid dynamics in photocatalytic reactors [11].

As mentioned earlier, one of the key issues is scaling up photocatalytic reactors, and this is precisely what a well-developed mathematical model can solve. Fig. 2 displays a flowchart explaining the scaling approach. The first phase (upper part of Fig. 2) depicts the derivation of a chemical kinetic expression that is independent of the reactor configuration, radiation source, and experimental conditions, and corresponds to the photocatalytic decomposition of a model compound in a laboratory-scale reactor [11]. Intrinsic kinetics is based on a thorough photocatalytic reaction scheme and includes elements such as irradiation circumstances, photocatalyst quantity, and compound's starting concentration [11, 16]. Typically, the kinetic parameters should be estimated using a nonlinear optimization tool to fit the model predictions to the experimental data [17]. The radiation model's main purpose is to assess how radiation absorption impacts the speed of the photocatalytic reaction. The simultaneous presence of absorption and scattering is critical for radiation modeling (radiation transport equation or RTE). Mass balances of photodegraded compounds and reaction intermediates are used to determine the theoretical evolution of the species involved. These should incorporate information from the kinetic and radiation models [11, 16].

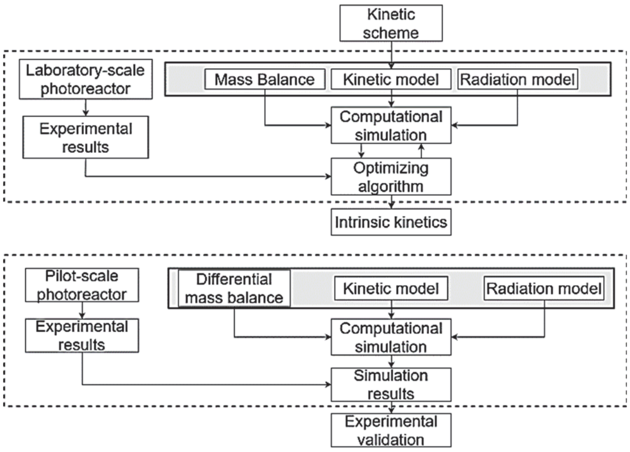

Figure 2 Flow chart of the scaling-up methodology of photocatalytic reactors [17]

In the second phase (lower part of Fig. 2), if the process scale (reactor size) is modified in the reactor model, the same kinetic model for the reaction as in the laboratory tests must be used. It is important to highlight that the local volumetric rate of photon absorption (LVRPA) must be determined by employing a different radiation balance which was estimated for the larger photoreactor. As a result, to predict LVRPA in a response space, RTE should be applied to the new reactor. The obtained expression should be included in the mass balance and used as the foundation for calculating the reactor output variables through the simulation technique. Finally, the simulation results acquired from the modeling process must be validated by comparing them to the experiments carried out in the new (pilot) reactor [11, 17].

For the purpose of modelling the annular reactor described in chapter 2 (annular reactor), COMSOL Multiphysics 6.1 software was used. The software itself is mathematical modeling software which is used for a variety of physics and engineering applications. It enables simulation of coupled physics phenomena like structural mechanics, fluid dynamics, heat transfer, electromagnetics, acoustics, and chemical reactions [18].

3.1 Fluid Flow Modelling

A precise photoreactor model should address the effect of hydrodynamic circumstances as represented by momentum balance. Photocatalytic reactors must take into account two sorts of conditions: free flow through the reaction system and flow through the porosity system [14, 19]. As is the cornerstone of the CFD approach, when modelling a given (reactor/fluid flow) system, it is important to first describe the motion of the fluid and solve this problem before solving the RTE [20].

There are various hydrodynamic models based on the flow's characteristics (laminar or turbulent). The Laminar Flow interface in COMSOL Multiphysics (which was used for modelling of the reactor) utilizes the Navier-Stokes equations to determine flow velocity and pressure. These equations define momentum balance under stationary conditions and govern fluid motion [21].

$$\rho\left(\frac{\partial u}{\partial t}+u\cdot\nabla u\right)=-\nabla p+\nabla\cdot\left(\mu\left(\nabla u+(\nabla u)^{T}\right)-\frac{2}{3}\mu(\nabla\cdot u)I\right)+F \tag{1}$$

In the above equation, u is the fluid velocity; p is the fluid pressure, Pa; ρ is the fluid density, kg/m^3; μ is the fluid dynamic viscosity, Nsm^{-2}. The various terms in Eq. (1) correspond to the inertial, pressure, viscous, and external forces applied to the fluid. The aforementioned equations are always solved along with the continuity equation [21].

$$\rho\nabla\cdot(u)=0 \tag{2}$$

The Navier-Stokes Eq. (1) represent momentum conservation, whereas the continuity Eq. (2) indicate mass conservation [21].

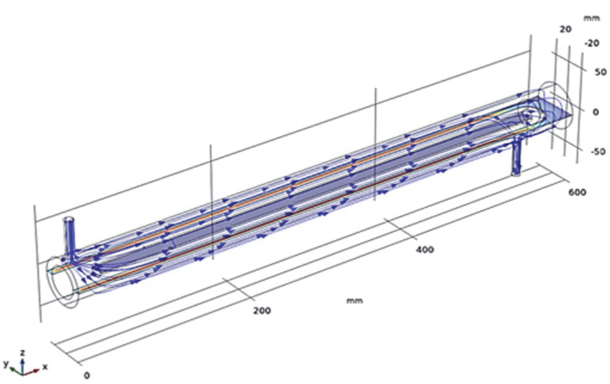

Figure 3 Visual representation of velocity contours in the modelled reactor

During the simulation, the Navier-Stokes equation is solved with no-slip boundary conditions to calculate the fluid's pressure and velocity in the model. These equations form the core of fluid flow modeling. In the given geometry of the model, solution of these equations enables the forecast of fluid velocity and pressure for the given boundary conditions (inlets, outlets, and walls). These equations have a limited number of analytical solutions due to their complexity. Previous research has demonstrated that such traditional Navier-Stokes equations are effective for determining the hydrodynamic properties of single-phase photoreactor systems [21].

3.2 Lamp Emission and Radiation Modelling

In photocatalytic reactors, there are three methods of lighting: direct illumination (as in immobilized photoreactors); with a lamp immersed in the reaction environment (suspension reactor); using reflecting devices (parabolic or elliptical) [22]. The preceding specifies the creation of the light bulb emission model. The lamp emission model is significant because of the effects of refraction, reflection, and absorption of radiation before substance enters the reaction space. Everything aforementioned needs to be incorporated as boundary conditions during CFD radiation modelling [22].

The discrete ordinates method (DOM) which is used in COMSOL Multiphysics software represents a numerical technique used for solving the radiative transfer equation (RTE) in problems involving thermal radiation for a collection of directions spanning the entire solid angle range of 4π around a point. This is important because RTE equation describes the transport of radiant energy through a medium, accounting for absorption, emission, and scattering. The RTE for a finite cylindrical medium that emits, absorbs, and scatters linearly and anisotropically can be expressed as follows [18, 23]:

$$\Omega\cdot\nabla I(\Omega,s)=\kappa I_b(T)-\beta I(\Omega,s)+\frac{\sigma_s}{4\pi}\int_0^{4\pi}I(\Omega,\Omega')\Phi(\Omega,\Omega')\partial\Omega' \tag{3}$$

where $I(\Omega, s)$ is radiation intensity at a given position s in the direction $\mathbf{\Omega}$; T is temperature; κ, β, σ_s are absorption, extinction, and scattering coefficients; $I_b(T)$ is the blackbody radiation intensity; $\Phi(\mathbf{\Omega}, \mathbf{\Omega}') = 1 + \alpha_1\mu_0$ where $\mu_0 = \mathbf{\Omega} \times \mathbf{\Omega}'$ is the cosine of the scattering angle [23].

The cylinder walls' boundary intensities are computed by adding the effective emitted intensity and the reflected incident intensity in the given direction [23]:

$$I_{i,bnd}(\Omega)=\varepsilon_w I_b(T)+\frac{\rho_d}{\pi}+q_{\text{out}} \tag{4}$$

for all such that $n\ \ \Omega < 0$

where ε_w is the surface emissivity, which is in the range [0, 1]; $\rho_d = 1 - \varepsilon_w$ is the diffusive reflectivity; n is the outward normal vector; q_{out} is the heat flux striking the wall [23].

$$q_{\text{out}}=\int_{n\cdot\Omega_j>0}(n\cdot\Omega)I(\Omega,s)\partial\Omega' \tag{5}$$

The equations above can be discretized in Cartesian coordinates for monochromatic or grey radiation as [23]:

$$\Omega_i \cdot \nabla I_i = \kappa I_b(T) - \beta I_i + \frac{\sigma_s}{4\pi}\int_0^{4\pi} I(\Omega, \Omega')\Phi(\Omega, \Omega')\partial\Omega' \quad (6)$$

The S_n approximation of the RTE in the direction i can be expressed as [23]:

$$\Omega_i \cdot \nabla I_i = \kappa I_b(T) - \beta I_i + \frac{\sigma_s}{4\pi}\sum_{j=1}^{n}\omega_j I_j \Phi(\Omega_j, \Omega_i) \quad (7)$$

The values of $\Omega_{i,1}$, $\Omega_{i,2}$ and $\Omega_{i,3}$ define the direction cosines of Ω_i, satisfying the condition $\Omega_{i,1}{}^2 + \Omega_{i,2}{}^2 + \Omega_{i,3}{}^2 = 1$. The index j in the equation above represents the direction of incoming radiation, which contributes to the direction Ω_i.

The equation for a diffuse reflecting surface on a wall boundary can be translated as follows [23]:

$$I_{i,bnd} = \varepsilon_w I_b(T) + \frac{\rho_d}{\pi} + \sum_{n \cdot \Omega_j > 0} \omega_j I_j n \cdot \Omega_j \quad (8)$$

for all Ω such that $n \ \Omega < 0$

So far, the DOM process for radiation prediction has proven to be an elegant and accurate way for simulating multidimensional heat transfer by radiation in cylindrical geometry [23].

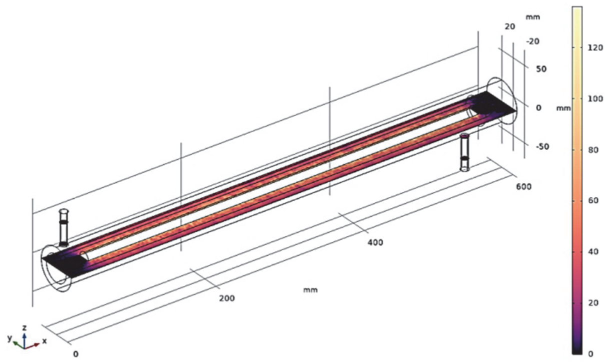

Figure 4 Visual representation of the intensity of UV radiation in the modelled reactor / mW cm^{-2}

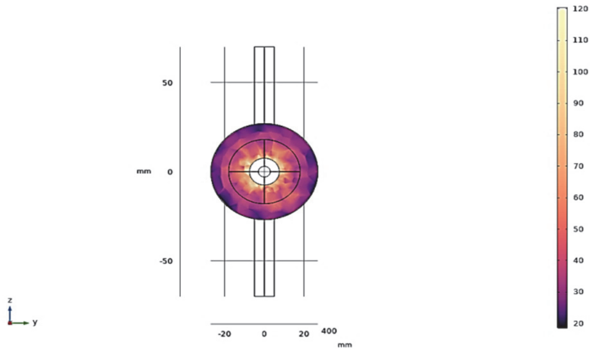

Figure 5 Visual representation of the intensity of UV radiation from the front side of the modelled reactor / mW cm^{-2}

3.3 Modeling of Chemical Reactions and Transport of Pollutants Through the Reactor

Simulations are useful in chemical reaction engineering because they allow to investigate and optimize a specific reaction process. Modelling chemical processes allows to better understand the chemical reactions that take place within the model, determine the best size and design of the system, and observe how it interacts with other physical aspects that may occur.

After establishing the fluid flow through the reactorr and the radiation emissions from the lamp, it is requiredd to characterize the chemical reactions that occur within the reactor. COMSOL Multiphysics allows to define the reaction mechanism using the Chemistry interface. This interface is a tool for creating a set of variables used to model chemical species and reaction systems. Variables are derived from species and reaction properties and are classified into two types [18]:

- rate expressions and heat sources for use in mass and heat balances,
- material property variables (mixture density, diffusivity, viscosity, and so on) for use in spatially dependent transport equations.

As photocatalysis is a process that uses light energy to catalyze chemical reactions with the help of a catalyst, it is necessary to define the reactants and the final product of the reaction. For example, if we want to oxidize methane (CH_4) into less harmful carbon dioxide (CO_2) with the help of photocatalysis, the reaction equation in which methane (CH_4) (pollutant) and TiO_2 (catalyst) are reactants, and carbon dioxide (CO_2) is the final product of the reaction can be written as:

$$\mathrm{CH_{4(g)}} + \mathrm{TiO_{2(ads)}} \Rightarrow \mathrm{CO_{2(g)}} \quad (9)$$

The arrow ("=>") signifies an irreversible reaction, as evidenced by the label itself. Other labels in the computer program include "<=>" for a reversible reaction and "=" for an equilibrium reaction. By doing the above, the program interface begins examining the substances involved in the chemical equation and automatically adds the associated features.

With the Transport of Diluted Species interface it is possible to calculate the transfer and reaction of pollutants in the reactor. The time-dependent advection and diffusion equation can be coupled to the stationary velocity field vector u to represent pollutant transfer (assuming an acceptable gas flow rate at the reactor inlet and constant ambient pressure):

$$\frac{\partial C_{pollutant}}{\partial t} = \nabla \cdot \left(D \nabla C_{pollutant}\right) - u \cdot \nabla C_{pollutant} \quad (10)$$

where $C_{pollutant}$ is the inlet concentration of pollutant in the reactor, molm^{-3}; D is mass diffusion coefficient of pollutant in air, m^{2}s^{-1}. Eq. (10) explains the evolution of pollutant concentration in the flow due to diffusion (first term on the right side of the equation) and advection (second term on the right side) of pollutant molecules.

3.4 Modelling of Adsorption and Desorption

Important stage in photocatalysis is the adsorption of pollutants on the catalyst surface. In a typical photocatalytic process using a semiconductor, the reactant species must first be adsorbed onto the surface of the photocatalyst. As a result, the efficiency of the photocatalyst is directly proportional to its adsorption capacity.

The adsorption process can be defined as the equilibrium reaction [24]:

$$\mathrm{A}_{(g)} \rightleftarrows \mathrm{A}_{(ads)} \tag{11}$$

In the above equation, the chemical species $A_{(g)}$ in the gas phase is called an adsorbate. In photocatalysis, adsorbate is adsorbed at a specific rate of adsorption and is then desorbed at a certain rate of desorption.

The way in which this equilibrium reaction is mathematically described is with the help of the Langmuir adsorption model, which results from the following assumptions [25]:

- There is a maximum surface concentration of adsorbate, c_{sat}, molm^{-2}, at which the surface of adsorbate becomes saturated.
- The partial coverage of the adsorbate has no effect on the adsorption rate constants, as all adsorption sites are equal and mutually independent.
- Adsorption is a second-order process with a rate that is proportional to both the concentration of the adsorbate in the mass phase at the surface and the proportion of vacancies.
- Desorption is a first-order process that occurs at a linear rate as the adsorbate is partially covered.

Using the above mentioned assumptions, the adsorption-induced flow of material to the surface can be described as follows [24]:

$$N_{ads} = k_{ads} \cdot C_A \cdot C_{sat} \cdot (1-\theta) \tag{12}$$

where N_{ads} is surface flux, mol m^{-2}s^{-1}; k_{ads} is adsorption rate constant, m^{3}mol^{-1}s^{-1}; C_A is concentration on the surface in the adjacent mass phase, molm^{-3}; C_{sat} maximum surface concentration of adsorbate, molm^{-2}; θ is fractional adsorbate coverage, which can be defined as:

$$\mathrm{C}_{A,ads} / \mathrm{C}_{sat} \tag{13}$$

$C_{A,ads}/C_{sat}$ is unitless, so $(1-\theta)$ in Eq. (12) represents the proportion of vacant sites.

Similarly, the flux of material from the surface due to desorption can be represented as [24]:

$$N_{des} = k_{des} \cdot C_{sat} \cdot \theta \tag{14}$$

where k_{des} is the desorption rate constant, s^{-1}.

The adsorbate's surface coverage is constant at equilibrium, hence fluxes to and from the surface must be equal. By equating and canceling common concepts, we get:

$$\frac{k_{ads}}{k_{des}} \cdot C_A \cdot \left(1-\theta\right) = \theta \tag{15}$$

The equilibrium constant for adsorption is defined as k_{ads}/k_{des}. The higher the equilibrium constant, the stronger the thermodynamic driving force for adsorption. Finally, by rearranging the statement Eq. (15), the partial surface coverage can be expressed as [24]:

$$\theta = \frac{K_{ads} \cdot C_A}{1 + K_{ads} \cdot C_A} \tag{16}$$

The Langmuir adsorption isotherm is represented by Eq. (16). For a particular temperature and K_{ads} value, the fractional covering of the adsorbent surface in equilibrium can be estimated as a function of its total concentration [24]. Langmuir's model represents a simplistic approximation. In realistic real-world systems, interactions between surrounding adsorbed molecules are commonplace so as fractional surface coverage increases, adsorbing new material becomes simpler or more difficult [24]. As a result, more complex mathematical models have been developed to better account for real-world adsorption processes. For example, the Freundlich isotherm has an additional empirical constant that can account for interactions between adsorbed molecules [24, 26]. The Brunauer-Emmett-Teller (BET) isotherm can be utilized in systems with multilayer adsorption, which means that the second and subsequent layers of adsorbed molecules are attached to molecules of the same type rather than the chemical substrate's underlying surface [24, 27].

Fig. 6 and Fig. 7 show the photocatalytic oxidation of pollutants in the gaseous phase in an annular reactor. An example of a pollutant is methane (CH_4), which oxidizes during the photocatalysis process and turns into much less harmful carbon dioxide (CO_2). Fig. 6 shows how methane molecules are adsorbed onto the surface of the photocatalyst material in a time period of 150 minutes, while Fig. 7 shows the carbon dioxide (CO_2) molecules that are produced in the reaction (desorption).

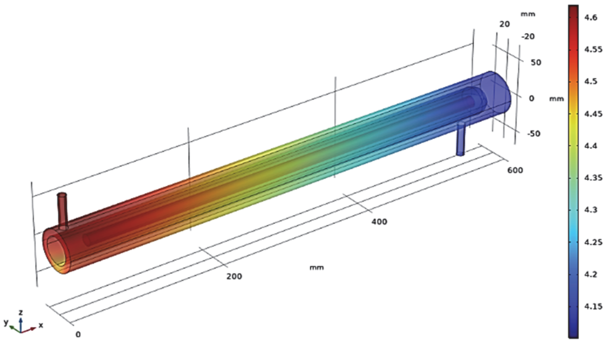

Figure 6 Photocatalytic oxidation of CH_4 into CO_2 in modelled annular reactor (CH_4adsorption), molm^{-3}

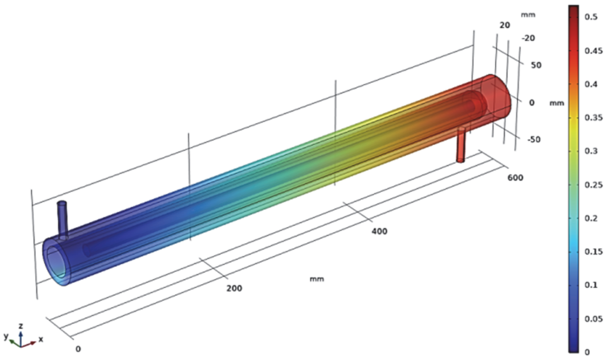

Figure 7 Example of photocatalytic oxidation of CH_4 into CO_2 in modelled annular reactor (CO_2desorption), molm^{-3}

4 DISCUSSION

Mathematical modeling in various softwares like COMSOL Multiphysics is used to simulate and analyze a wide range of physical phenomena in a variety of engineering and scientific fields. It enables development of mathematical representations of physical systems and solves complex partial differential equations (PDEs) that control these systems to forecast their behavior under various scenarios.

A variety of factors can influence photocatalyzation's effectiveness. Modeling allows the optimization of the entire system in order to find the most efficient one for one's purpose. It enables the testing of various design configurations, material qualities, and operating circumstances in order to reach specified performance objectives. Optimization algorithms built into the software can further optimize the design to fulfill specific objectives, such as lowering power usage or increasing efficiency. It is because of modelling that significant cost and time savings can be achieved compared to traditional experimental methods. By conducting virtual experiments through simulations, a wide range of design scenarios can be explored without the need for physical prototypes. As photocatalytic oxidation is an interplay of various factors and processes involved and is influenced by a multitude of factors, this accelerated design iteration process reduces development cycles and associated costs. Therefore, it is important to conduct several studies in order to find the optimal parameters for the most efficient photocatalytic oxidation of the target pollutant. In case of multiple contaminants, several experimental sets should be done. Each contaminant must be studied individually to check both adsorption and oxidation. In some cases, contaminants could be treated like a group during the modelling [28].

Since photocatalysis is a process where pollutants are degraded or converted into less harmful substances using light-activated catalysts, its efficiency of photocatalysis depends on several factors. These factors can be broadly categorized into catalyst-related factors, environmental conditions, and properties of the pollutants being treated.

Through modeling, it can be seen how the following critical parameters affect the efficiency of the photocatalytic degradation of a certain pollutant in a relatively short time [29]:

- Catalyst morphology (e.g., particle size, shape, and surface structure) influences surface area, light absorption, and catalytic activity. A bigger surface area and clearly defined crystal faces can enhance photocatalytic activity.
- Light intensity: Higher light intensity increases the number of electron-hole pairs formed in the photocatalyst. In this method, photocatalytic activity is increased. However, too much light can degrade the catalyst or create adverse effects, thus it is critical to select light that will ideally excite the chosen catalyst.
- Temperature and humidity: Temperature influences the reaction kinetics in the process, whereas humidity influences pollutant adsorption on the catalyst surface. These parameters within the reactor are thus critical for ensuring efficient photocatalytic degradation.
- Pollutant concentration and type: Higher pollutant concentrations can saturate the active sites on the catalyst's surface, resulting in the reduction efficiency of photocatalytic oxidation. Aside from the foregoing, contaminants' chemical type and structure influence their reactivity and degradation kinetics.
- Adsorption affinity: The adsorption affinity of pollutants to the catalyst might influence their availability for oxidation and the overall efficiency of the process.
- Air flow: The speed of the air flow can play a crucial role in influencing the photocatalytic oxidation of a certain pollutant, since it determines the mass transfer of the pollutant to the surface of the photocatalyst within the reactor itself. Higher air velocities can promote better mixing and distribution of reactants in such a cylindrical space, ensuring more efficient contact with the photocatalyst. Also, the speed of air flow affects the stagnation of pollutants (gas) inside the reactor itself, which can lead to an uneven distribution of reactants and thus to a reduced efficiency of the photocatalytic process. By optimizing the speed of the air flow, the time required for the reactants to spend in contact with the photocatalyst is also optimized, which reduces the unnecessary retention time of the reactants in the reactor.
- The length of the tube of the annular reactor. The length of the pipe can potentially have a significant impact on the effective oxidation of pollutant in the photocatalysis process since the length of the pipe determines the retention time of the reactants in the reactor. The aforementioned affects the way that polluting substances (reactants) have to travel a longer path which results in an extended retention time. This enables more opportunities for photocatalytic oxidation.
- Reactor geometry and configuration: The design of a photocatalysis reactor influences light distribution, residence time, and catalyst use. The reactor's geometry should be tuned to maximize photon penetration while minimizing photon loss.

By optimizing the above-mentioned factors, the efficiency of photocatalytic oxidation can be improved for various environmental remediation and purification applications. In this way, the influence of certain parameters on the efficiency of the photocatalytic processes can be clearly predicted. Experiments and system optimization involving trial-and-error by simulating certain optimization conditions can take hours (depending on the level of detail of the modeled reactor) instead of days or weeks. This refers mostly to the scaling of the system itself, since in real life scenarios each reactor for the photocatalytic process will need to be adapted for specific use. More practical implementation of other types of CFD models can be found in [30-33].

5 CONCLUSION

Photocatalytic oxidation has yielded promising results in studies on the breakdown of organic contaminants in air and water. It has been shown to successfully degrade a wide range of organic chemicals, including volatile organic compounds (VOCs), ammonia (CH_3), methane (CH_4), insecticides, and dyes, into innocuous components like carbon dioxide (CO_2) and water (H_2O). As a result, it is required to create new technologies for using photocatalysts in a variety of basic applications.

Traditional experimental methods for improving photocatalytic reactors can be very time-consuming so computer modelling represents alogical step-up in development of reactors for photocatalytic oxidation. Computer modeling eliminates the need for actual prototypes and thorough testing, considerably lowering the costs and time required to develop such a system for application at the source of pollutant release. The use of computational fluid dynamics allows for rapid iteration through various designs or scenarios to maximize performance without the requirement for physical prototypes, resulting in quicker product development cycles and adaption to real-world systems. While CFD modeling offers great capabilities for simulating fluid dynamics, it does have inherent limits that can impair the accuracy and application of its results. Most notable limitations would be high computational demand, user's knowledge of the very physics that need to be used for specific purposes in modeling, software limitations and need to validate data against experimental data to ensure reliability (which can be expansive time-consuming).

Modelling of photoreactors is today primarily focused on Computational Fluid Dynamics (CFD) technologies which are primarily tools for general purpose and are not specifically designed for use in photocatalytic processes. Because of this, adopting such simulations requires a significant amount of time and specialized knowledge. Because photocatalytic oxidation is becoming an increasingly common way of breaking down organic contaminants in a fluid, it would be required to adapt the present computer tools to this method so that they could be utilized more simply and in today's laboratory experiments. This could potentially ease the development of suitable technology for use in various real systems.

In commercialization of photocatalytic processes, scaling up of photocatalytic reactors can be considered a key step. There are several processes and parameters to consider throughout the scaling process, thus methods based on correctly built mathematical models such as hydrodynamics, reaction kinetics and radiation are required. This ensures a reliable prediction of the proposed photoreactors' performance, allowing them to be manufactured and potentially deployed in the real world at pollution sources (such as gas wells on waste landfills for example).

6 REFERENCES

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