Chapter

Hydrodynamic Analysis on a Photocatalytic Reactor Using ANSYS Fluent®

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Abstract

Solar technology includes a wide variety of developments in environmental applications that include photovoltaic cells and photocatalytic devices, among others. Sunlight usage as a clean energy source is highly desirable in technology applications. The main interest of this proposal is to carry on with hydrodynamic analysis in photocatalytic reactors applications where sunlight is used to activate a chemical reaction to degrade water pollutants and calculations are based in computational fluid dynamics (CFD) using ANSYS®. The different steps, geometric domain, preprocessing steps, setup, and postprocessing steps, are described to display an analysis of a numerical calculation during the design of a photocatalytic reactor using the commercial software ANSYS Fluent®. This work may help as a guide for chemical reactor design and includes a numerical solution of one case for a photocatalytic reactor during its design process. In addition, simplifications are explained which enable the designer to make an efficient process of the numerical calculation. Calculations and analysis are carried over in ANSYS Fluent® a powerful multi-physics program suite to develop photocatalytic reactors.

Keywords: hydrodynamics, CFD, ANSYS®, photocatalysis, chemical reactor

1. Introduction

Chemical reactor design is a complex task that requires multiple disciplines working together to obtain an efficient design. Among the different tools that can be used during the chemical reactor design development, computational fluid dynamics (CFD) is one that has attracted attention due to the interesting extent of simulation capabilities that latest code versions offer. In this chapter, the main focus relates to the first step that needs to be resolved during a CFD simulation, that is, fluid dynamic simulation.

Supported by brief theoretical fundamentals as design guidelines and software tools such as computer-aided design (CAD) and ANSYS Fluent®, a case of study for

a photocatalytic reactor is presented in this chapter. The case of study focuses in the fluid dynamic simulation for practical reasons in regard to the extent needed to be explained further from this simulation. The chapter intends to capture the essence of the first step in the CFD simulation task on the reactor design development and be a general guide for other developments of similar reactors.

2. Chemical reactors

Chemical reactor design is a complex task that requires multiple disciplines to interact, so a final product may be achieved. Due to the high complexity involved, there are extensive literature covering the chemical reactor design. The present chapter intends to be a brief view to a case where a chemical reactor design intends to simulate the hydrodynamics of the reactor [1, 2].

Chemical reaction engineering (CRE) is mentioned in several sections assuming the reader has an idea of this area, but the case displayed in this chapter only simulates hydrodynamics without going further in the process to develop CRE. For more information related to CRE, the authors recommend to consult textbooks on this matter.

A chemical reactor may be defined as an equipment unit in a chemical process (plant) where chemical transformations (reactions) take place to generate a desirable product at a specified production rate, using a given chemistry. Usually, the performance of the chemical reactor plays a pivotal role in the operation and economics of the entire process since its operation affects most other units in the process (separation units, utilities, etc.), so an efficient reactor design will reflect deeply in the plant performance [2].

2.1 Chemical reactor brief background

Classifying chemical reactors is a difficult task due to the great variation available; in fact, reactor features may be as unlimited as the designer's imagination. In general, reactors may be classified by three main characteristics:

1. Mode of operation (e.g., batch, continuous, semi-batch).

2. Geometric configuration (e.g., tubular, agitated tank, radial flow).

3. Contacting patterns between phases (e.g., packed bed, fluidized bed, bubble column).

Another practical classification is based in reactor operations that may be based in the way their temperature (or heat transfer) is controlled. Three operational conditions are commonly used:

i. Isothermal operation—the same temperatures exist throughout the reactor.

ii. Adiabatic operation—no heat is transferred into or out of the reactor.

iii. Non-isothermal operation—the operation is neither isothermal nor adiabatic.

There are terms commonly used that are recommended to at least have an idea of what they mean, for example, batch reactors, semi-batch reactor, distillation reactor, continuous reactor (flow reactors), residence time, etc. These terms are explained in textbooks related to reaction engineering or chemical reactor

design. Also, there are common configurations of continuous reactors that a designer should have at least an idea of them, such as tubular reactor, continuous stirred-tank reactor (CSTR), and cascade of CSTRs, among others. For multiphase reactions, the contacting patterns are used as a basis for classifying the reactors. Common configurations include packed-bed reactor, moving-bed reactor, fluidized-bed reactor, trickle-bed reactor, bubbling column reactor, and others (e.g., spray reactor, slurry reactor, membrane reactor, etc.) [1–4].

2.2 Photocatalytic reactors

Photocatalysis is based in the photocatalyst absorption of radiant energy (visible or UV), normally an oxide semiconductor, which accelerates the reaction rate. The photocatalysis main advantage relates to the use of solar energy as a clean primary source of energy in its processes. The difference between photocatalysis and catalysis is found at the method to activate the catalyst, because the former uses photonic energy for activation in substitution of thermal activation used in conventional catalysis [4].

The photocatalytic process starts when the semiconductor receives photonic energy from the light source with an energy equivalent or higher than band gap ($h\upsilon \geq E_g$) and a pair electron hole ($e-/h+$) with opposite charge is generated. Charges $e-/h+$ generated migrate to the semiconductor surface. The electron at the interphase may be transferred to an acceptor or oxidant molecule in such a way that the excited electron in the conduction band produces the reduction semi-reaction. In contrast, the electron transfer from a reducing molecule to fill a hole in the valence band produces the oxidation semi-reaction, which potentially will generate the hydroxyl radicals or other radical species considered responsible of the photocatalytic activity. The simultaneous oxidation reduction reactions occur at the catalyst surface, at the interphase between the excited solid and the fluid (liquid or gas). During the design process, electronic transfer process effectiveness needs to be considered taking into account that there is a competition with the electron–hole recombination because this last process dissipates in heat the energy absorbed by the photon.

Another consideration the designer needs to account for is the operation mode for the reactor. For example, it may be continuous with single step or in batch. If degradation occurs in a single step, then reactor size and flow rate need to be carefully defined to make sure the desired pollutant degradation is reached, and it may be possible to increase the number of reactors for that purpose. In discontinuous mode or batch mode, the fluid is stored in a tank and is recirculated continuously through the reactor until the desired pollutant concentration is reached. Batch mode operation is the most used option [1–3].

A photoreactor specifically with two features is considered more important; these features are (a) catalyst load and configuration and (b) light source type.

TiO_2 photoactivation requires light radiation with a wavelength of at least 384 nm and a maximum absorbance approximated to 340 nm. The required radiation may be generated by artificial illumination (lamps) or with sunlight illumination. Artificial light sources are in general multidirectional, and it is common to use reflectors to direct or focus the light emitted to the reactor. In contrast, sunlight is considered unidirectional. In consequence, reactor design depends on the light source since its geometry and dimensions are oriented to capture the most ideal way to capture available light [3, 4].

2.3 Chemical reactor design highlights

Due to the diversity of applications and numerous configurations of chemical reactors, a generic design procedure is impossible in order to describe reactor

operations. It is necessary to identify the characteristics of the chemical reaction and the main features that the reactor should provide and from there define the next steps. Once these are identified, the appropriate physical and chemical concepts are applied to describe the selected reactor operation [1–5].

3. Computational fluid dynamics

Computational fluid dynamics (CFD) is the analysis of systems involving fluid flow, heat transfer, and associated phenomena such as chemical reactions by means of computer-based simulation. This methodology is very powerful and may be used in a wide range of industrial and nonindustrial application areas. For hydrodynamic simulations, CFD is the proper methodology that may be used during reactor design procedures.

3.1 CFD methodology

CFD codes may be considered a series of numerical algorithms that can resolve fluid flow problems. Commercial CFD packages include sophisticated user interfaces to facilitate the process of input problem parameters and to examine the results, and our interest within this chapter is the code ANSYS® [6, 7]. Most codes contain three main elements: (a) a preprocessor, (b) a solver, and (c) a postprocessor. There are external functions that can be coded as additional or complementary functions that can add up to the calculations and results; for ANSYS Fluent® these functions are known as user-defined functions (UDFs) [8]. Briefly, the function of each of these elements within a CFD code is mentioned [1–5].

3.1.1 Preprocessing

Preprocessing consists of the input of a flow problem to a CFD program by means of an interface and the subsequent transformation of this input into a data ready to use by the solver. The user activities at the preprocessing stage involve geometry definition (domain), grid generation (mesh), physical and chemical phenomena to be modeled, fluid properties, and boundary conditions.

3.1.2 Processing

There are three different schemes for numerical solution techniques: finite difference, finite element, and spectral methods. In this work only finite volume method will be considered, a special finite difference formulation that is central to the most well-established CFD codes including the program used in our case of study ANSYS Fluent®. The numerical algorithm to resolve the problem at hand consists of the following steps: governing equations, discretization, and solution of algebraic equations.

3.1.3 Postprocessing

In this step, results are available, and thanks to the visualization code tools, the data may be presented in different ways to facilitate the results analysis. The leading CFD packages are equipped with versatile data visualization tools. These may include domain geometry and grid display, vector plots, line and shaded contour plots, 2D and 3D surface plots, particle tracking, and view in perspective (translation, rotation, scaling, etc.), and more recently, animation has been included.

Most codes produce trusty alphanumeric output and have data export facilities for further manipulation external to the code which also represents a possibility to enhance the result analysis and solution presentation/explanation procedures.

3.2 Governing equations

The governing equations of fluid flow represent mathematical statements of the conservation laws of physics: (a) mass conservation, (b) momentum conservation, and (c) energy conservation.

The fluid will be subject to the theory of the continuum. For the analysis of fluid flows at macroscopic length scales (around 1 μm and larger), the molecular structure of matter and molecular motions may be ignored. The behavior of the fluid is described in terms of macroscopic properties, such as velocity, pressure, density and temperature, and their space and time derivatives. These may be thought of as averages over a suitable large number of molecules. We will save the mathematical development because it is beyond the scope of this chapter and recommend the reader to consult CFD textbooks for such purpose.

4. Hydrodynamic calculations

As mentioned in prior sections, the design of a chemical reactor involves several steps and disciplines, and simulation hydrodynamic calculations are the first to be carried on. Fluid kinematics deals with describing the motion of fluids without necessarily considering the forces and moments that cause the motion. In this section, we introduce fundamental kinematic concepts related to flowing fluids. We discuss briefly the material derivative and its role in transforming the conservation equations from the Lagrangian description of fluid flow (following a fluid particle) to the Eulerian description of fluid flow (pertaining to a flow field).

The kinematics of experiments under the Lagrangian description involves keeping track of the position vector of each object, x_A, x_B,. ..., and the velocity vector of each object, V_A, V_B, ..., as functions of time. When this method is applied to a flowing fluid, we call it the Lagrangian description of fluid motion. From a microscopic point of view, a fluid is composed of billions of molecules that are subject to continuous collisions into one another, somewhat like billiard balls, but the task of following even a subset of these molecules is quite difficult, even for our biggest computers.

A more common method of describing fluid flow is the Eulerian description of fluid motion. In the Eulerian description of fluid flow, a finite volume called a control volume is defined, through single piece of volume fluid flows in and out. We do not need to keep track of the position and velocity of a mass of fluid particles of fixed identity. Instead, we define field variable functions of space and time, within the control volume [3–5]. For example, the pressure field is a scalar field variable for general unsteady tridimensional fluid flow in Cartesian coordinates:

Pressure field:

$$\vec{P}=P\left(\vec{x},\vec{y},\vec{z},t\right) \tag{1}$$

We define the velocity field as a vector field variable in a similar fashion:

Velocity field:

$$\vec{V} = V\left(\vec{x},\vec{y},\vec{z},t\right) \tag{2}$$

Likewise, the acceleration field is also a vector field variable:

Acceleration field:

$$\vec{a} = a\left(\vec{x},\vec{y},\vec{z},t\right) \tag{3}$$

Collectively, these (and other) field variables define the flow field. The velocity field of Eq. 2 is expanded in Cartesian coordinates (x, y, z) and (i, j, k) as:

$$V = \left(\vec{u},\vec{v},\vec{w}\right) = u(x,y,z,t)\hat{i} + v(x,y,z,t)\hat{j} + w(x,y,z,t)\hat{k} \tag{4}$$

We will leave for other texts the mathematical development of the Lagrangian and Eulerian descriptions since we are interested in a qualitative interpretation more than the mathematical concepts. In the Eulerian description, we do not really care what happens to individual fluid particles, but we are concerned with the pressure, velocity, acceleration, etc., of whichever fluid particle happens to be at the location of interest at the time of interest. The Eulerian description is often more convenient for fluid mechanic applications. Furthermore, experimental measurements are generally more suited to the Eulerian description [3–5].

4.1 First hydrodynamics

In this work, the intention is to resolve and analyze one of the most important steps during the chemical reactor design process, in particular, for a case related to a photocatalytic reactor. This section establishes the importance of hydrodynamics in chemical reactor design for water remediation focusing in photocatalytic reactors. The fluid dynamics is a part of the reactor design process that among the simulation activities should be resolved in the first place. Fluid dynamic results can be complemented by chemical reaction simulation, chemical species, radiation from light source effects, etc.

4.2 Proposed model to incorporate CFD calculations in chemical reactor design

In this type of reactors, the phenomena occurring in the device may be explained by four different processes: (i) fluid mechanics, (ii) heat transfer (radiation), (iii) mass transport, and (iv) chemical reaction. These different processes may be considered the steps to follow or a design methodology. It works better if used as a recirculated cyclic process because at some point some experimental parameters will be needed. For example, a kinetic intrinsic model for the chemical degradation of the selected pollutant(s) is needed as input. The kinetic parameters are obtained from experimentation and will be used as input data in the CFD modeling. Another advantage obtained from CFD is the possibility to build new scenarios using these input data, for example, the use of a bigger size or more complex reactor under different flow dynamics or optical conditions.

A photocatalytic reactor used a light source or sunlight as energy source to trigger the chemical reaction. Modeling facilitates the designer to run the chemical reactor under different scenarios that may be later compared with results obtained with experimentation when a physical device is available. There are different chemical reactor methodologies or guidelines; in **Figure 1** the reader may find a general methodology proposed for the specific case of photocatalytic reactor design.

In the design of a chemical reactor, knowledge of the chemical kinetics process involved is needed. Kinetic parameters should follow a mechanistic model, so they may be used during the simulation beyond the operational limits used to obtain them. The reaction modeling is an area under development due to the difficulty of accurate methodologies to obtain appropriate kinetic parameters that may be used during the

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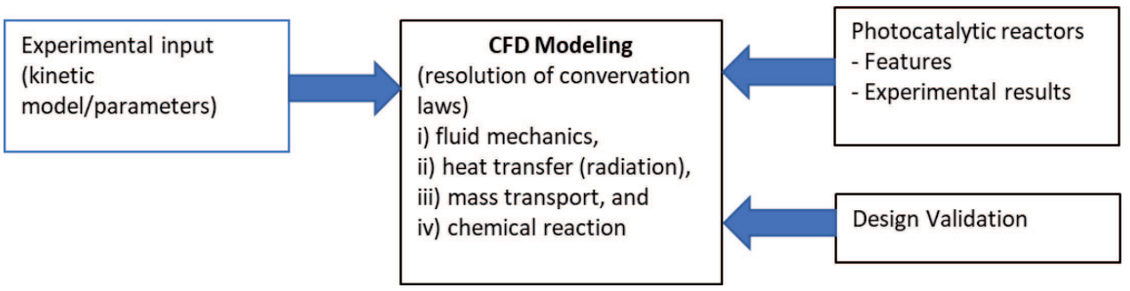

Figure 1.
Proposed methodology for photocatalytic reactor design.

simulation. For each specific reactor type, the recommendation is to consult the latest literature to define the guidelines in order to define the kinetic parameters [3–5].

4.3 CFD calculations

As mentioned in prior sections, this chapter will deal with hydrodynamic calculations related to a photocatalytic reactor. While any intelligent, computer-literate person can run a CFD code, the results obtained may not be physically correct. The case proposed within this chapter has been included as an academic example only. Therefore, the goal of this chapter is to present guidelines or the basic steps for a hydrodynamic simulation.

The examples presented here have been obtained with the commercial computational fluid dynamic code ANSYS Fluent® [6, 7]. Other CFD codes would yield similar but not identical results. Sample CFD solutions are shown for incompressible laminar flow, without heat transfer and chemical reaction.

5. Case of study

In this case, an academic example of a photocatalytic reactor design process is included. More specifically, the intention is to develop the hydrodynamic simulation of the photocatalytic reactor. The data that can be obtained from hydrodynamic simulation permits a detailed definition of the flow motion features, for example, fluid speed in the reaction zone, fluid pressure distribution, and the use of these data as input for further calculations such as distribution of energy from light source, photocatalytic reaction, etc. To achieve these calculations, literature and operational basic requirements were studied in order to define fundamental criteria to assign basic dimensions to the reactor geometry.

With the definition of basic dimensions, it is possible to start using CAD tools to build 3D models that will provide the reactor geometric features that will be needed during CFD simulations. Creo 4.0 and SolidWorks 2016 were used to develop the 3D models of the proposed reactor. For hydrodynamic calculations ANSYS Fluent® versions 18.2 and 19 were used [6, 7].

5.1 Initial calculations

To be able to grow an understanding of the basic reactor design criteria, it was needed to consult the bibliography in different functional areas. The design intent is to build a photochemical reactor of an appropriate size to support laboratory capabilities for testing of nanoparticles after those are synthetized by our research group. It is important for this design to simplify as much as possible the reactor operation.

The basic dimensions defined for the reaction zone container are 300 x 40 x 25 mm. From these dimensions everything else was defined until a 3D model was ready for each component of the reactor including a file with the part assembly that contains the whole reactor. Also, the basic dimensions allow fundamental initial calculations such as volume, inlet/outlet diameter, Reynolds number, etc. Some of the initial assumptions made for this reactor relate to the shape of the reaction zone container which was defined as cuboid (a rectangular hexahedron or a polyhedron bounded by six quadrilateral faces) as will be displayed in the next pages. Within this reaction zone, polluted water will be subject to a chemical reaction to degrade the pollutant into harmless components. So, the fluid chosen is water with a pollutant in low concentration.

Another criterion that needs to be covered in this initial part is the pollutant that will be considered during the design procedures. For this case hydrogen peroxide (H_2O_2) at very low concentrations (20 mg/L) was selected, so for hydrogen calculations the effects of the pollutant may be ignored, and the fluid may be considered as water. Inlet velocity is considered completely axial to the inlet face, and this face is considered exposed to the atmospheric pressure (P_{abs} = 1 atm). All the walls in the domain are considered steady nonslip conditions. The analysis was performed in steady state (nondependent of time) and in laminar regime considering that Reynolds number can be calculated with the next equation:

$$Re = \frac{V \rho Lc}{\mu} \tag{5}$$

V = velocity in m/s.
ρ = density in kg/m3.
L_c = characteristic length in m.
μ = dynamic viscosity in Pa-s.

For the geometry employed in the reactor, characteristic length may be calculated with the next equation (for rectangular ducts):

$$L_c = \frac{4 \times A}{I} \tag{6}$$

So, we can calculate for a velocity with the next value: V = 0.025 m/s:

$$A = 0.25\,m \times 0.003\,m = 75 \times 10^{-6} m^2$$

$$P = (2 \times 0.025\,m) + (2 \times 0.003\,m) = 0.056\,m$$

$$L_c = \frac{4 \times (75 \times 10^{-6}\,m^2)}{0.056\,m} = 0.00535\,m$$

$$Re = \frac{0.025\,{}^{m}/_{s} \times 998.2\,{}^{kg}/_{m^3} \times 0.00535\,m}{0.001003\,{}^{kg}/_{m-s}} = 133.10$$

Then, the values for Re may be calculated for different inlet velocities (**Table 1**).

For the hydrodynamic simulation, the inferior face to work as the reaction surface as well as the inlet and outlet flow face was defined. The liquid selected will be water, and the properties are defined as explained in prior pages. The properties that will be used for water are:

Density = 998.2 kg/m^3.
Viscosity = 0.001003 kg/(m-s).
Inlet velocity = 0.05 m/s.
Temperature = 288.16 K = 15.01 C.

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5.2 Tridimensional models using CAD tools

With the initial parameters mainly in the reaction zone, the CAD 3D models were developed to continue further building the rest of the components. After designing each one of the components, the assembly of the whole reactor was built, and engineering prints were also generated to complete the CAD development. In this chapter the reaction zone will be the main focus for calculations. The rest of the assembly will be displayed to complement the reactor context. Engineering prints will be mentioned only, but the information within the prints which is intended to manufacture the components falls out of the scope of this chapter. The assembly of the reactor design is displayed in **Figure 2**.

Once the geometry definition of the reactor is completed, then it is needed to define the domain where the hydrodynamic calculations will be performed. The reaction zone was defined from the beginning and is considered the central part of the reactor. From the reaction zone, the volume that will be used for hydrodynamic calculations is extracted using CAD software and ANSYS Fluent® tools. The geometry of the reaction zone is shown in **Figure 3**. This domain is the central part of

Item	Inlet velocity (m/s)	Reynolds number	Residence time in the reaction zone (s)
1	0.05	266.2	5.00
2	0.10	532.4	2.50
3	0.15	798.6	1.33
4	0.20	1064.8	1.25
5	0.25	1331.0	1.00

Table 1.
Effects of cell count for an experiment under V = 0.05 m/s during the mesh analysis.

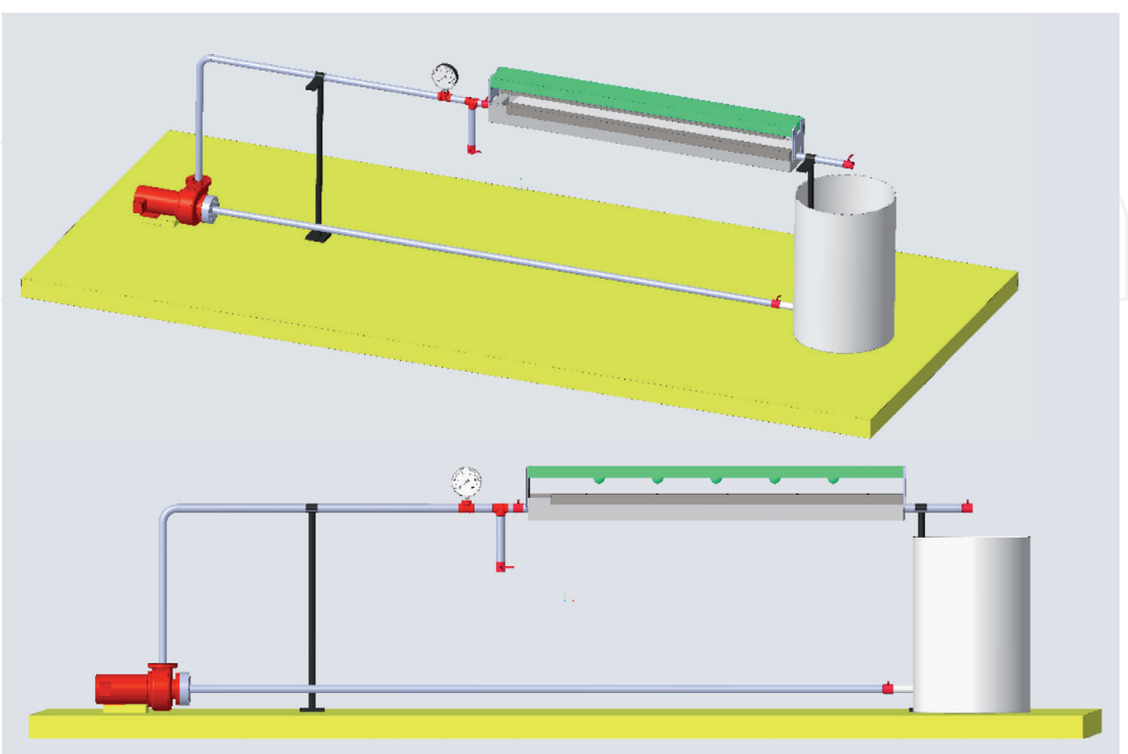

Figure 2.
Photocatalytic reactor proposed. (a) Reactor assembly isometric view and (b) reactor assembly side view.

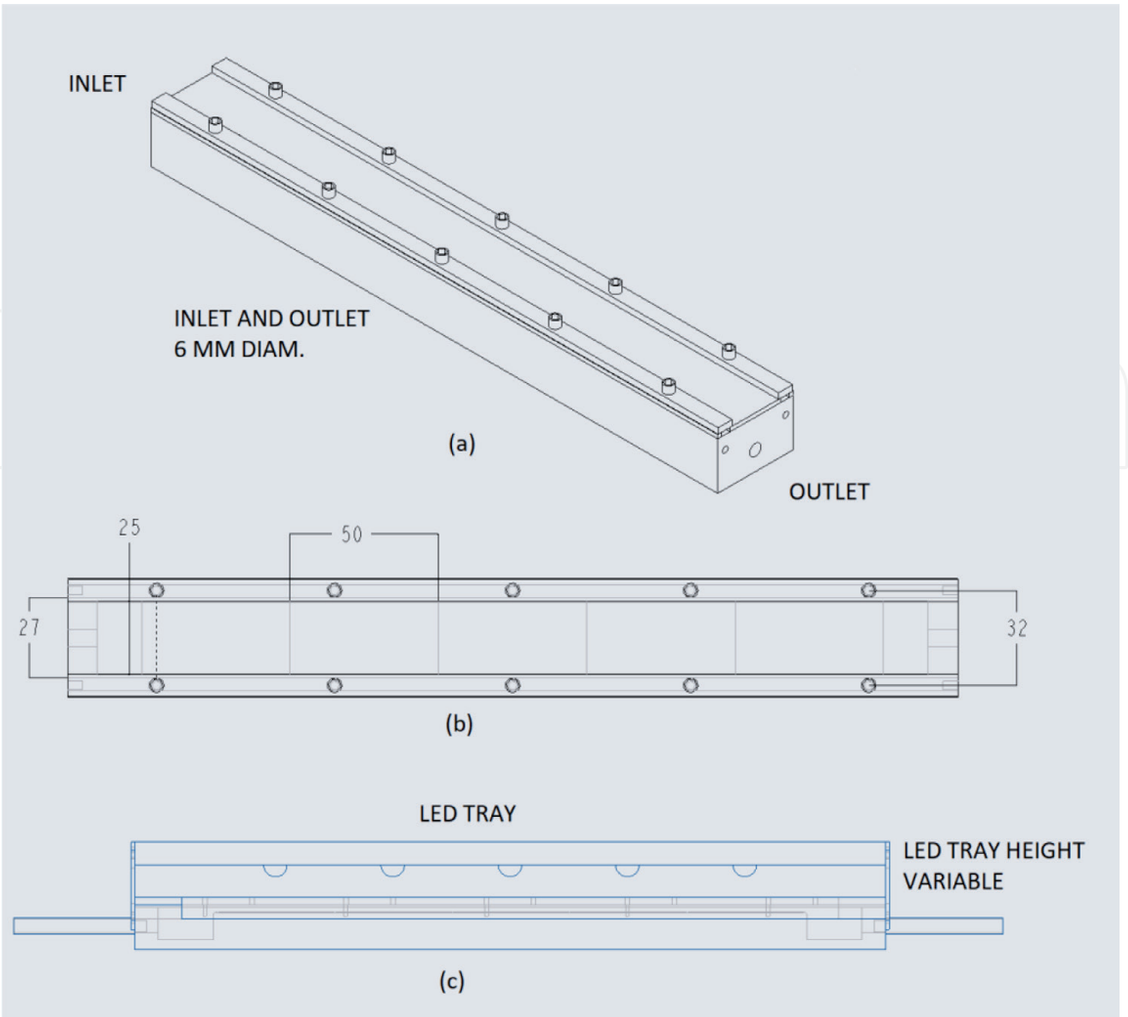

Figure 3.
Reaction zone, (a) isometric view of reaction zone, (b) top view of reaction zone, and (c) lateral view of reaction zone including LEDs.

CFD calculations because the methodology used is finite volume. For that purpose, the domain will be processed using the software by first discretizing the domain in small control volumes where the governing equations will be resolved with the help of numerical methods to obtain valuable results.

Finite volume methodology is based in dividing the domain in a number of control volumes (cells or elements), the elements should not overlap among them, and the variable of interest is located at the centroid of each element. If the nodes in the border wall of each consecutive region are unidentical, the mesh is nonconformed. The walls should connect through their interphase, and calculated flows through these walls may be assigned from a mesh to the other.

Conformed mesh is the most precise connectivity between regions. Nonconformed mesh may reduce the complexity of the meshing process but would increase the error, at least the local error. In this work, there is an effort to obtain the conformed mesh during the discretization process.

5.3 Photocatalytic reactor general operation

The reactor operation is simple; the design intent is having an inlet circular port with a diameter of 6 mm and arrives into a rectangular cavity which is filled until reaching the reaction zone level. Then the fluid circulates through the reaction zone under a laminar flow regime. The fluid reaches the outlet and finally goes

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out through a 6-mm-diameter outlet port. The reaction zone has the dimensions of 3 mm x 25 mm x 250 mm, and from there the calculated volume is 18,750 mm3. With these dimensions the reactor complies with one of its purposes since it is intended for laboratory testing. **Figure 4** shows an image of the domain.

The reactor has a cover made of a transparent material that allows light to pass through; in this case we selected Pyrex glass with dimensions of 40 x 300 mm, and it will be fastened to the main block using ten fasteners and two fixing devices made of metal with dimensions of 7.5 x 300 mm.

The light source will not be analyzed in this chapter, but initial estimations will be mentioned in this section. The distance to locate the light source from the reaction zone is adjustable. For the light source, it is intended to use 10 lamps which will be UV LED devices with 365 nm mounted in a bench that will have dimensions of 25 x 300 mm. LEDs are distributed along the reaction zone in 250 mm of the total length. Light source selection is based in some of the advantages this device offer such as low electric consumption, long life cycle, and easy control of light intensity using low-cost electronic devices.

The inlet and outlet have a 6 mm diameter with a threaded connection. The centerline of the inlet is located at a height of 18 mm with respect to the reactor base. The outlet is located at a height of 10 mm with respect to the reactor base with the intention of helping out the fluid.

5.4 Mesh details

An initial mesh of m (0.75 mm) hexahedral-type cubic cells was used considering the geometry is simple enough, applying a meshing method known as hexa-dominant within the native options within ANSYS® Mesh. The initial meshing process generated 52,615 cells. This is the first step in an iterative process where the cell count increases in order to find the optimal cell count where the effect of the number of cells in the calculation is minimized. This is done comparing the iterative residual values in a simple calculation; when the difference between one experiment and the subsequent is minimum, then the cell count may be considered irrelevant, and this may be considered the optimum cell count for the problem.

The option facing was used to standardize the cell size and its orthogonality (these are native options within ANSYS® Mesh). During the mesh analysis,

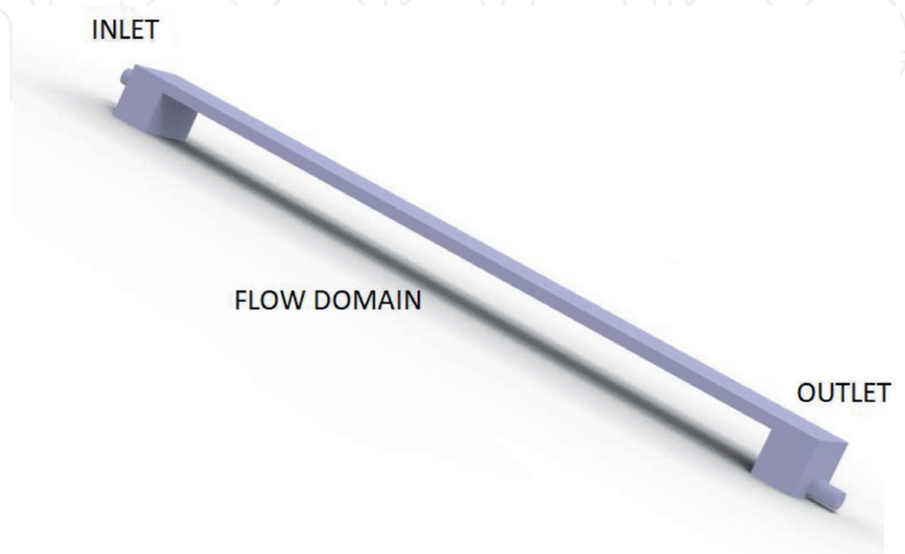

Figure 4.
Definition of reaction zone for CFD simulations.

AANSYS® version 19.2 was also used. For this analysis, the cell count was increased until reaching 500,000 cells. The simulation was performed in the reaction zone which has a simple geometry that facilitates all the meshing process and in general reduces the problem complexity. The results of the mesh analysis are displayed in **Tables 2** and **3**, and the best choices for the meshing process are marked *.

CFD will resolve governing equations for mass, momentum, and energy. The discretization process is also known as the meshing process. In this process ANSYS Fluent® has improved a lot, and since the geometry was simple for this reactor, meshing was resolved easily. There are two meshing types: structured mesh and nonstructured mesh. Examples of structured and nonstructured cases are shown in **Figure 5**.

In the former the mesh is identified by a triple index (i, j, k), in three dimensions. The cell borders form continuous lines of meshing with the adjacent cells which help a lot in the subsequent steps. In nonstructured meshing, cells and nodes do not have an exact match and cannot identify easily between neighboring cells.

Meshing has been regarded as the most difficult process in a CFD simulation. The latest versions of ANSYS® incorporate new tools that have enhanced the program capabilities and make the job easier for the users. Among the different tools incorporated, the known tools have been improved. An important factor to consider while meshing the domain is the cell shape. For this case, the geometry is a regular shape, so the cell shape was resolved easily. Conformed mesh is the desired status for the mesh because the nodes and boundaries will work smoothly if the individual cells are conformed.

In this way, the user needs to consider the interphase interaction, for example, interaction between the walls and the fluid and others. Discretized domain is shown in **Figure 6**.

Different scenarios were calculated with variants in the mesh, so the results can be compared in search for the optimum mesh as shown in **Tables 2–4**. Results such as velocity, pressure, and mainly the residuals were used to reach a conclusion on which mesh and how many cells are the best choice for this work.

Item	Mesh size (m)	Adjustments used	Cells generated
1	7.5 e-4	54,615	1e-3, 1e-4, 1e-5 y 1e-6
2	5.00E-04	200000*	1e-3, 1e-4, 1e-5 y 1e-6
3	4.00E-04	385020*	1e-3, 1e-4, 1e-5 y 1e-6

** Optimized value for elements quantity.*

Table 2.
Effects of cell count for an experiment under V = 0.05 m/s during the mesh analysis.

Inlet velocity (m/s)	Maximum pressure absolute (Pa)	Likeliness between values	Outlet pressure at central zone (Pa)	Likeliness between values
0.1	27.906	91.6	11.310	92.6
0.1	27.906	91.6	11.310	92.6
0.1	29.802	97.8	11.265	92.2
0.1	29.804	97.8	11.265	92.2
0.1	30.481	100.0	12.218	100.0
0.1	30.482	100.0	12.218	100.0

Table 3.
Effects of cell count for an experiment under V = 0.05 m/s during the mesh analysis.

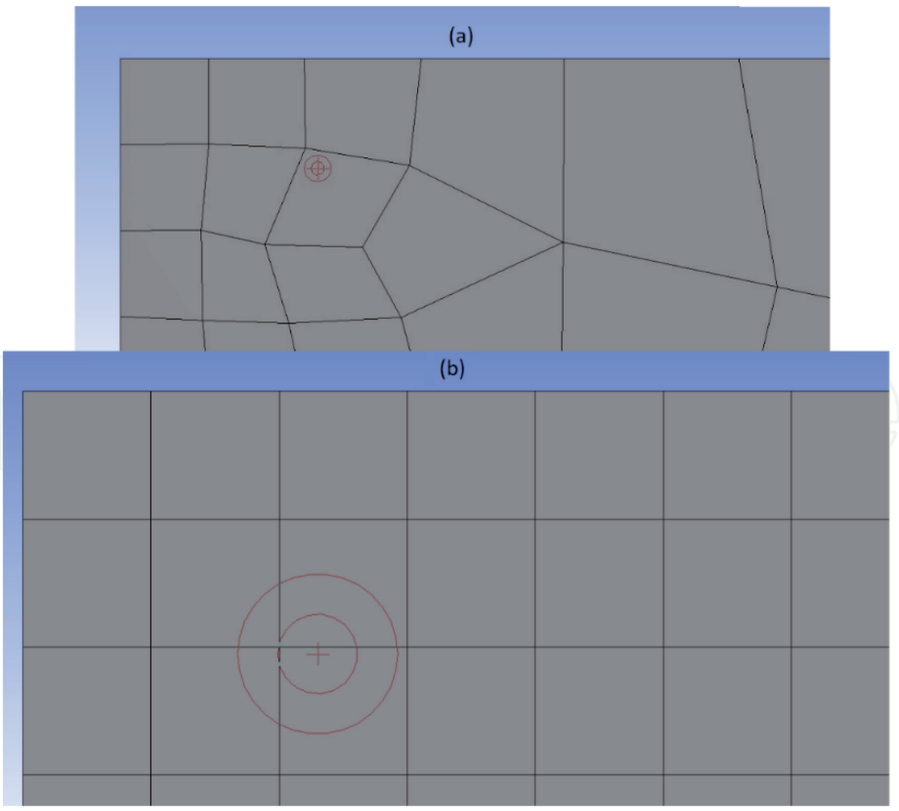

Figure 5.
Mesh examples: (a) non-structured mesh and (b) structured mesh.

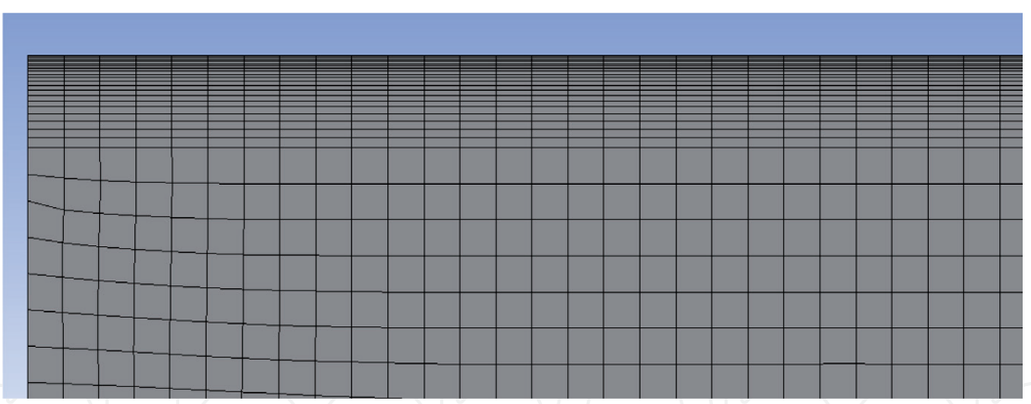

Figure 6.
Discretized domain using tools incorporated in ANSYS fluent® version 19.2.

5.5 Processing and resolution of governing equations

As mentioned in prior sections, flow dynamics is the first step during the design development of a photocatalytic reactor. A good velocity field with an appropriate distribution will be important for the photocatalyst distribution and to avoid possible nonuniform zones. Since the estimated operational parameters indicate Reynolds will oscillate between 266.2 and 1331.0, calculations will be carried on under laminar flow regime. Since the regime and the fluid conditions may be considered homogeneous, calculations can be performed in steady state and assume one can proceed on to resolve the continuity equation (Eq. 7) and the tridimensional classical equation of Navier–Stokes (Eq. 8):

$$\nabla(\rho\bar{v}) = 0 \tag{7}$$

Inlet velocity (m/s)	Maximum pressure absolute (Pa)	Outlet pressure at central zone	Minimum pressure absolute (Pa)	Mesh variant	Inlet velocity (m/s)	Outlet velocity (m/s)	Residuals
0.1	27.906	11.310	0.245	1	0.103	0.151	1.00E-05
0.1	27.906	11.310	0.245	1	0.103	0.151	1.00E-06
0.1	29.802	11.265	0.007	2	0.100	0.160	1.00E-05
0.1	30.481	12.218	0.004	3	0.101	0.154	1.00E-05
0.1	29.804	11.265	0.007	2	0.100	0.160	1.00E-06
0.1	30.482	12.218	0.004	3	0.101	0.154	1.00E-06

Table 4.
Effects of cell count for an experiment under V = 0.05 m/s during the mesh analysis.

$$\nabla\cdot(\rho\bar{v}\bar{v}) = (-\nabla P) + (\nabla\cdot\bar{\bar{\tau}}) + \left(\rho\vec{g}\right) \tag{8}$$

where ∇ is the delta operator and ρ, $\bar{v}$, P, $\bar{\bar{\tau}}$, and are the fluid density, velocity vector, pressure, stress tensor, and gravity acceleration, respectively. These equations and Newton's viscosity law as a constitutive equation to relate the stress tensor with the continuous fluid motion will enable the user to calculate the velocity field for this reactor. Since we are interested only in fluid dynamics, we will skip energy equation. The resolution of these equations keeps representing one of the most complicated problems analytically and numerically in fluid mechanics for complex geometries. An analytical solution is unavailable, but a reasonably accurate solution may be reached numerically using methodologies such as finite volume as it was described briefly in prior sections.

In this case the resolution algorithm semi-implicit, linked equations (SIMPLE) was used. In this algorithm an initial value for pressure from there calculates the velocity and verifies that the outlet flow is identical to the inlet value and increases or decreases the input according to the best option. The program will resolve numerically for each of the finite volumes created during the discretization process or in other words will resolve the equations in the centroid for each cell in the mesh. This step may be considered a numerical solution for the discrete volumes but need an integration to display global results. The integration is done by producing an algebraic version of the differential equations, and the solution for this version is reached with a matrix. The processing means the software will resolve the governing equations according to the inputs provided. The inputs include the geometry, the mesh, fluid properties, boundary conditions, the algorithm to be used, and other details that the software will require if following its natural sequence as coded by ANSYS Fluent®.

5.6 Result analysis and postprocessing

When the processing step completes its respective work cycle, the governing equations are resolved for the centroid of each cell, and the integration process was also completed for global results.

From these results the program offers a module to create views of the domain geometry that facilitate the analysis by the users or the presentation of the results to a specific audience. In this problem, the results obtained relate to the reactor zone

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hydrodynamics. A useful tool generates contours of the domain for the desired parameters such as velocity, pressure, drag force, residuals, mass imbalances, etc.

The analysis of pressure for the system and in specific regions of the reaction zone may be an interesting contour to start with the analysis procedures. **Figure 7** shows the results obtained for pressure within the domain by generating an image at the inlet and outlet. In **Figure 8**, one may see another interesting vector graphic to display the velocity profile at the inlet and outlet considering an inlet velocity of 0.1 m/s. The maximum pressure calculated at the inlet is 29.8 Pa, while the minimum pressure at the outlet is 0.0742 Pa. Then, with this data the designer has an idea of the pump dimensions considering the inlet pressure is needed, so the flow can pass through the reaction zone under the selected conditions. Pressure losses due to the interaction of the fluid with pipes and other reactor components in its way to the inlet in the reaction zone will not be included within this chapter but can easily be resolved by the designer.

Reaction zone pressure in addition with pressure losses will provide the minimum value needed to dimension the appropriate pump for a correct operation of this reactor. An interesting tool that helps to know the exact value in a specific location within the domain may be completed with the help of the probe tool. With this tool the software is capable of calculating this parameter on a specific location, for example, if the user would like to know the average velocity, the probe tool should

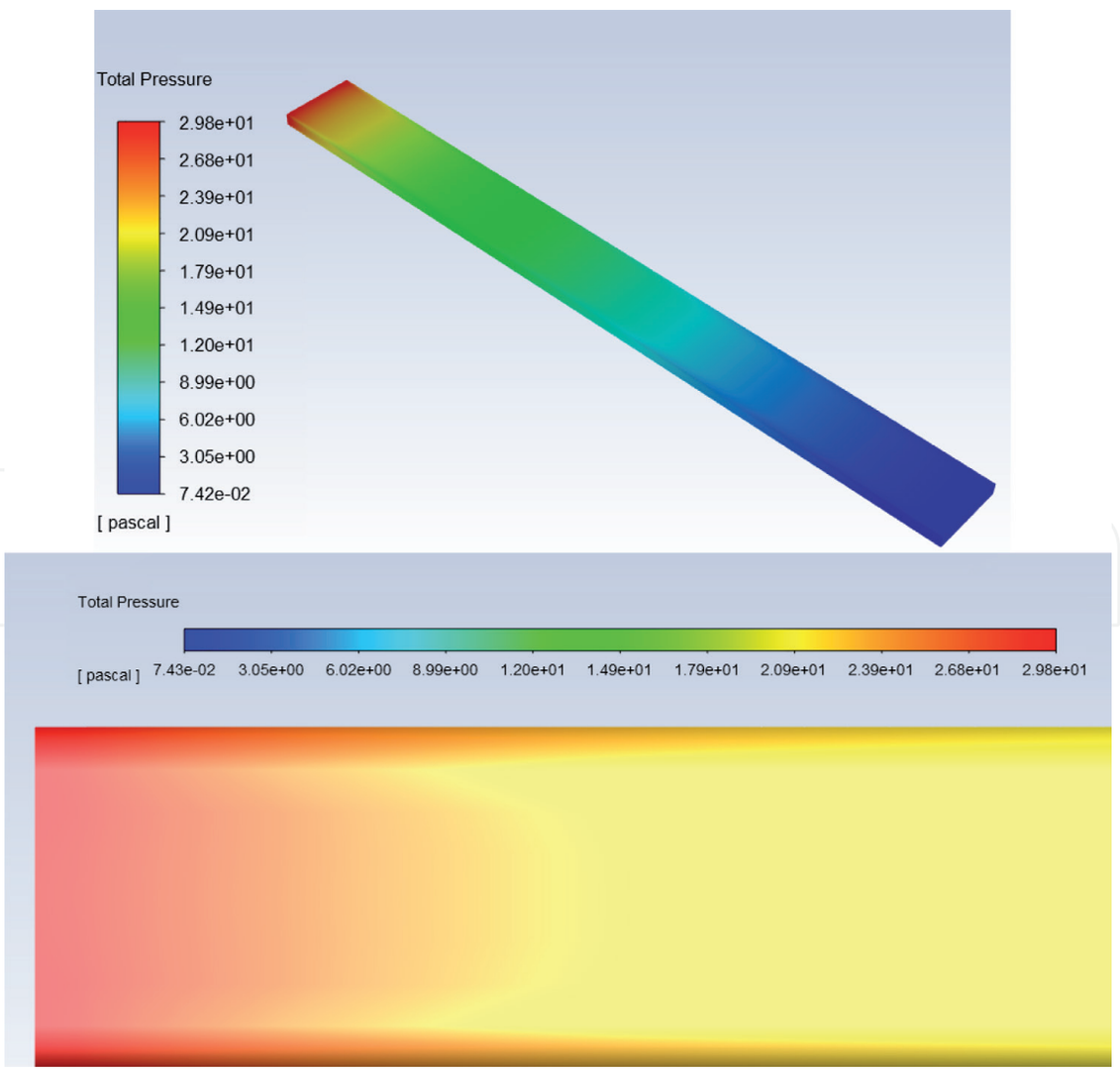

Figure 7.
Postprocessing contour for pressure distribution in the reaction zone in (a) isometric view and (b) lateral view.

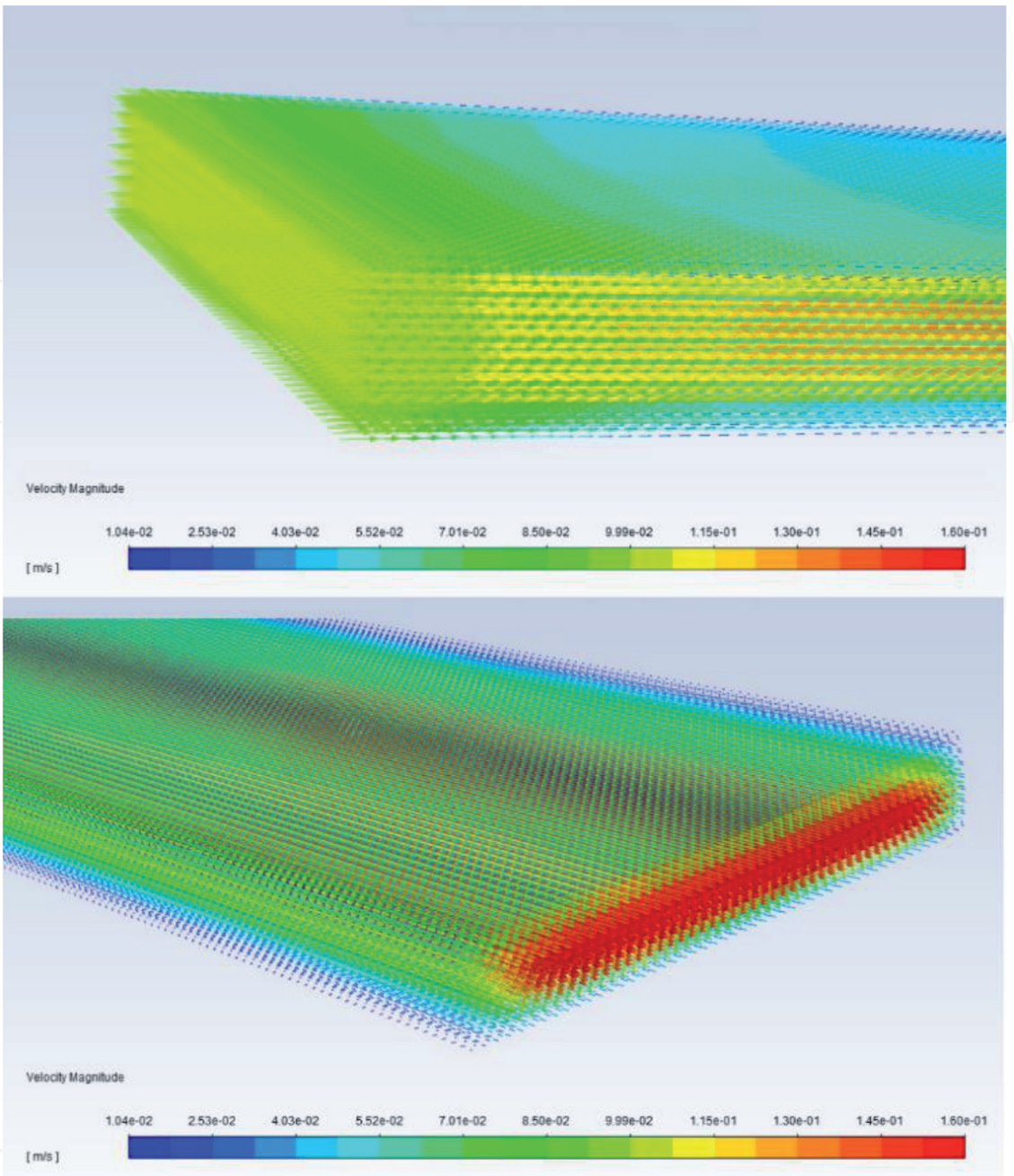

Figure 8.
(a) The graph showing velocity vectors at the inlet in the reaction zone considering an inlet velocity of 0.1 m/s and (b) velocity profile at the outlet considering the case of an inlet fluid velocity of 0.1 m/s.

indicate the specific region and the desired parameter, and, in this case, the average velocity at central region is 0.1000459 m/s. In this measurement it is interesting to observe that the expected value was 0.1 m/s for the inlet speed at the central region and the software calculated 0.1000459 m/s instead. The difference is very small, so a conclusion that may be reached is that the calculation accuracy is acceptable for the case of the velocity in this location. The minimum pressure obtained was 0.0742 Pa, for a velocity of 0.1 m/s in the reaction zone. **Figure 9** shows the velocity contour.

ANSYS® in its latest version offers a whole module to carry on with the postprocessing procedures. This module facilitates a lot the designer work and allows the user to generate a great deal of graphics, charts, animations, etc. which will be of great help for the presentation of results. In this example the graphics generated so far will be considered enough to illustrate the analysis done but represent only a few of the potential analysis tools that can be obtained.

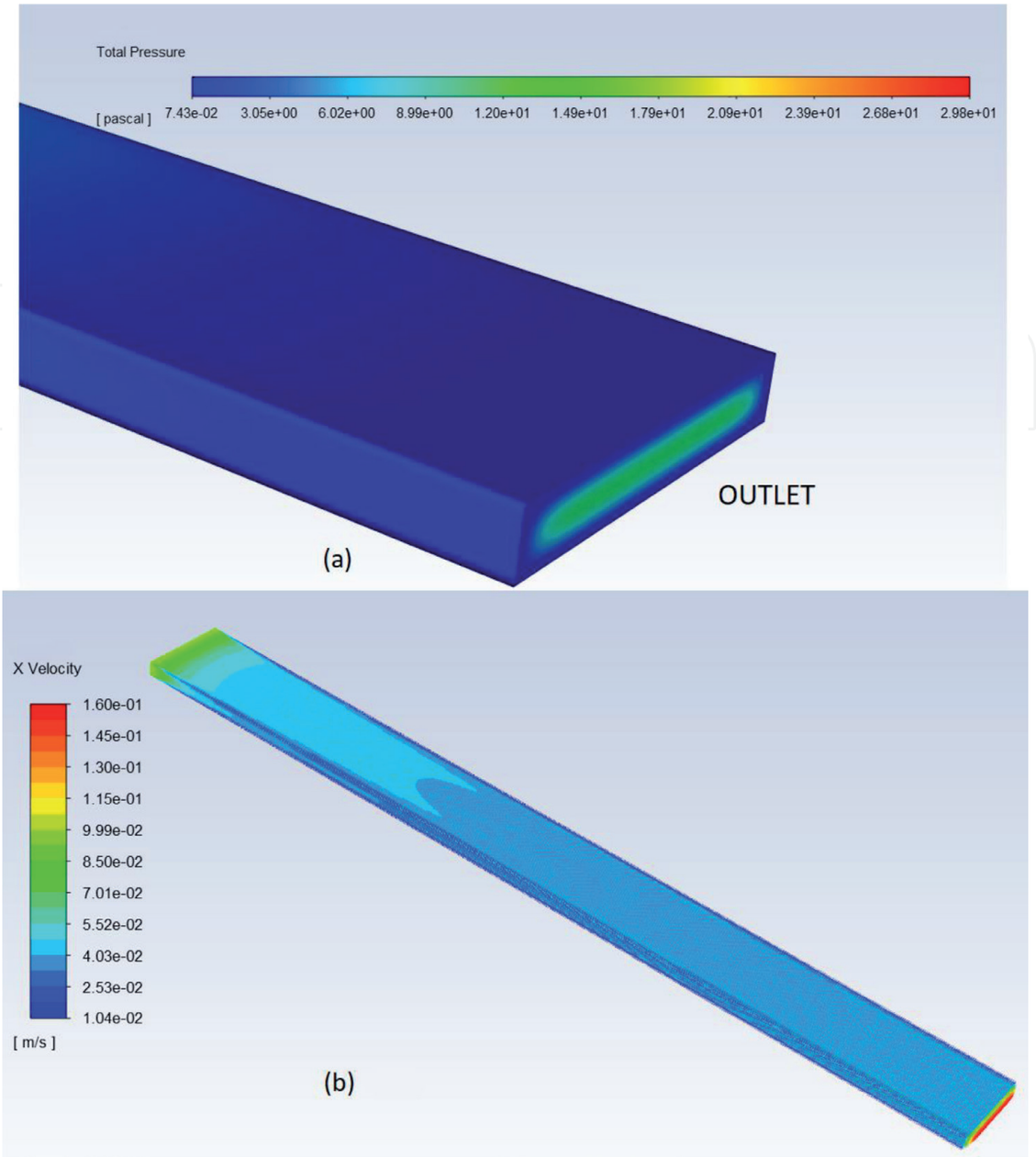

Figure 9.
(a) Contour graphic for pressure obtained at the outlet of the reaction zone. (b) Contour graphic for velocity in the reaction zone with an inlet velocity of 0.1 m/s.

6. Conclusions

In conclusion, CFD codes are becoming common tools used in chemical reactor design development. The simulation possibilities are quite interesting and include resolving the governing equations for fluid dynamics but also may include chemical species and multiphase, among other, additional possibilities for the simulation of the chemical reactor operation under different scenarios. CAD tools complement the CFD code because the geometry is the central piece of information required to carry on with CFD simulation. Discretization process required a formidable amount of efforts in the past, in particular for complex geometries, but this problem has decreased in the latest versions of CFD codes. In particular, ANSYS® has incorporated a series of tools at different stages of the simulation process that facilitate in a great deal in the meshing process.

In the case of study, a simple geometry was used for the reaction zone of the chemical reactor proposed for a laboratory scale, and a mesh with 385,020 elements was

proposed as the best choice to carry on with the calculations. The analysis developed for the case of study provided interesting results for the fluid dynamics in the reaction zone which were used to generate graphics and images that facilitate the result presentation and explanation. Additional simulation may be performed which will be included in future publications. A future case of study that may complement our work presented herein may involve chemical reactions and the radiation effects caused by the light source since this case analyzes only the hydrodynamics of a photochemical reactor.

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Conflict of interest

Authors state that this research was completed without any conflicts of interest related with the funding to develop the present work.

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