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EVALUATION OF TURBULENCE MODELS FOR A MILI-PHOTOREACTOR

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Abstract. *The crescent need for pollutants mitigation measures has also stimulated the use of process intensification techniques in the effluent treatment area. Process intensification technologies focus in the size reduction of unit operations, besides the increasing of process speed and safety control. In this sense, reactors of micro and meso-scale, such as NETmix, gain importance. The NETmix is a mili-photoreactor that can be used for the photo-catalytic oxidation of volatile organic compounds (VOCs) dispersed in gaseous streams. The flow inside this type of reactor can be laminar or turbulent. In this work, the choice of turbulence model is investigated through computational fluid dynamics tools. Two $k-\varepsilon$ approaches were analysed, for a flow with a Reynolds number of approximately 150. Both Standard $k-\varepsilon$ and RNG $k-\varepsilon$ returned similar results, with slightly greater conversion when employing RNG $k-\varepsilon$ model.*

Keywords: *Micro-channel, $k-\varepsilon$, NETmix, Photocatalysis*

1. INTRODUCTION

Air quality is a growing area of research, especially after massive incidents such as the one that occurred in London in 1952, where several deaths were attributed to poor air quality. Contemporary incidents, include the pollution smog around Chinese cities in recent years. The impact of air pollution goes beyond the respiratory system, around 20% of cardiovascular and stroke deaths have some kind of relation with air pollution. Air quality is also appointed as cause factor for several different types of cancers. Autoimmune afflictions, osteoporosis, conjunctivitis, skin and cognitive problems, among several other illness, including diabetes and anemia are linked to air quality problems (Kelly and Fussell, 2019; Schraufnagel *et al.*, 2019).

Poor air quality can be due to the presence of many chemical compounds such as nitrogen oxides, particulate matter, ozone and volatile organic compounds (VOCs). By definition VOCs are organic substances with boiling point inferior or equal to $250°C$ at atmospheric pressure. VOCs occur naturally in places like wetlands, forests, oceans and volcanoes, however the big pollution problem by these compounds is related to human activities. The VOCs emissions are present at several industrial processes besides transportation, stationary combustion of fossil fuels, biomass burning and solvent utilization (Li *et al.*, 2019; He *et al.*, 2019).

Several techniques can be applied to solve the VOCs emission problem. The pollutant removal can be based on physical, chemical or biological methods. Industrial plants can either focus on the recovery or on the destruction of VOCs compounds. Among the recovery methods are absorption, adsorption, condensation, and membrane separation. The destruction methods consists of bio-filtration and oxidation methods, including reverse flow reactor and thermal or catalytic oxidation (Kelly and Fussell, 2019; Berenjian *et al.*, 2012; Kim, 2011; Khan and Kr. Ghoshal, 2000).

In this work, the fluid dynamic of an oxidation process is evaluated using a photocatalytic reactor. The reactor in question, is known as NETmix, and was developed by the researchers of the Laboratory of Separation and Reaction Engineering and Laboratory of Catalysis and Materials (LSRE-LCM) from University of Porto - Portugal (Laranjeira *et al.*, 2011).

The NETmix is a static mixer that is commonly employed as mili-photoreactor. The reactor is composed by a metallic plate, where a pattern of channels and chambers are engraved. On top of this plate, a flat glass plate, coated with the TiO_2 catalyst, completes the reactor. A luminous source is positioned above the glass to activate the catalyst and promote the pollutant degradation. The pattern of this meso-scale reactor is composed by a net of cylindrical chambers interconnected by a series of prismatic channels as described by Da Costa Filho *et al.* (2017). The cylindrical chambers have a diameter of 6.5 mm, while the prismatic channels have only 1 mm width and 2 mm in length. As show in Fig 1, the depth of the engraved pattern is equivalent to 3 mm.

In this work, the degradation of perchloroethylene is simulated considering that the catalyst is homogeneously illuminated. The fluid flow regime inside the reactor is taken into account as a possible transition to turbulent regime, with a Reynolds number of 150 at the prismatic channels. The aim of the current work is to compare two $k-\varepsilon$ turbulence models for the photocatalytic degradation of gaseous pollutants in the NETmix mili-photoreactor. Therefore, the Standard $k-\varepsilon$ and the RNG $k-\varepsilon$ models are compared through CFD simulations of a VOC oxidation.

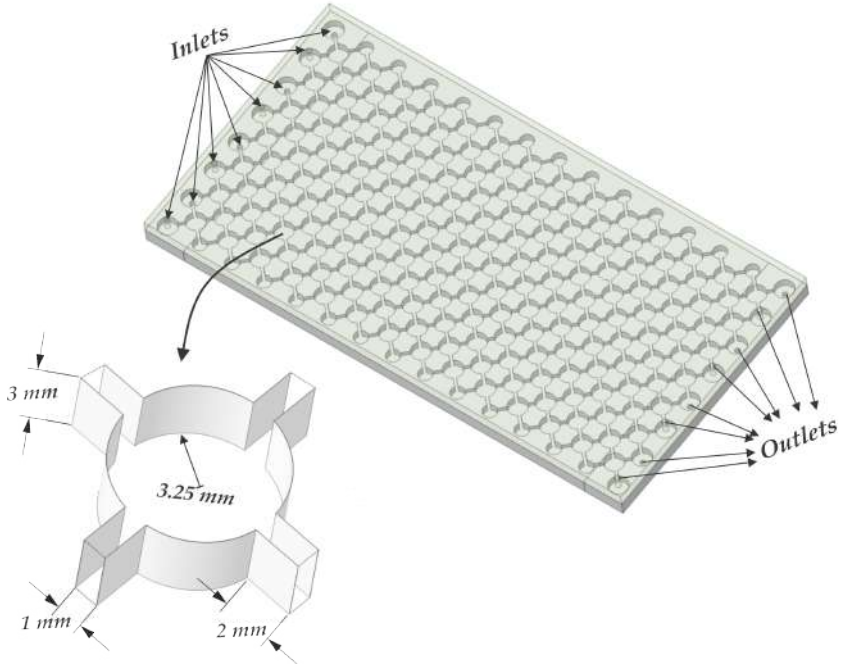

Figure 1. NETmix meso-scale reactor

2. METHODOLOGY

The mass, energy, momentum and species conservation equations that describe the reactor were solved employing the ANSYS 2019R2 software suite, using the ANSYS Fluent as a solver. NETmix is a repetition of channels and chambers of the same length and radius, therefore, in order to reduce the total number of cells in the mesh, only a slice of the reactor, in the same direction of the flow, is drawn and simulated, as illustrated in Fig. (2). This simplification, allows a significant reduction in simulation time, since only around $1/6$ of the hole geometry is simulated. The 3D hexahedral mesh used for the simplified geometry of NETmix, consist of 5,590,559 elements, and a symmetry boundary condition is imposed for both sides of the simplified geometry.

The kinetic rate employed to describe the photo-oxidation of perchloroethylene is the one proposed by Imoberdorf *et al.* (2007), introduced in the ANSYS Fluent solver via a UDF (user defined function). This model takes into consideration quantum efficiencies and incident photon flux in its formulation, as described in Eq. (1).

$$r_{PCE} = \alpha \frac{C_{PCE}}{1 + K_{Water} C_{Water}} e^{a,s} \tag{1}$$

where, α is equivalent to $154\ m^3/E$, C_{PCE} is the pollutants concentration, C_{Water} is the concentration of water, K_{Water} coresponds to $3.21x10^{-4}\ m^3/mg$ and $e^{a,s}$ is the local superficial rate of photon absorption.

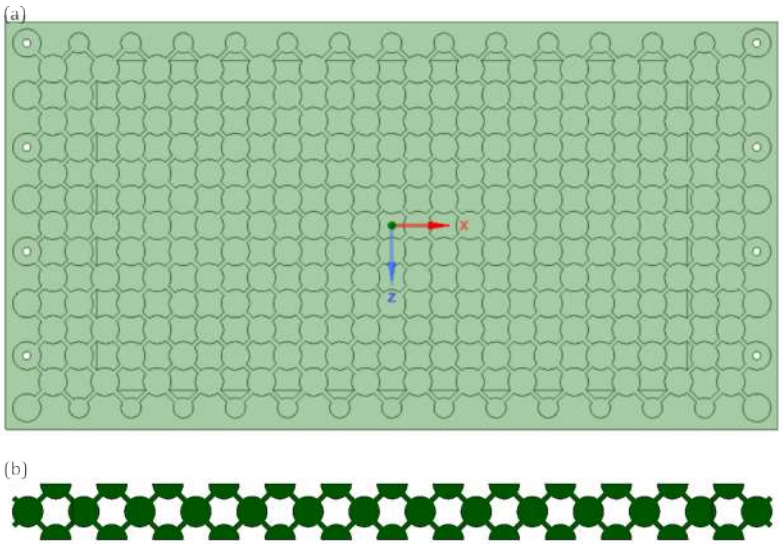

Figure 2. Geometry of the reactor
(a) Full reactor, (b) simplified geometry

The turbulence was evaluated employing two distinct $k-\varepsilon$ models, the Standard $k-\varepsilon$ and the RNG $k-\varepsilon$. For the boundary conditions, the prescribed velocity was employed at the reactor entrance, with the inlet velocity set as $1.28m/s$, and for the reactor outlet, the prescribed pressure was selected, with atmospheric pressure set at the outlet of the reactor.

The reactor feed stream is composed by wet air, with a relative humidity of 30%, and a pollutant concentration equivalent to $3.19x10^{-3}\ mol/m^3$. The degradation reaction is conducted in a temperature of $298\ K$, and the irradiation is considered to be constant in every point of the catalyst surface, and equivalent to $38.4\ W/m^2$.

3. RESULTS AND DISCUSSION

In Fig. (3), a color map comparison of the velocity along the reactor show that both standard $k-\varepsilon$ and RNG $k-\varepsilon$ have very similar velocity magnitude, as expected. The streamlines in Fig. (4), show the re-circulation patterns of the flow inside the circular chambers, and how they vary from one turbulence model to the other. This figures allow the observation of the fluid dynamics inside the NETmix, where the fluid gains velocity when crossing the prismatic channels, and soon after, it disperses inside the cylindrical chambers promoting an intense mixing of the flow.

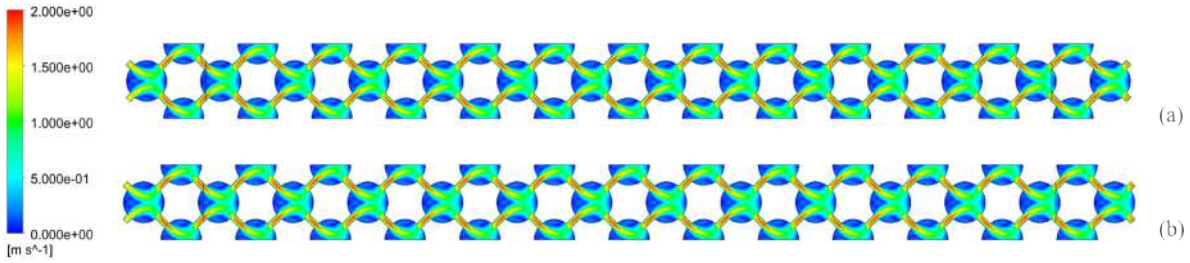

Figure 3. Velocity along the reactor
(a) Standard $k-\varepsilon$, (b) RNG $k-\varepsilon$

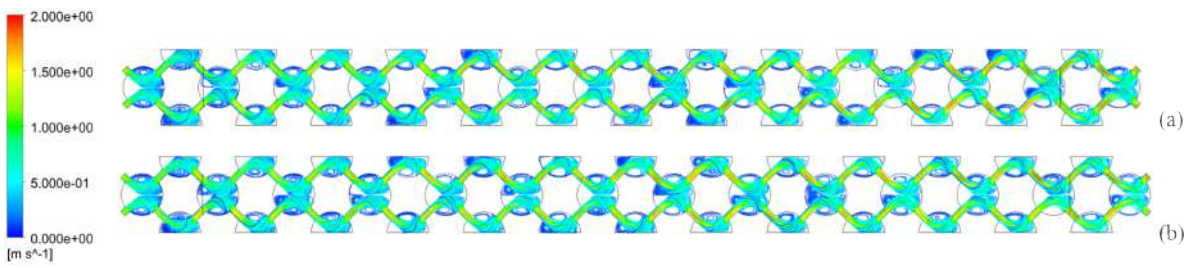

Figure 4. Representation of Flow Streamlines
(a) Standard $k-\varepsilon$, (b) RNG $k-\varepsilon$

In order to compare the velocities found with each turbulence model in a more quantitative form, the velocity profile inside a cross-section of one of the cylindrical chamber was plotted, as shown in Fig. (5). Although very similar, the velocity inside a chamber vary slightly with the turbulence model choice. In Fig. (5), the blue line represents the velocity obtained when the turbulence model employed is the Standard $k-\varepsilon$, for the majority of the cross-section the velocities of both models are equivalent, and the Standard $k-\varepsilon$ presents higher velocity values at the region where the velocity is already more accentuated. However, in this peak region, the Standard $k-\varepsilon$ reaches a velocity no more than 4% greater than the RNG $k-\varepsilon$.

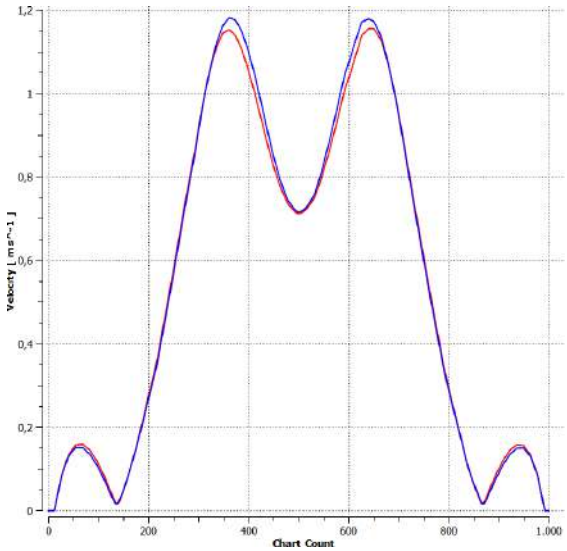

Figure 5. Velocity inside a specific chamber
— Standard $k-\varepsilon$, — RNG $k-\varepsilon$

When observing the turbulent kinetic energy, Fig. (6), the opposite can be said. In this case the profile still similar, but the Standard $k-\varepsilon$ has the lesser magnitude. The more accentuated differences are localized in the center of the chamber, where the RNG $k-\varepsilon$ exhibit a turbulent kinetic energy value almost 7% greater than the Standard $k-\varepsilon$.

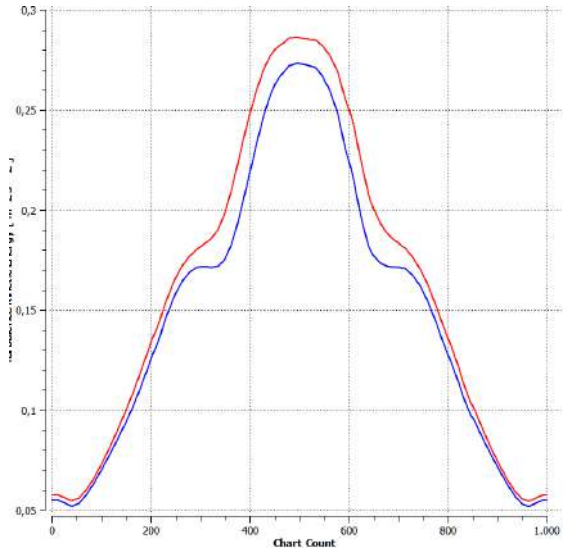

Figure 6. Turbulent Kinetic Energy inside a specific chamber
— Standard $k-\varepsilon$, — RNG $k-\varepsilon$

The slight differences in the velocity patterns that each turbulence model give, result in mixing changes that alter the concentration of the pollutant in space. Figure (7) illustrates how the molar concentration of the pollutant can vary from the Standard $k-\varepsilon$ (blue line) to RNG $k-\varepsilon$ (red line). Both models follow the same profile with Standard $k-\varepsilon$ showing a molar concentration up to 1% higher.

These changes also affect the reaction rate. Figure (8) illustrates the reaction rate at the surface of the catalyst for each turbulence model. The rate of reaction is very similar for both cases, and is possible to notice that the areas of greater rate are the ones with greater velocity magnitude, therefore, where a higher mixing degree is found. In Fig (8), is possible to

observe that in the firsts and lasts chambers no reaction occurs since no catalyst is deposited in these regions. It is also noticeable that the reaction rate is stronger in the beginning of the reactor, this is expected once the pollutant concentration is higher close to the entrance of the reactor.

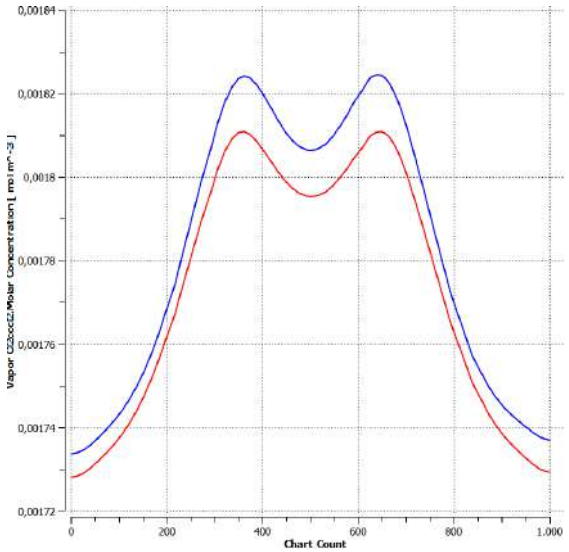

Figure 7. Molar Concentration of Pollutant inside a chamber
— Standard $k-\varepsilon$, — RNG $k-\varepsilon$

The reaction rate for the Standard $k-\varepsilon$ case is equivalent to $1.4756x10^{-5}mol/m^2s$, while the RNG $k-\varepsilon$ achieves $1.4851x10^{-5}mol/m^2s$. Therefore, the pollutant conversion is slightly higher when employing the RNG $k-\varepsilon$, 51.21% against 50.87% from the Standard $k-\varepsilon$, a difference of only approximately 0.7%.

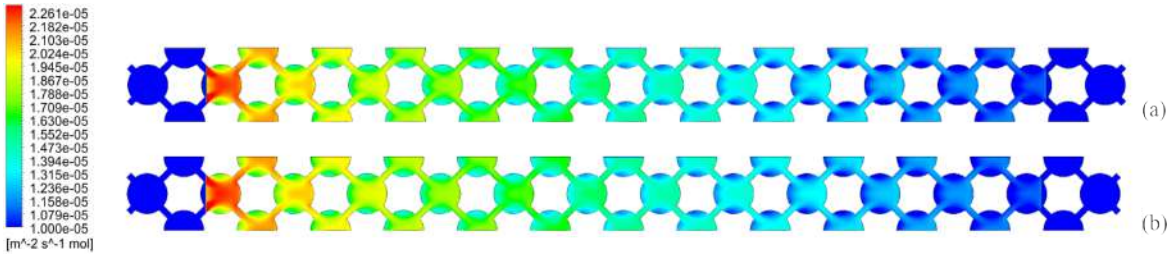

Figure 8. Kinetic Rate along the reactor
(a) Standard $k-\varepsilon$, (b) RNG $k-\varepsilon$

4. CONCLUSIONS

The photocatalytic oxidation of perchloroethylene using titanium dioxide as catalyst inside a meso-scale reactor was investigated using two $k-\varepsilon$ approaches, Standard $k-\varepsilon$ and RNG $k-\varepsilon$. The reaction was conducted in a mili-reactor known as NETmix, for a Reynolds number of approximately 150. The pollutant contained in the gaseous stream was successfully degraded in NETmix, achieving a conversion of approximately 51%.

The Standard $k-\varepsilon$ and the RNG $k-\varepsilon$ were compared. The models give similar results, with a slight impact on kinetic parameters. As expected, both $k-\varepsilon$ approaches, result in similar velocity profiles. The variable analysed that showed the greatest discrepancy between the models was the turbulent kinetic energy, however the distinct magnitude between the models do not exceed 7%. Therefore, the choice of either Standard $k-\varepsilon$ or RNG $k-\varepsilon$ turbulence model presented little impact on the final results. Further comparison with experimental data is still necessary in order to validate the $k-\varepsilon$ approach for the gaseous photocatalytic oxidation.

Furthermore, future works can compare other turbulence approaches, as well as, investigate the impact of distinct Near-Wall treatments, besides the influence of the turbulence models at different Reynolds numbers.

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