Influencing Parameters on Supercritical Water Reactor Design for Phenol Oxidation

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Abstract – For accurate and reliable process design for phenol oxidation in a plug flow reactor with supercritical water, modeling can be very insightful. Here, the velocity and density distribution along the reactor have been predicted by a numerical model and variations of temperature and phenol mass fraction are calculated under various flow conditions. The numerical model shows that as we proceed along the length of the reactor the temperature falls from above 430 °C to approximately 380 °C. This is because the generated heat from the exothermic reaction is less that the amount lost through the walls of the reactor. Also, along the length, the linear velocity falls to less than one-third of the initial value while the density more than doubles. This is due to the fall in temperature which results in higher density which in turn demands a lower velocity to satisfy the continuity equation. Having a higher oxygen concentration at the reactor inlet leads to much faster phenol destruction; this leads to lower capital costs (shorter reactor will be required); however, the operational expenditures will increase for supplying the needed oxygen. The phenol destruction depends heavily on the kinetic parameters and can be as high as 99.9%. Using different kinetic parameters is shown to significantly influence the predicted distributions inside the reactor and final phenol conversion. These results demonstrate the importance of selecting kinetic parameters carefully particularly when these predictions are used for reactor design.

Key words: Supercritical water oxidation, Numerical modeling, Plug flow reactor, Advanced oxidation, Reaction engineering

1. Introduction

At temperature and pressure close to the critical point, the properties of water begin to drastically change. Supercritical water oxidation (SCWO) is an oxidation method based on the particular properties of supercritical water. Under supercritical conditions, nonpolar organic compounds and gasses such as oxygen become completely soluble in water because their dielectric constant decreases to amounts close to those of nonpolar organic solvents such as benzene. During the oxidation process, nonpolar organic compounds react with an oxidant, most commonly oxygen, in a single phase reaction producing carbon dioxide and water. The nitrogen present in inorganic compounds leads to the production of N_2 and small amounts of N_2O [1].

Many advantages have been stated for supercritical water oxidation. For example, no polluting gases such as NO_x and SO_x are produced. The destruction efficiency of organic wastes in SCWO is similar to that of incineration, while SCWO has fewer environmental hazards [2]. Supercritical water oxidation typically occurs at temperature

above 500 °C and pressure of 24~50 MPa. The reaction time can range from several seconds to no more than several minutes [1]. Often, the SCWO process is capable of degrading more than 9999 out of every 10,000 pollutant particles (destruction efficiency higher than 99.99%). Therefore, the exit stream of the process can be released into the environment without the need of any further treatment.

Also, since SCWO reactions are homogeneous, mass transfer does not cause restrictions [3]. This is one of the main reasons leading to shorter reaction times achieving higher reaction efficiency. However, there are also some challenges and limitations to SCWO technology, namely, the high costs, the high corrosion and need for special alloys, and possible sediment deposition [1,4].

So far, a range of various wastewaters including streams containing pharmaceuticals [5], different types of sludge [11], and fenuron and nitrogen containing compounds [6] have been treated with SCWO. Also, textile sludge [7], 3-4-trinitrotoluene [8], and oil-based drill cuttings [9] have been targeted. The removal of phenol from oil/gas produced water [10] has been investigated using this technology.

Modeling the degradation of various chemicals and waste streams based on the proposed mechanisms in supercritical water has been an area of study [12-14]. For example, Fourcault et al.[15] investigated supercritical water oxidation of phenol and modeled the profile of temperature and phenol concentration. Also Ghoreishi et al. [16]

modeled the effect of some parameters such as feed phenol concentration and reactor residence time on phenol conversion.

The heat transfer of supercritical water oxidation systems is also different from fluids in normal conditions. Numerous numerical models and semi-empirical models have been suggested [17,18]. As a result, extensive information is available on the reaction of numerous compounds in various conditions of supercritical water oxidation. These conditions are dependent on the type of reactor as well as the reacting compounds.

Being aware of the behavior of a supercritical oxidation reactor is vital for improving the safety and efficiency of the unit. However, due to the extreme operating conditions, obtaining real data from inside the reactor is difficult. Hence little experimental data is available for specific conditions. In addition, experimentation on a reactor can create serious risks for the reactor itself.

A mathematical model can thus be very useful for design and scale up. A model is also capable of providing more information than limited experimental data and can predict possible problems caused by the thermal behavior of the reactor. Computational fluid dynamics and process simulation are significant tools for designing and optimizing such chemical processes.

In this paper, a new and comprehensive numerical model is developed to predict phenol mass fraction and temperature distributions in an SCWO reactor under steady conditions. There are some experimental studies regarding the destruction of phenol and phenolic compounds via supercritical water oxidation [19-23]; however, few studies have investigated effective process parameters numerically. Remediation of wastewaters containing phenols is of high importance because of their high toxicity even at low concentrations.

2. Modeling procedure

A plug flow reactor was modeled under the wall boundary conditions with heat transfer to the surroundings for calculating the temperature and concentration under various flow conditions. The explanations of the computational scheme used to model the process and the mathematical equations describing the physical and chemical phenomena inside the reactor are described below.

2-1. Flow specifications and assumptions

The geometry of the study was a tubular reactor. Due to high mixing and uniformity of temperature and pressure the diameter of the reactor is considered to be small and the regime of the flow to be turbulent. In an ideal reactor, there is no axial mixing, and all fluid elements spend an equal duration of time in the reactor [15]. The following assumptions were made in this study:

1) Diffusion of the species and energy as well as turbulent mixing processes along the flow direction are negligible. Thus, axial diffusion is slow compared to convection.

2) At any cross section of the reactor, the temperature, composition and pressure are uniform. So, radial mixing is very fast.

3) The radial velocity profile is considered flat [15].

The flow conditions considered in this study are summarized in Table 1.

2-2. Fluid properties

Since the dominant bulk of the fluid inside the reactor is water, as well as the fact that water is a product of the reaction inside the reactor, the properties of the fluid are considered to be that of water. This assumption has also been used by other researchers [15,24,25]. Properties of pure water were obtained from the National Institute of Standards and Technology (NIST) [26].

2-3. Kinetic parameters

The mechanism of the oxidation of phenol involves many stages and intermediate species [25]. The reaction in its general form is expressed as:

$$C_6H_6O + 7O_2 \rightarrow 3H_2O + 6CO_2 \tag{1}$$
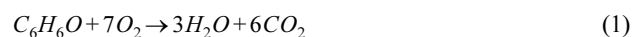
From the kinetics point of view, based on Arrhenius' law, the rate of the reaction is dependent on the temperature. The rate of the reaction is also dependent on the concentration of the reactants, namely, the phenol and oxygen. Therefore, the overall reaction rate equation is:

$$r = K exp\left(\frac{-E_a}{RT}\right) C_{C_6H_6O}^a C_{O_2}^b C_{H_2O}^c \tag{2}$$

where K is the pre-exponential factor, E_a the activation energy, R the gas constant, T the temperature, $C_{C_6H_6O}$ the phenol concentration, C_{O_2} the oxygen concentration, C_{H_2O} the water concentration and a and b and c the reaction orders with respect to phenol, oxygen and water, respectively [27-29].

Various kinetic parameters can be found in the literature based on the species (phenol, oxygen and water) that are considered in the equation of reaction rate. Five sets of kinetic parameters are considered in this study (A, B, C, D and E). The conditions under which the kinetic parameters were obtained are summarized in Table 2.

Since the entire reactor is at a supercritical state, the oxidant is completely mixed with the supercritical water, the process is turbulent, and the diameter of the oxidant injection pipe is small, it is assumed that upon entering the reactor the oxidant is immediately mixed and reacts uniformly [15].

Table 1. Flow conditions at the reactor inlet

Inlet Pressure (MPa)	Flow Rate of Waste (l h^{-1})	Phenol Concentration (g l^{-1})	Temperature of Waste (°C)	Flow Rate of Air (g s^{-1})	Temperature of Air (°C)
25	12.5	5	450	3.69	200

Table 2. Conditions under which the kinetic parameters were obtained

Sets of kinetic parameters	Reaction conditions	Reference
A	The temperature range of the study was between 573 to 773 (K) and phenol concentration was between 33 to 593 mg/L. Oxygen concentration was varied between 11 to 476 percent of amount that was needed for complete stochiometric oxidation of phenol.	[28]
B	Initial concentration of phenol was varied from 0.6 to 0.77 mg/L and the temperature range was 677 to 715 (K). The pressure was 25 MPa.	[29]
C	The temperature range was between 653 to 723 (K) and the pressure was adjusted between 23 to 26.5 MPa. The phenol concentration was from 500 to 1000 mg/L and the oxygen concentration was changed in the range of 0.3 to 12 g·L^{-1} (50% to 1000% excess oxygen)	[27]
D	The temperature and pressure range was between 653 to 713 (K) and 19 to 27 MPa, respectively. The inlet oxygen concentration ranged from 0.053 to 0.18 mol/L (100% to 1750% excess oxygen).	[19]
E	The temperature was between 573 to 693 (K) and the pressure was varied from 19 to 28.2 MPa. The inlet phenol concentration was 50 to 330 ppm, while the inlet concentration of oxygen ranged from stoichiometric up to 1100% excess oxygen.	[30]

2-4. Conservation equations

The simplified governing equations for a compressible Newtonian fluid with the assumptions mentioned earlier are as follows:

2-4-1. Conservation of Mass (Continuity)

$$\frac{\partial}{\partial x}(\rho u) = 0 \tag{3}$$

where x denotes the reactor length, u the axial fluid velocity, and ρ the fluid density.

2-4-2. Conservation of Momentum (Navier-Stokes)

$$\frac{\partial}{\partial x}(\rho u u) = \frac{\partial \tau_{xx}}{\partial x} - \frac{\partial P}{\partial x} + S_u \tag{4}$$

where τ_{xx} denotes the stress tensor, P the static pressure, and S_u the volumetric forces such as ρg.

2-4-3. Conservation of Energy

$$\frac{\partial}{\partial x}(\rho u h) = u\frac{\partial P}{\partial x} + \varphi + S_h \tag{5}$$

where h denotes the enthalpy of the mixture, φ specifies the positive-definite viscous dissipation function, and S_h denotes the source term (for example, reaction heat or heat loss) and is expressed as:

$$S_h = -W_{lost} - r\Delta_r H \tag{6}$$

where $\Delta_r H$ represents the heat of reaction, and r the reaction rate. W_{lost} is the heat loss by the reacting medium. The volumetric heat loss according to Newton's law is expressed as:

$$W_{lost} = \frac{4H}{d}(T - T_{ext}) \tag{7}$$

where H, T_{ext} and d are relevant to the heat transfer with the surroundings, the external temperature, and the internal diameter of the reactor, respectively. The parameters H and T_{ext} can either be constant or be functions of temperature or the length of the reactor. In this study, model predictions for when the reactor exchanges heat with the environment were examined.

2-4-4. Conservation of Species

$$\frac{\partial}{\partial x}(\rho u y_i) = S_{y_i} \tag{8}$$

where y_i denotes the mass fraction of species i, and S_{y_i} refers to the source term of species i (for example because of the reaction). S_{y_i} is expressed as:

$$S_{y_i} = M_i \gamma_i r \tag{9}$$

where M_i denotes the molar weight of species i and γ_i is the stoichiometric coefficient of the same species.

Phenol concentration can be related to its mass fraction using the following equation.

$$C_{C_6H_6O} = \frac{y_{C_6H_6O}}{M_{C_6H_6O}}\rho \tag{10}$$

where $M_{C_6H_6O}$ denotes the molar weight of phenol, $y_{C_6H_6O}$ is the mass fraction of phenol, and ρ is the density of the reacting medium.

2-5. Solution method

From the conservation of mass under steady-state conditions, it is concluded that ρu is constant. The entrance boundary conditions are the fluid temperature, pressure, mass fraction, and velocity (found from the input mass flow rate). The changes of the physicochemical properties of a supercritical fluid are highly nonlinear and predicting the flow behavior may be considered as a special example of variable property flow modeling. The problem is difficult to solve because the equations of conservation are coupled and must be solved simultaneously. In this study, the set of seven equations are solved by the Euler method. The solution starts with an initial guess of temperature and the final solution is found via iterations for 101 points in the solution domain. The numerical program is developed in MATLAB software. The results of the base numerical model are validated by the experimental results reported by Fourcault et al. [15].

3. Results and discussion

3-1. Effect of considering only phenol concentration in the equation of reaction rate

In this part, two different sets of kinetic parameters, A and B (Table 3), are used and the results are compared.

Fig. 1 shows the model predictions for temperature variations along the reactor. It is clear that the temperature decreases along the reactor. This can be a result of the slow reaction rate due to the low mass fraction of phenol. In this situation, the temperature distribution is affected more by the heat loss from the reactor to the surroundings rather than the heat generated by the reaction. Note that the fluid leaves the reactor at just under 380 °C. The choice of kinetic parameters does not affect the results greatly due to low phenol concentration and high environmental heat transfer.

Theoretically, it may seem that an increase in temperature could also help speed up the process. However, experimental data does not support this notion. This can be justified by the fact that at higher temperatures the water density is reduced, causing a decrease in concentration [30]. Also, increasing the reaction time may be of greater importance than temperature. This is because aromatic phenolic compounds may have a lower than expected conversion rate in SCWO [32] due to conjugated π-bond (especially in higher molecular weight structures). Polymerization is also possible [31]. In one experimental study, GC-MS was used to examine the effluent of the SCWO, showing that some primary dimers such as dibenzofuran, 2-polyphenol, and phenoxyethanol persisted, although they could be completely removed by increasing the reaction time [33].

The variation of the mass fraction of phenol along the reactor was investigated and shown in Fig. 2. It is observed that kinetic parameters A give results closer to the experimental data. The conversion efficiency of kinetic parameters A and B is 68.52% and 87.96%, respectively.

Fig. 3 shows the importance of considering density to be variable throughout the reactor. The density is at its lowest at the entrance of the reactor where temperatures are higher and increases along the reactor as the temperature decreases and heat is transferred to the environment. Unlike density, velocity has a decreasing trend to satisfy the continuity equation.

Water density is one of the most critical parameters which determines the mechanism of hydrothermal reactions. When the density is high (lower temperatures) the ionic mechanism is dominant. Conversely, when the density is low (temperatures are higher) the free radical reaction mechanism plays the dominant role [34]. Since supercritical water oxidation occurs at relatively high temperature, the free radical mechanism can be used to explain the reactions.
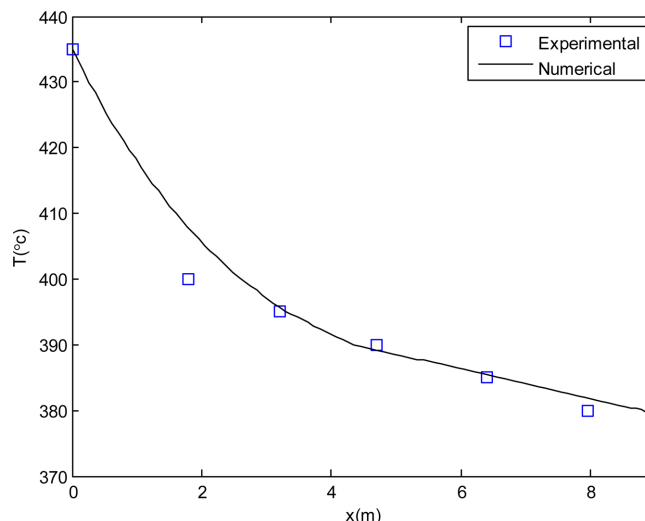

Fig. 1. Temperature distribution along the reactor; comparison of experimental data from [24] with the results predicted by the numerical model.
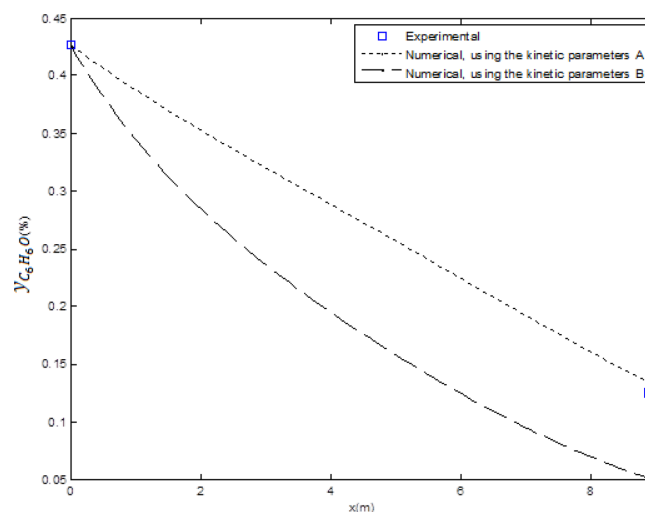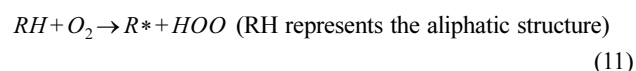

Fig. 2. Waste mass fraction distribution along the reactor; comparison of experimental data from [15] with the results predicted by the numerical model.

For example, in aliphatic structures, free radicals are produced efficiently by oxygen attack at weak bonds, such as the C-H bond [31]:

$$RH + O_2 \rightarrow R* + HOO \quad \text{(RH represents the aliphatic structure)}$$
(11)

$$RH + HOO* \rightarrow H_2O_2 + R*$$
(12)

$$H_2O_2 + M \rightarrow 2\ OH*$$
(13)

where (M) represents a homogeneous or heterogeneous partner of the collision. The free hydroxyl radical ($OH*$) has been recognized as the most active oxidant in SCWO, since its electrophilic reac-

Table 3. Kinetics parameters for oxidation of phenol

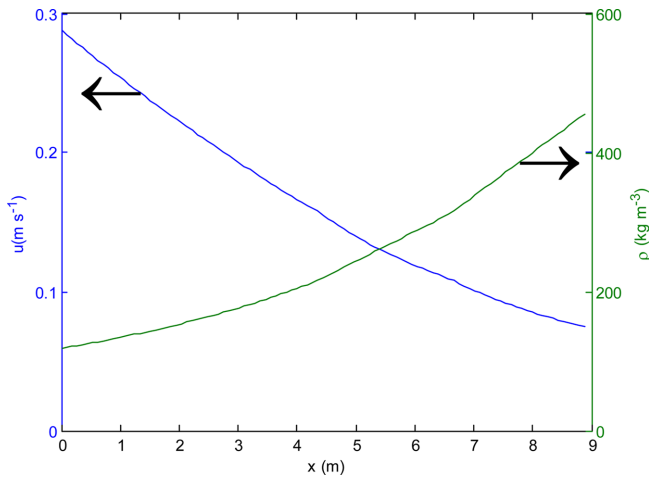|	K (s⁻¹)	E_a (kJ mol⁻¹)	a	b	c	Reference
A	$10^{1.34 \pm 0.77}$	39.2 ± 10.7	1	0	0	[28]
B	1970	60.8	1	0	0	[29]

Fig. 3. Velocity and density distributions along the reactor predicted by the numerical model using the kinetic parameters B.

tivity can oxidize all compounds having hydrogen [31]. $R*$ can be produced from the free hydroxyl reactions, leading to the following reactions:

$$RH + HO* \rightarrow R* + H_2O \tag{14}$$

$$R* + O_2 \rightarrow ROO* \tag{15}$$

$$ROO* + RH \rightarrow ROOH + R* \tag{16}$$

3-2. Considering the effect of phenol concentration on the mixture density

The literature shows that at lower pressure, the density of a mixture is a stronger function of the solute concentration [35]. Here, in the high temperatures and pressures under investigation, it is useful to examine to what extent the results are affected when considering phenol concentration and its effect on the density of the mixture. Unlike normal conditions where the simple van der Waals equation is often adequate, the Peng-Robinson equation is used in supercritical systems for higher accuracy [36]. Thus, here the density is calculated by the Peng-Robinson equation by using the law of mixtures [36]. To calculate mixture parameters, it is necessary to designate the interaction coefficients. Experimental data confirm that for binary systems interaction parameters have a linear relationship with temperature [36,37].

The two functions presented below are used to calculate the parameters of interaction for water-phenol and phenol-water systems [38]:

$$k_{Phenol-Water} = -1.629599T + 228.684 \tag{17}$$

$$k_{Water-Phenol} = -1.90779T + 14.75222 \tag{18}$$

Fig. 4 shows variation of the phenol mass fraction along the reactor for both kinetic parameters. It is observed that considering phenol concentration has a significant effect on the mass fraction.
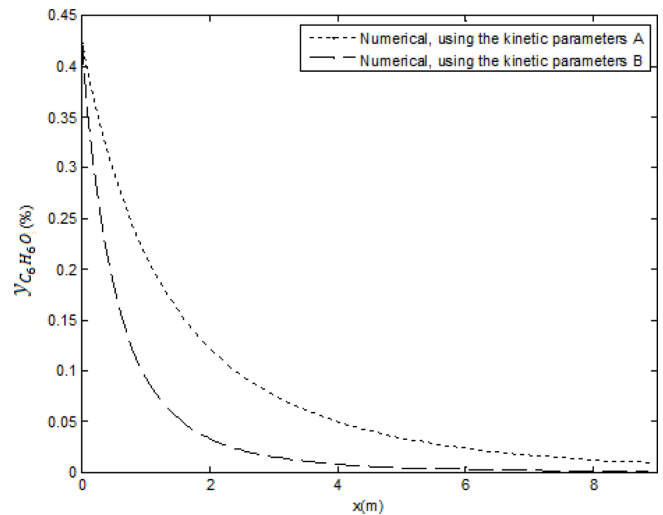

Fig. 4. Phenol mass fraction distribution along the reactor with considering the effect of phenol concentration on the fluid density.

In the beginning section of the reactor, the phenol concentration and hence the destruction efficiency are higher but they gradually decrease. The conversion efficiency when considering kinetic parameters A and B is 97.89% and 99.89%, respectively.

3-3. Effect of considering oxygen concentration in the reaction rate equation

The kinetic parameters for the case where the oxygen concentration is considered in the reaction rate equation are presented in Table 4.

Fig. 5 shows the variation of the phenol mass fraction along the reactor for kinetic parameters C for the following cases:
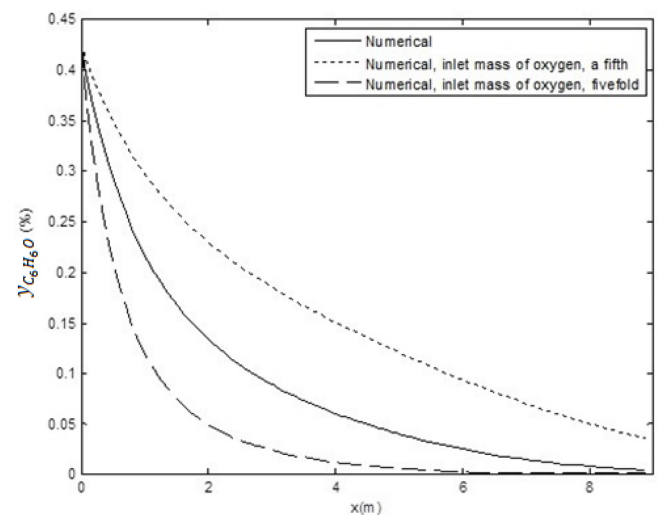

Fig. 5. Phenol mass fraction distribution along the reactor when oxygen concentration is considered in the equation of reaction rate (kinetic parameters C).

Table 4. Kinetic parameters for oxidation of phenol for the case where oxygen concentration is considered in the reaction rate equation

	K ((mol l⁻¹)$^{1-a-b-c}$ s⁻¹)	E_a (kJ mol⁻¹)	a	b	c	T, K	P, MPa	Reference
C	$4.9A \times 10^8$	124.8	1.04	0.38	0	653-723	23-26.5	[27]

1. The inlet mass flow rate of oxygen is unchanged, yielding a conversion efficiency of 99.04%.

2. The inlet mass flow rate of oxygen is a fifth of the initial value, yielding a conversion efficiency of 91.62%.

3. The inlet mass flow rate of oxygen is fivefold the initial value, yielding a conversion efficiency of 99.97%.

As clearly shown in Fig. 5, if the amount of initial oxygen varies, the phenol conversion efficiency changes significantly throughout the reactor.

The free radical mechanism of supercritical water oxidation can be used to explain this observation [31]. As the concentration of the oxidant is increased, it can logically be assumed that more radicals will be formed, which will accelerate the oxidation reaction [40]. However, if the concentration of the oxidant is too much, it has been observed that termination reactions of radicals may prevail, leading to stable products. This will result in a much slower increase in the conversion rate of the pollutant. Thus, there is an optimal value for excess oxygen, after which the increased investment will not be justifiable due to minimal increases in conversion efficiency [29].

Here, such a phenomenon is observed: the final conversion efficiency for the case of increasing the oxygen mass flow rate is very close to that of the base case. So the use of excess oxygen is not recommended due to economic considerations. Nonetheless, one advantage of having excess oxygen could be the need for a shorter reactor (because the conversion could happen more quickly), leading to reduced capital expenses.

In the beginning section of the reactor, the oxygen concentration and hence destruction efficiency are higher and they decrease gradually as phenol concentration decreases along the reactor.

3-4. Effect of considering water concentration in the reaction rate equation

After reviewing the effects of water on high-temperature and supercritical water reactions, Akiya and Savage [40] stated that several roles could be envisaged for water during supercritical oxidation. It is noteworthy that these may become conflicting when it comes to their effects on kinetics. They could include water acting within steps of the reaction, some solvation effects, and physical effects such as diffusion limitations and energy transfer of collisions [40]. It is also possible that the properties of density-dependent water support different chemistries (ionic vs. free-radical). This is particularly interesting because there may be regions having lower or higher density in the system [41]. In short, water can take part in the reaction as a reactant generating active radicals. The corresponding kinetic parameters used for such a condition are presented in Table 5.

The oxygen concentration also affects the reaction rate and a Langmuir-type model is used here to describe its effect [17].

$$phenol + O_2 \xrightarrow{k_1, k_{-1}} intermediate\ species \xrightarrow{k_2} products \qquad (19)$$
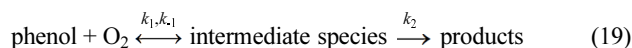
$$K_1 = \frac{k_1}{k_{-1}} \qquad (20)$$

where k_1, k_{-1} and k_2 are the reaction rate constants.

The reaction rate equation considering the Langmuir model can be simplified as:

$$r = \frac{K_1 k_2 C_{phenol} C_{oxygen}}{K_1 C_{oxygen} + 1} \qquad (21)$$

According to Equation 21, when the concentration of oxygen is high so that $K_1 C_{oxygen} \gg 1$, r approaches $k_2 C_{phenol}$ and thus the effect of oxygen content on the reaction rate is negligible. That is when b is zero (Table 5).

The mass fraction of phenol in the reactor using kinetic parameters D is shown in Fig. 6. The destruction efficiency is much lower when water concentration is considered in the reaction equation.

As it is clear from Fig. 6, unlike what was previously observed, the phenol conversion rate is lower in the beginning section of the reactor and increases gradually towards the reactor outlet. Water is the product of the reaction and so as expected (and Fig. 7 shows), water concentration increases along the reactor. This increases the reaction rate because water produces free radicals which have an important role in the progress of the reaction. Also, water has an order higher than unity (c) in the reaction rate equation, which means that as its concentration increases the reaction rate increases.

Since the concentration of water is small everywhere in the reactor and it appears in the reaction rate equation with a power
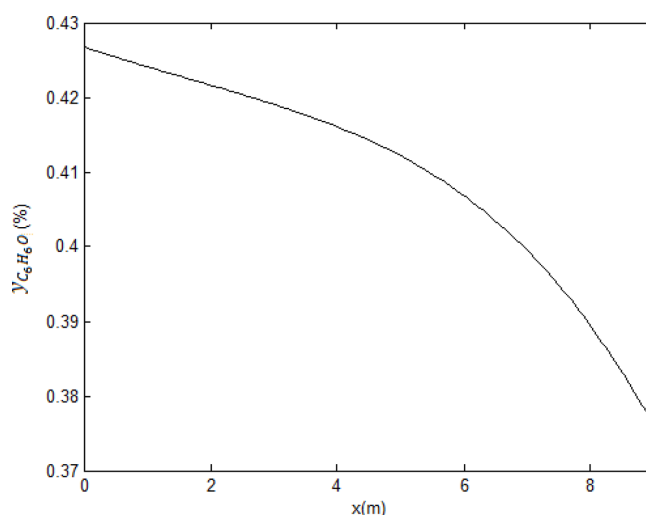
Fig. 6. Phenol mass fraction distribution along the reactor when water concentration is considered in the reaction rate equation (kinetic parameters D).

Table 5. Kinetic parameters for phenol oxidation with respect to water concentration in the reaction rate equation

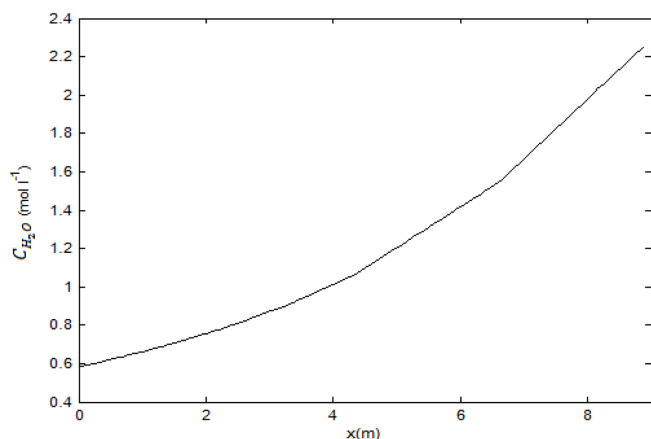|	K ($(mol\ l^{-1})^{1-a-b-c}$ s^{-1})	E_a (kJ mol^{-1})	a	b	c	T, K	P, MPa	Reference
D	8.91×10^4	99.6	1	0	1.38	653-713	19-27	[17]

Fig. 7. Distribution of water concentration along the reactor when water concentration is considered in the reaction rate equation (kinetic parameters D).
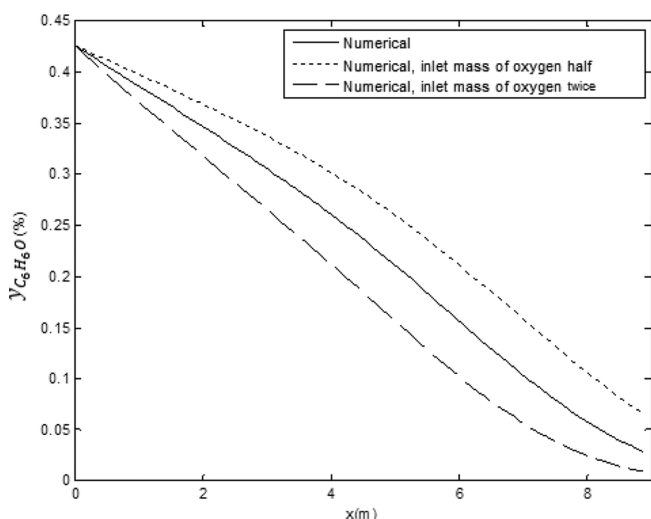

Fig. 8. Phenol mass fraction distribution along the reactor when concentrations of both oxygen and water are considered in the reaction rate equation (kinetic parameters E).

greater than one (c > 1), it is expected for the reaction rate to be very low all along the reactor. This results in the overall destruction efficiency to decrease.

3-5. Effect of considering both oxygen and water concentration in the reaction rate equation

Under certain circumstances, the reaction rate is dependent on the concentration of both oxygen and water. The kinetic parameters in Table 6 are used to study this situation.

Fig. 8 shows the distribution of the mass fraction of phenol using the kinetic parameters E for the following three cases:

1. The oxygen inlet mass has a fixed value. This leads to a destruction efficiency equal to 93.31%.

2. The oxygen inlet mass is half the value of case 1. This yields in a destruction efficiency of 84.67%.

3. The oxygen inlet mass is twice the value of case 1. The destruction efficiency increases to 97.96% in this case.

So, increasing the amount of the inlet oxygen increases the destruction efficiency of phenol along the reactor. It can be seen that at the beginning of the reactor, the oxygen concentration and the rate of destruction are higher. Understandably, these parameters gradually decrease as oxygen concentration decreases along the length of the reactor.

4. Conclusions

To better design a supercritical water oxidation unit one must be able to predict the variations of the parameters such as temperature and phenol mass fraction along the length of the reactor under various conditions. In addition, the temperature rise along the reactor should be noted, in order not to cause harm to the constructing materials of the reactor body.

In the present study, a plug flow reactor was modeled to investigate the oxidation process of phenol in a supercritical water environment under steady operating conditions.

Since the oxidation of phenol in supercritical water is an exothermic reaction, depending on the conditions, the fluid temperature may increase, remain constant, or decrease along the reactor. The numerical model showed that in this particular case, as we proceeded along the length of the reactor the temperature fell from above 430 °C to approximately 380 °C. So it can be concluded that although the oxidation of phenol is an exothermic reaction, the temperature decreases along the reactor because there is heat transfer with the surroundings.

Also, the linear velocity falls to less than one-third of the initial value, while the density more than doubles. The density increases due to the decrease in temperature, which forces a decrease in velocity to satisfy the continuity equation.

Using the developed numerical model, the effects of various kinetic parameters on phenol mass fraction and temperature along the reactor were studied. The conversion efficiency for the phenol depends heavily on the kinetic parameters and can be as high as 99.9%. Using different kinetic parameters is shown to significantly influence the predicted distributions inside the reactor and final phenol conversion. These results demonstrate the importance of selecting kinetic parameters carefully, particularly when these predictions are used for reactor design.

One of the most important findings of the current study was that although increasing the initial concentration of oxygen leads to much faster destruction of phenol, if adequate length of reactor is provided (long residence time) the effects of excess initial oxygen

Table 6. Kinetic parameters for phenol oxidation with respect to oxygen and water concentration in the reaction rate equation

	K ((mol l^{-1})$^{1-a-b-c}$ s^{-1})	E$_a$ (kJ mol^{-1})	a	b	c	T, K	P, MPa	Reference
E	303	51.8	1	0.5	0.7	573-693	19-28.2	[30]

concentration become less pronounced. Thus, an increase in oxygen at the inlet to above stochiometric values will allow a much smaller reactor to be constructed, and hence use fewer construction materials. However, this will lead to higher operation expenditures for supplying the oxygen. Hence a trade-off is present and the initial oxygen concentration should be optimized in order to minimize the combination of capital as well as operational expenditures.

Conflict of Interest

On behalf of all authors, the corresponding author states that there is no conflict of interest.

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