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Supercritical water oxidation of phenol with air. Experimental results and modelling

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ABSTRACT

Hydrothermal oxidation is an efficient and clean way for the treatment of wastewater containing organic matter. Because of its specific properties, supercritical water ensures high conversion of a wide range of organic load in the presence of an oxidant. The purpose of this work is to develop a mathematical model for a continuous flow tubular reactor devoted to hydrothermal oxidation. This reactor has a low ratio diameter length with one air injection. The mathematical model is based on plug flow assumption. The governing equations are: momentum, mass, species and energy balances. According to this model, the profiles of temperature and concentration of chemical species are computed along the reactor. The numerical predictions of the model are compared to experimental profiles obtained in the case of supercritical oxidation of phenol. These comparisons show very good agreement.

1. Introduction

Treatment of toxic and dangerous industrial wastes has become a very important topic for environmental protection. It is necessary to combine Chemistry and Environmental Engineering for searching new technologies for the disposal of toxic wastes. An important part of these industrial wastes are composed of water and are indexed as aqueous wastes. When their organic content is more than 1%, they are too concentrated to undergo a biological treatment, while, when it is less than 10%, their treatment by incineration is too expensive because it requires extra-gas.

Hydrothermal oxidation in supercritical water is an alternative way to dispose of these effluents. It mixes pressure and temperature like reaction activator: the pressure moves the reaction equilibriums between the phases, allowing an intimate contact between organic matter and oxidant, while the temperature increases the kinetics of the reactions according to the Arrhenius law. Depending on the operational conditions, the hydrothermal oxidation divides into two: wet oxidation and supercritical water oxidation. Wet oxidation, also known as wet air oxidation (WAO), refers to the process for oxidizing dissolved materials in liquid water with dissolved oxygen at high temperature. If operational conditions (temperature and pressure) are above the critical point of pure water (22.06 MPa, 647.13 K), the oxidation will become a supercritical water oxidation. It is a high-efficiency thermal oxidation process able to dispose of a wide range of industrial and urban wastes. The main advantage of this technology is that the by-products of the process are not toxic. Indeed, carbon is oxidized into carbon dioxide, hydrogen into water while hetero-atoms are converted into mineral salts [1–5]. Moreover, this technology allows to recover an important part of the energy released by the exothermic reaction of oxidation.

Because of the high pressure conditions that prevail, it is very difficult to obtain physical data inside the reactor. A mathematical model can be an efficient way to tackle this problem. Indeed, once validated by comparisons with experiments, such a model can provide further data and especially data concerning the inner part of the reactor. Moreover, a validated model might be very useful for the scale up of supercritical reactors at industrial scale.

The aim of this paper is precisely to develop such a model. In some previous attempts [6–8], a methodology was developed in order to predict supercritical water oxidation of model compounds in different kinds of reactors developed at l'Institut de Chimie et de la Matière Condensée de Bordeaux. However, these models were developed in the specific case of oxidation with pure oxygen what could limit the scope of the modelling procedure. In this work, oxidation with air is addressed.

The Supercritical Fluids Laboratory of the University of Cadiz has developed an experimental apparatus, which is presented in a first part. This device is of tubular type and experiments were carried out using phenol as model compound. Then, in the second part, the model, which translates into mathematical formalism the physical and chemical processes occurring in the reactor, is presented.

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Nomenclature

C_j	molar concentration of species j (mol m^{-3})
d	inner diameter of the reactor (m)
E_a	activation energy of oxidation reaction (J mol^{-1})
h	specific enthalpy of the reactive medium (J kg^{-1})
H	external heat transfer coefficient (W m^{-2} K^{-1})
L	total length of the reactor (m)
$\dot{m}_{O_2}$	mass flow rate of oxygen at injection (kg s^{-1})
M_k	molar weight of k (kg mol^{-1})
P	pressure of the reactive medium (Pa)
r_i	rate of reaction i (mol m^{-3} s^{-1})
R_j	chemical reaction rate of species j (kg m^{-3} s^{-1})
S	cross sectional area of the reactor (m^2)
S_{energy}	volumetric source term of energy in Eq. (13) (J m^{-3} s^{-1})
S_{mass}	volumetric source term of mass in Eq. (5) (kg m^{-3} s^{-1})S
S_{mom}	volumetric source term of momentum in Eq. (7) (kg m^{-2} s^{-2})
T	temperature of the reactive medium (K)
T_{ext}	external temperature (K)
u_{O_2}	velocity of oxygen at the injection point (m s^{-1})
w_{lost}	volumetric thermal power lost by the reactive medium to the surroundings (W m^{-3})
y_k	local mass fraction of species k

Greek symbols

$\Delta_r H_i$	enthalpy of reaction I (J kg^{-1})
$\Delta\xi/\Delta x$	lineic pressure drop (Pa m^{-1})
μ	dynamic viscosity of the reactive medium (Pa s)
ρ	density of the reactive medium (kg m^{-3})
τ_{xj}	stress tensor in direction x linked to velocity gradient in direction j.

Finally, the comparison between the numerical prediction and the numerical results are presented, with a very good agreement.

The results presented in this paper are new as regards supercritical water oxidation: firstly, experiments are carried out in a new facility developed at the University of Cadiz, which uses air as the oxidant, and, secondly, those experimental results are compared to the numerical prediction of the mathematical model that was previously written [6]. The fact that the comparison shows very good agreement emphasizes the reliability of the above-mentioned model.

2. Experimental apparatus

Fig. 1 sketches the experimental apparatus of *Supercritical Fluids Laboratory of the University of Cadiz*. The SCWO pilot plant consists of a continuous flow tubular reactor and other additional elements.

The liquid feed is stored in a stirred tank to keep it homogeneous. Waste is pumped through a high pressure pump from the feed tank to the first heat exchanger devoted to liquids. The air is pressurized by a high pressure compressor and is introduced into a second heat exchanger. Both feed streams are separately preheated.

The pilot plant has a coaxial counter-current heat exchanger with a total length of 11.5 m. This heat exchanger is used to preheat the liquid feed with the reactor effluent excess energy. In this equipment the effluent of the reactor, at high temperature and pressure, flows through the internal pipe giving calorific power to the cold feed, which flows through the annular space between the two coaxial pipes.

The main equipment is the continuous flow reactor, which is made of stainless steel AISI 316L. The internal diameter is about 12.32 mm and the external diameter is about 19.05 mm. It consists in three 3/4 in. pipes, the length of each one is 2920, 2960 and 3000 mm, respectively; they are horizontal and connected by Hoke connections used for high pressure applications. Two vertical pipes with a length of 69.3 and 69.9 mm, respectively connect the three pipes. The total volume of the reactor is 1229.553 cm^3. The inlet temperature in the reactor is around 400 °C and the outlet temperature can be raised up to 550 °C. In order to minimize the loss of the heat produced by the wastewater oxidation reactions, this reactor is surrounded by a thermal shield. When the reactor is used to determine kinetics data, it has to be isothermal. The reactor is not totally adiabatic; so we have to specify the heat loss coefficient by making a preliminary experiment with pure water. Seven thermocouples are placed along the reactor in order to measure the temperature profile generated in the reaction system.

The effluent of the reactor crosses the first heat exchanger, a coaxial counter-current heat exchanger for liquid feed, where the hot fluid goes through the internal tube and the cold fluid goes through the external tube. According to the calculations, the inlet and outlet temperatures are around 25 °C and 420 °C respectively for the cold fluid, and around 600 °C and 250 °C respectively for the hot fluid. The calorific power of the heat fluid is used to preheat the liquid feed stream. Then the effluent crosses a second coaxial counter-current heat exchanger, which is used to preheat the air feed. The characteristics of the heat exchanger for air are similar to the heat exchanger for liquid. The inlet and outlet temperatures of the air (cold fluid) are around 100 °C and 200 °C respectively, while the hot fluid goes in at 250 °C and goes out at 200 °C. Both heat exchangers are insulated so that this system can operate autothermally.

Once cooled, the effluent is depressurized by a back pressure regulator and the product stream is then separated into liquid and vapour phases in a gas–liquid separator.

In order to ensure that the temperature of the reactor effluent decreased below 50 °C, a multi-stage heat exchanger is used; it is refrigerated by water and the flow is controlled by an automatic valve.

To start up the pilot plant, it is necessary to increase the waste temperature before the reactor inlet to activate the oxidation reaction. So the pilot plant has an electric preheating system: resistors which are wound around the pipe where the liquid flows before going in the reactor. There are two kinds of resistors: the first one has a power of 1250 W and the second one has two units with a power of 3000 W each one. The total heating power is 7250 W.

The pilot plant is fully automated using the PLC and SCADA software developed by Schneider Electric. The automatic control system makes it possible to improve the performance and safety in the installation.

3. Mathematical modelling

The elaboration of the mathematical model describing the processes occurring within the supercritical water oxidation reactor is a complex task. Before deriving the governing equations it is necessary to discuss the assumptions on which it relies. This is the aim of the first part of this section. Secondly, the mathematical model is derived using mass, momentum, energy and chemical species balances. The main steps of the solving procedure are then explained.

3.1. Assumptions

Because of the high water content (more than 70%) inside the reacting medium and according to previous work [6–8] the reacting medium is assumed to be pure water. Thus thermo dynamical prop-

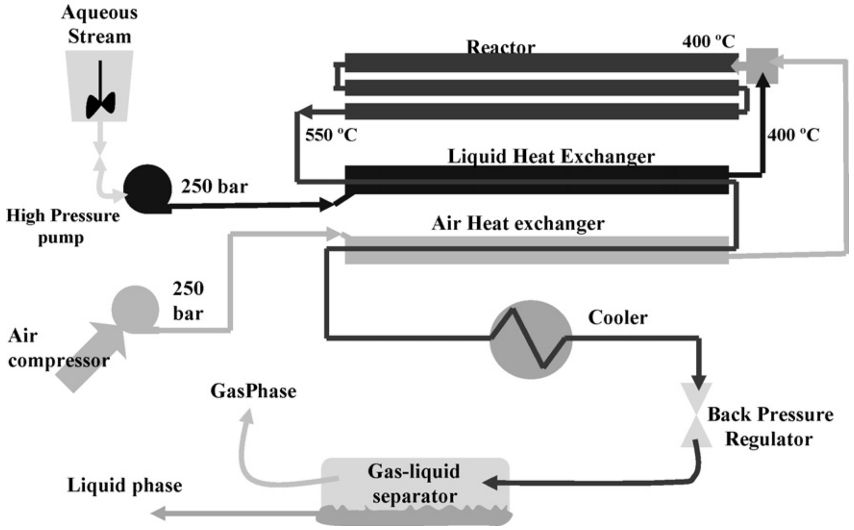

Fig. 1. Sketch of the Cadiz University Super Critical Water Pilot Plant.

erties of the medium are computed from the IAPWS formulation for pure water [9].

So the first assumption is:

A1: Thermodynamical properties (specific enthalpy, density) of the reacting medium are assumed to be equal to pure water properties.

The second assumption (which is closed to the first one) is relative to the transport properties of the reacting medium. Indeed, with the same justification than assumption A1, we postulate:

A2: Transport properties (thermal conductivity, density and viscosity) of the reacting medium are equal to pure water properties.

Given the general operating conditions (temperature at inlet is above 400 °C, pressure is 25 MPa and the mass flow rate is above $10\,\text{kg}\,\text{h}^{-1}$), the Reynolds's number at the entrance of the reactor can be estimated: $\text{Re} = 2.5 \times 10^4$. Thus turbulence inside the reactor is expected to be fully developed and this is the reason why we assume a plug flow mode of operation for this reactor. Moreover, this study is devoted to the stationary mode of operation. Thus the state variables of the system are one-dimensional. This leads to the third assumption:

A3: In stationary mode of operation, the system under study is considered as one-dimensional.

In this study, the choice has been made to focus on phenol as a possible model waste. A complete description of the oxidation of this species would require a detailed chemical mechanism including a lot of intermediate species. However, for high computation efficiency reasons, the reaction mechanism is lumped into the following global one step reaction

$$C_6H_6O + 7{\cdot}O_2 \rightarrow 3{\cdot}H_2O + 6{\cdot}CO_2 \tag{1}$$

A4: The chemical oxidation of phenol is described as a one step global reaction.

From the kinetics point of view we expect the rate of reaction to be dependent upon the temperature as postulated by Arrhenius. Moreover, we assume that this rate depends on the local concentrations of waste and oxygen. Thus, the rate of reaction is expressed as follows:

A5:

$$r = k^{\circ} \exp\left(\frac{-E_a}{RT}\right) \cdot C^{m}_{C_6H_6O} \cdot {C_{O_2}}^{n} \tag{2}$$

In Eq (2), k° stands for the pre-exponential factor of Arrhenius law, E_a for the activation energy of reaction (1) while $C_{C_6H_6O}$ and C_{O_2} represent respectively the local concentration of phenol and oxygen. m and n stands for the order with respect to waste and oxygen. In order to give insights into the importance of this set of parameters, two of them will be tested in this paper [10,11].

Although the whole apparatus is thermally insulated, it is obvious that thermal losses exist. They have to be taken into account into the energy balance of the reactor. To compute these losses, we assume that at each location of the reactor, a specific heat flux is lost according to Newton's law for heat transfer. For convenience, we relate this external specific heat flux to a volumetric power lost by the reacting medium.

A6: The volumetric power lost by the reactor by thermal losses is expressed as:

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

In this expression, H stands for the overall heat transfer coefficient with the surroundings, d the inner diameter of the reactor, and T and T_{ext} stand respectively for the local temperature and the external temperature.

Because of turbulence phenomena, some important mechanisms exist that might increase the rate of transport of species and energy under gradients of concentration and temperature respectively. However, because of the high value of the ratio L/d we assume the axial diffusion of species to be negligible with respect to the convective process [12]. Assuming further that Lewis's number equals unity, we draw the same conclusion for thermal transport processes.

A7: Axial diffusions of species and energy are negligible.

As it has been pointed out in the introduction, one of the main advantages to use supercritical water is that air is completely miscible within the reacting medium. Because everywhere in the reactor supercritical conditions prevail, because the process operates under turbulent conditions and because of the small diameter of the injector, we assume that

A8: Air is instantaneously and completely mixed with the reacting medium once it is injected in the reactor.

3.2. Governing equations

One of the aims of a mathematical model is to provide more information than experimental results can yield. For example, in our case, we expect the model to be able to describe the evolution of species concentration as well as the temperature along the reactor.

In order to obtain such information, we need to write some mathematical equations that translate physical and chemical phenomena into mathematical formalism. Basically, these equations postulate that in stationary mode of operation, mass, species, momentum and energy are conserved over a control volume of our choice.

In the following paragraph we show the governing equations in their “derivative” form inside each of the three reactors.

Total mass conservation

$$\frac{\partial \rho u}{\partial x} = 0 \tag{5}$$

where ρ stands for the local density of the mixture and u for its velocity. This equation states that within the reactor mass is neither created nor disappeared.

Momentum conservation

As it has been quoted into assumption A3, we consider the system as one-dimensional. However, a complete formulation of the momentum equation should include a two-dimensional formulation of this equation because of shear stress at the wall of the reactor. Indeed, this shear stress results in high radial gradients at this location. Thus the momentum balance is written as follows:

$$\frac{\partial \rho u u}{\partial x} = -\frac{\partial P}{\partial x} + \frac{\partial \tau_{xj}}{\partial x_j} \tag{6}$$

where P stands for the local pressure of the reacting medium, and τ_{xj} for the stress tensor, in direction x, linked to a gradient of velocity in the direction j.

Moreover, in turbulent mode of operation, the stress tensor should include the Reynolds’s stress tensor and an appropriate model to compute it. This would drastically complicate the mathematical description of the process. Thus, the choice that has been made here is to compute the divergence of the stress tensor as the local pressure drop over the control volume under consideration. This computation has been done according to Churchill’s correlation, valid for any Reynolds’s number [13]. The resulting balance equation is then

$$\frac{\partial \rho u u}{\partial x} = -\frac{\partial P}{\partial x} - \frac{\Delta \xi}{\Delta x} \tag{7}$$

where $\Delta\xi/\Delta x$ represents the local linear pressure drop inside the reactor.

Species conservation

We use the classical formulation of chemical engineering to describe the chemical reaction. Indeed if a set of species $J = \{1,2,\ldots,j,\ldots,N_{sp}\}$ is submitted to a set of chemical reactions $I = \{1,2,\ldots,i,\ldots,N_{reac}\}$, the total chemical reaction rate R_j (on a mass basis) of a species j is linked to the rate of reactions according to

$$R_j = M_j \sum_{i=1}^{N_{reac}} \partial_{i,j} r_i \tag{8}$$

where $\partial_{i,j}$ stands for the stoichiometric coefficient of species j in reaction i and M_j for the molar weight of species j. Given this formalism, the species balance can be written as

$$\frac{\partial u \cdot \rho y_j}{\partial x} - R_j = 0 \tag{9}$$

where y_j stands for the mass fraction of species j.

Energy conservation

Following the formalism used to derive the divergence of the stress tensor, one is able to compute the dissipation (both viscous and turbulent) as [14]:

$$\Theta = u \frac{\Delta \xi}{\Delta x} \tag{10}$$

Then the balance of energy over the control volume is expressed as:

$$\frac{\partial \rho u h}{\partial x} = u \frac{\Delta \xi}{\Delta x} + u \frac{\partial P}{\partial x} - w_{lost} - \sum_{i=1}^{N_{reac}} r_i \Delta_r H_i \tag{11}$$

where $\Delta_r H_i$ stands for the standard heat of reaction i, and h for the enthalpy to weight of the medium.

Models for density, enthalpy to weight and viscosity:

Then, one needs to write equations for the computation of density, viscosity and enthalpy. These equations stem from the IAPWS formulation for pure water [9] (see assumption A1) and they are written as:

$$\rho = \rho_m(P, T) \tag{12}$$

$$h = h_m(P, T) \tag{13}$$

$$\mu = \mu_m(P, T) \tag{14}$$

3.3. Boundary conditions

Boundary conditions are required at the input of the reactors. Indeed, because of the assumption A8 (instantaneous mixing of air with the supercritical fluid) the conditions prevailing at the input of the reactor are computed using a balance on an adiabatic, completely stirred tank reactor defining the injector.

If we denote h_0, P_0, T_0, ρ_0, u_0, $y_{j,0}$ and h_0 the conditions prevailing at the output of the preheater, P_{in}, T_{in}, ρ_{in}, u_{in}, $y_{j,in}$ and h_{in} the effective conditions at the input of the reactor under consideration, and $\dot{m}_{air}$, u_{air} and h_{air} the mass flow rate, velocity and enthalpy of air at the injector, then we write:

- *Mass balance*

$$U_{in} = \frac{\rho_0 u_0 S + \dot{m}_{air}}{\rho_{in} S} \tag{15}$$

- *Enthalpy balance*

$$h_{in} = \frac{\rho_0 u_0 h_0 S + \dot{m}_{air} h_{air}}{\rho_{in} u_{in} S} \tag{16}$$

- *Oxygen balance*

$$y_{O_2,in} = \frac{\rho_0 u_0 y_{O_2,0} S + y_{O_2,0} \dot{m}_{air}}{\rho_{in} u_{in} S} \tag{17}$$

- *Nitrogen balance*

$$y_{N_2,in} = \frac{\rho_0 u_0 y_{N_2,0} S + y_{N_2,0} \dot{m}_{air}}{\rho_{in} u_{in} S} \tag{18}$$

- *Species balance (except oxygen and nitrogen)*

$$y_{j,in} = \frac{\rho_{out} u_{out} y_{j,out}}{\rho_{in} u_{in}} \tag{19}$$

- *Momentum balance*

$$P_{in} = \frac{(\rho_0 u_0^2 + P_0) S + \dot{m}_{O_2} u_{O_2}}{S} - \rho_{in} u_{in}^2 \tag{20}$$

In the above expressions, S stands for the cross sectional area of the tubular reactor.

Models for density, enthalpy to weight and viscosity:

$$\rho_{in} = \rho_m(P_{in}, T_{in}) \tag{21}$$

$$h_{in} = h_m(P_{in}, T_{in}) \tag{22}$$

$$\mu_{in} = \mu_m(P_{in}, T_{in}) \tag{23}$$

Table 1
Operating parameters used for the evaluation of h_{ext}.

Inlet Pressure (MPa)	Flow rate of waste ($\mathrm{l\,h^{-1}}$)	Mass fraction of phenol	Mass fraction of water	Temperature of waste (°C)	Flow rate of air ($\mathrm{g\,min^{-1}}$)	Temperature of air (°C)
25	10.58	0	1	450	66.36	180

Modelling and simulation of hydrothermal oxidation of organic compounds.

Table 2
Review of kinetics parameters for oxidation of phenol from literature.

k° $(\mathrm{mol\,l})^{-1-m-n}\,\mathrm{s^{-1}}$	E_a ($\mathrm{kJ\,mol^{-1}}$)	m	n	References
$10^{1.34\pm0.77}$	39.2 ± 10.7	1	0	[10]
22 ± 9	39.6 ± 6	1	0	[11]

Modelling and simulation of hydrothermal oxidation of organic compounds.

3.4. Solving

The mathematical system under consideration is composed of 7 ordinary differential equations (total mass, momentum, energy, CO_2, O_2, N_2, phenol conservation) and 3 algebraic equations (model for enthalpy, density and viscosity of the mixture). Such a system cannot be directly fed to a computer to get the proper solution. Thus the choice has been made here to discretize the differential equations in order to get a purely algebraic system. Among the discretization methods, the finite volume method [15] is very attractive because the balance equations are satisfied over each control volume that constitutes the mesh. That is why we have derived the algebraic equations according to the divergence formulae:

$$\int_v div(\vec{\phi})dV = \oint_s \vec{\phi} \cdot d\vec{S} \tag{24}$$

where $\vec{\phi}$ stands for any vectorial data.

In our case the oxidation reaction is very fast, and mainly takes place near the injection of air.

This stiffness of the systems requires an appropriate meshing in order to make the mathematical system more stable. For this reason, we have chosen a grid with a step size following a geometrical common ratio from the injector to the output:

$$\Delta x^{i+1} = q\Delta x^i \tag{25}$$

where Δx^i stands for the size of the control volume number i (Fig. 2).

To conclude with the finite volume method, one needs to add an interpolation scheme allowing to define the state variables at the surface of the control volume as functions of the state variables inside the surrounding control volume. Because of its better stability, we have chosen the upwind scheme for interpolation.

Finally, the algebraic system obtained after discretization is solved using Newton–Raphson's method for algebraic systems of non-linear equations.

4. Results

In this section, we present the results of specific experiments obtained from both the experimental and numerical point of view.

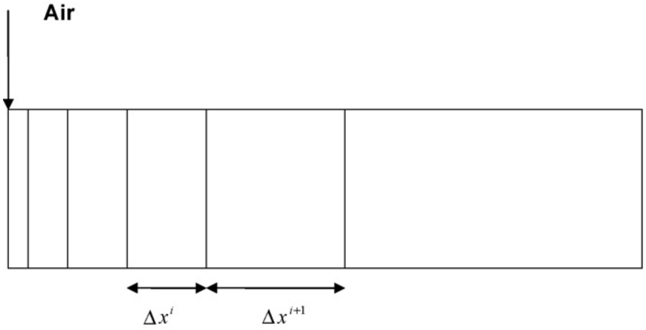

Fig. 2. Illustration of the adaptive mesh used for the discretization of differential equations.

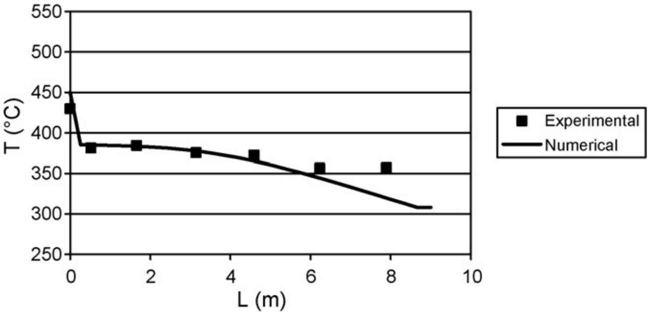

Fig. 3. Determination of the convective external heat transfer coefficient.

Nevertheless, the mathematical model requires a value of the convective heat transfer featured in Eq. (4). That is why, as a preliminary result, we present an analysis that allows the prediction of thermal losses of the device.

4.1. Determination of the convective external heat transfer coefficient

The value of this global coefficient (*i.e.* the thermal losses) is computed from a test with pure water, in the absence of chemical reaction and oxygen supply. This is a way to estimate the heat transfer between the experimental apparatus and the surroundings. These experimental tests were carried out in our experiments conditions. The operating data are summed up in Table 1 for the chosen experiment, and the temperature profile obtained is represented in Fig. 3. This temperature profile is compared with the one obtained by numerical predictions. The best results are obtained with a value of the global heat transfer coefficient of $30\,\mathrm{W\,m^{-2}\,K^{-1}}$.

Table 3
Operating parameters used for each experiment.

Experiment number	Inlet pressure (MPa)	Flow rate of waste ($\mathrm{l\,h^{-1}}$)	Phenol concentration ($\mathrm{g\,l^{-1}}$)	Temperature of waste (°C)	Flow rate of air ($\mathrm{kg\,s^{-1}}$)	Air in excess (%)	Temperature of air (°C)
1	25	12.5	5	450	3.69	484.16	200
2	25	9.98	10	500	3.32	292.7	200

Modelling and simulation of hydrothermal oxidation of organic compounds.

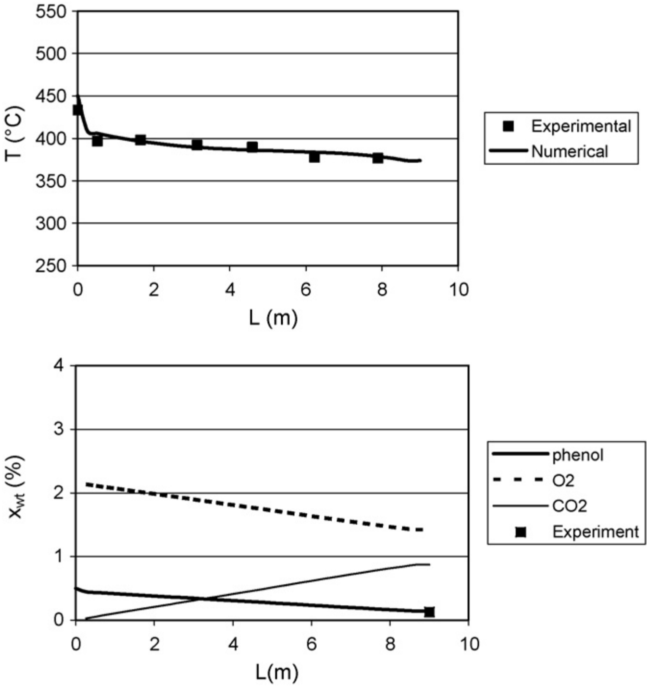

Fig. 4. Comparison between experiments and numerical predictions for temperature profile and conversion ratio, experiment 1, kinetic data from [10].

4.2. Oxidation of phenol

The supercritical oxidation of phenol has been chosen for the comparison between experiment and numerical prediction. Indeed this compound can be preheated above the critical temperature of pure water without being damaged. Moreover, some studies have already been performed on this compound and on the same experimental design in order to determine kinetic data [6,7]. The authors published their kinetic results with a range of uncertainty. For our simulations, we have chosen to compare two kinetic data. Table 2 summarises these kinetic data (in terms of energy of activation, E_a, as well as pre-exponential factor, k_0).

These values have been chosen for they have already been estimated in our operating conditions. Because the experimental device can only provide temperature profile, we have chosen this particular state variable to make the comparison between experiments and simulations. Two experiments are presented here. Table 3 resumes the operating conditions of each experiment.

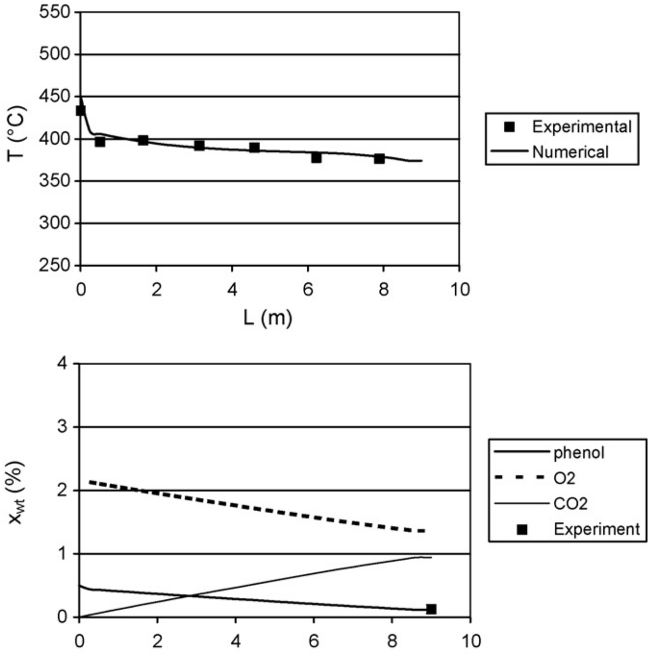

Fig. 5. Comparison between experiments and numerical predictions for temperature profile and conversion ratio, experiment 1, kinetic data from [11].

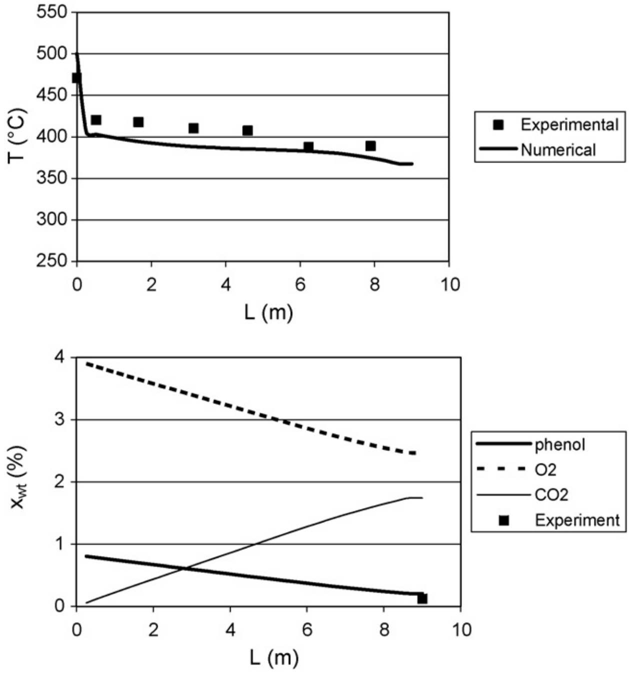

Fig. 6. Comparison between experiments and numerical predictions for temperature profile and conversion ratio, experiment 2, kinetic data from [10].

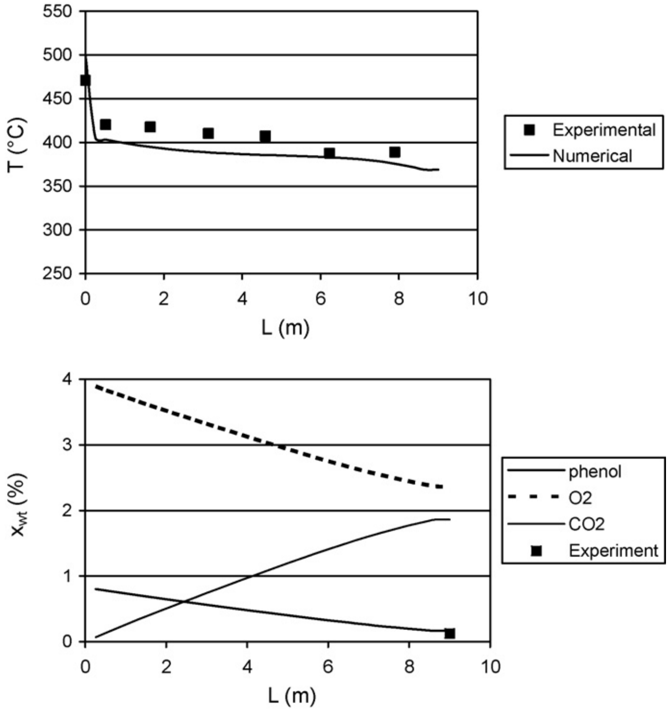

Fig. 7. Comparison between experiments and numerical predictions for temperature profile and conversion ratio, experiment 2, kinetic data from [11].

Figs. 4 and 5 show the comparisons of the temperature and conversion ratio between experiments and simulations for the first experiment, while Figs. 6 and 7 show the same comparisons for the second experiment.

From the experimental point of view, these Figures prove that the phenol oxidation process is valuable.

From the validation point of view, we can see that the numerical predictions fit quite well the experimental results. Numerical temperature profiles cohere with the experiments, and at the output, the conversion ratios obtained in numerical and experimental cases are the same (error is between 3 and 10%). Both kinetics data give basically the same results. Given the good prediction of the temperature profile inside the reactor, we assume the model to be validated. In our operating conditions both kinetic data are useable.

5. Conclusion

A mathematical model for the oxidation of organic compounds into supercritical water has been presented in this paper. This model relies on several assumptions that have been discussed in a devoted section. This model is based on the conservation of total mass, chemical species, momentum and energy written in steady state mode of operation. It allows the prediction of temperature and species profiles what give a detailed description of the phenomena occurring within the reactor. The results of this model have been compared to experimental data coming from Cadiz University facilities, in the case of phenol oxidation. As it has been discussed the numerical prediction highly depends upon the physical properties in a supercritical medium. Here enthalpy, viscosity and density should have been calculated with mixing laws and equation of state valuable for supercritical mixing. However, this model gives excellent prediction of the temperature profile along the reactor. This indicates that the different assumptions that have been formulated are valid. Thus this model can be used in order to give more information than the experimental apparatus can yield, as well as for the scaling up of supercritical water oxidation reactors.

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