Numerical Study of the Influence of Geometrical and Operational Parameters in Behavior of a Hydrothermal Flame in Vessel Reactor

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Supercritical water oxidation (SCWO) is a promising technology for waste elimination with great possibilities in energy recovery, but its commercialization faces some resistance due the problems of corrosion and salt deposition associated to this technology, as well due its high energetic consumes. The application of reactors working with a hydrothermal flame as a heat source contributes to overcome many of the challenges presents in this technology. Injection of the reagents over an hydrothermal flame can avoid the reagents preheating as the feed can be injected into the reactor at low temperatures, avoiding plugging and corrosion problems in a preheating system. Also the kinetics is much faster allowing complete destructions of the pollutants in residence times lower than 1 s. Next to this the high temperatures associated to the hydrothermal flames contribute to a better energy recovery of the reaction heat for electricity production. For safety and material limitations the flame has to be properly insulated or kept in distance from the pressure vessel wall. The configuration of the reactor and fluid injection nozzle has to be specially projected for this purpose. In this work, influence of reactor configuration is evaluated by experimental and simulation ways. Geometrical parameters studied are the distance between injector's outlet and reactor's ceiling and the injector inner diameter. Influence of operational parameters like flow velocity and inlet temperature are also verified. The CFD-model provides a good prediction of the experimental results and can be used for designing of reactors looking for performance and flame stabilization.

INTRODUCTION

Supercritical water oxidation (SCWO) is a promising technology for the total destruction of waste with residence times of a few seconds and even in residence times lower than one second if the reactor works in hydrothermal flame regime. It takes advantage of the special solvation properties of water above its critical point (374ºC, 22.1 MPa) to achieve the complete destruction of organic waste. Oxidation of organics dissolved in supercritical water (SCW) can be carried out in a homogeneous phase due to the complete miscibility of gases (oxygen) and organics with SCW. However, some challenges have still to be overcome for the successful and profitable commercialization of this technology. The industrial development of the process has been delayed due to the main challenges of this technology: corrosion, salt deposition and high energetic demand ([1],[2]). Corrosion and salt deposition problems, as well as heat recovery optimization can be overcome by the use of appropriate materials and reactor designs.

Several research groups have developed reactors working with a hydrothermal flame as a heat source ([3],[4]), since the formation of hydrothermal flames was proved by Franck and coworkers [5]. Hydrothermal flames are combustion flames produced in aqueous environments at conditions above the critical point of water [6]. SCWO reactors with a hydrothermal flame have a number of advantages. It allows the destruction of the pollutants in residence times of a few milliseconds and it is possible to initiate the reaction with feed injections temperatures near to room temperature [7]. This last point supposes an advantage from the operational and the energetic integration points of view, as avoid problems of plugging and corrosion in a preheating system. Next to this, the higher operation temperatures improve the energy recovery. The High Pressure Process Group (HPPG) of the University of Valladolid (UVa) (Spain) showed the formation of hydrothermal flames in tubular reactors [8] and modeled those using the combustion approach based on mixing model [9]. With this simple device, extinction temperatures of the flame could not be reduced under 370ºC. Vessel reactors have demonstrated to be more successful in maintaining steady stable hydrothermal flames with injection temperatures near to room temperature ([3],[4],[10]). The flame stability is related to injection temperature and flow velocity, and vessel reactors provide flow velocities that are compatible with hydrothermal flame velocities [11]. It is thought that vessel reactors provide a space for the recirculation where the cold reagents are preheated to the ignition temperature and brought into contact with the radicals already formed, making possible the flame formation. CFD simulations of these reactors show the existence of a flame front where most of the reaction takes place [12].

In this work a CFD model has been used to make an analysis of the behavior of a vessel reactor, a new cooled wall reactor design (CWR) with and internal hydrothermal flame developed in the University of Valladolid, focussing in its behavior. The geometry of the reactor and operational parameters have been analysed.

EXPERIMENTAL

Results of CFD model simulations were compared to experimental data provided by the new cooled wall reactor working at the pilot plant of the University of Valladolid. The cooled wall reactor consists of a cylindrical reaction chamber of 2.2 L (1 m length and 53 mm diameter), limited by a Ni-alloy wall contained in a stainless steel pressure shell with a volume of 4.3 L. Cold water flows in space between the reaction chamber and the pressure shell in order to keep the pressure vessel at temperatures lower than 400ºC.

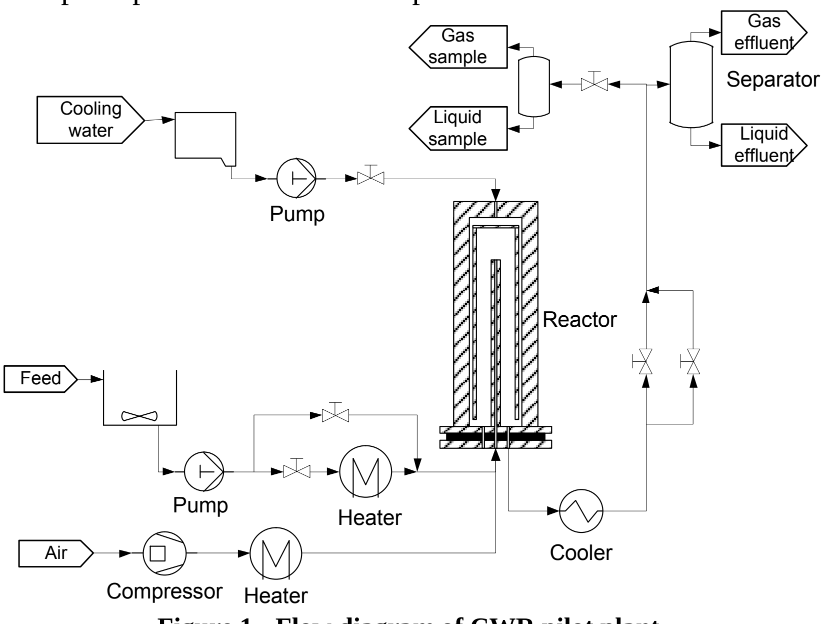

Figure 1 - Flow diagram of CWR pilot plant.

Feed and air are introduced into the reactor through its lower part, and flow through an injector up to the upper part of the reaction chamber, where the reaction takes place. The streams flow down and decontaminated water leaves the reactor through its lower part. In order to follow the reaction, the temperature is measured in several points of the reaction chamber. The flow diagram of the pilot plant is shown in Figure 1.

Injectors with different configurations were proved. For each configuration a series of experiments at different flows and temperatures were performed, in order to obtain a set of design parameters. All the injectors are Ni-alloy empty tubes. All the experiments were performed using isopropyl-alcohol (IPA) as contaminant-model, and air as oxidant.

MODEL

A CFD model was performed in order to study the internal fluid dynamic behavior of the cooled wall reactor. The main elements of the reactor have been included in the model geometry, including the metallic injector, the reaction chamber, and the space between the pressure shell and the chamber. A simplification, consisting of the assumption that the effluent leaves the reactor through an annular space on its lower section, was considered. This assumption was essential to allow modelling the reactor as an axisymmetric 2D system instead of as a 3D system, which considerably reduces the complexity and computer-time requirements of the model. Nevertheless, the simplification has no further influence on results since we are interested in region of flame formation, which means the injector outlet and the upper part of reactor.

The model includes the mass, energy and momentum transport equations. For the description of the oxidation kinetics, has been used a kinetic model fitted from tubular reactor data of our group [8]. The k-ε model has been used to model turbulence, as suggested by Sierra-Pallares et al. [13], and due to low velocity flow on reaction chamber, the low-Reynolds method [14] was activated. Heat transfer by conduction through both the metallic walls of the injector and of the reaction chamber has been considered in the energy equation. The physical properties required by the model are the volumetric, thermal and transport properties of the mixtures of the five species that constitute the system: water, oxygen, nitrogen, carbon dioxide and isopropyl-alcohol. Specific heat (and enthalpies) of the mixture is calculated with Peng-Robinson Equation of State (PR-EoS) [15]. Mixture density is calculated with the Peng-Robinson Equation of State with constant volume translation (VTPR-EoS) [16]. Thermal conductivities are given by TRAPP method for high pressure systems [17]. The remaining properties have been calculated as a mass-fraction average of the properties of the pure components.

The model was solved on the commercial CFD software Fluent®. Changing de injector configuration and the feed flow, we obtain a list of 6 model cases that show the behavior of the reactor (Table 1).

Table 1 – Cases to be simulated for study of parameters of cooled wall reactor.

# Simulation	Feed flow	Nominal diameter	Length
S1	13 kg/h	1/4”	95 cm
S2	13 kg/h	1/4”	50 cm
S3	13 kg/h	1/8”	95 cm
S4	23 kg/h	1/4”	95 cm
S5	23 kg/h	1/4”	50 cm
S6	23 kg/h	1/8”	95 cm

RESULTS

Figure 2 shows a comparison of experimental and predicted temperatures. Dashed line corresponds to temperature inside the injector that arises slowly due to heat transfer through injector’s wall. Continuous line is the prediction for the temperature on the reaction chamber, which is higher at upper part, where flame is formed. The triangles are experimental measurements of temperature and show a good agreement to the model. Dotted line represents the temperature of cooling water flowing between the reactor wall and the pressure shell.

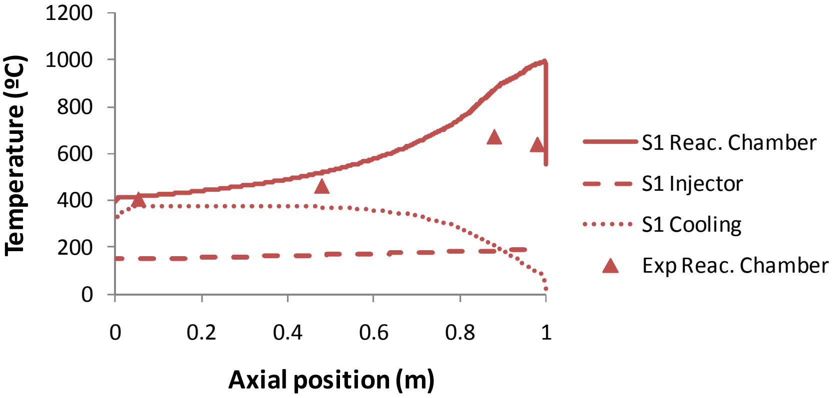

Figure 2 – Temperature profiles inside CWR: Experimental and simulation prediction for case S1.

More detailed information can be observed in Figure 3 that presents the contours of mass fraction of IPA. The shape of contours points to the existence of a flame at injector outlet, where most of the fuel (IPA) is consumed. Flame is maintained by the recycling zone at upper part of reaction chamber that allows cold feed to be brought in contact with hot products.

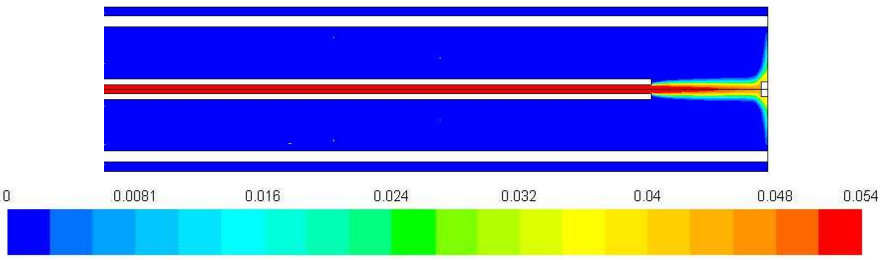

Figure 3 – Contours of IPA mass fraction, for case S1.

Study of injector's length

Experimental measurements and simulation results suggest that the flow of reagents "collides" against reactor's ceiling, which could be the cause for the back mixing phenomena when the injector is 95 cm long. In order to evaluate the influence of distance between injector outlet and reactor's ceiling, the injector was reduced to 50 cm. With that configuration, the flow has sufficient space for stabilizing with no influence of ceiling.

Figure 4 compares the temperature contours inside the injector and at reaction chamber for cases S1 and S2 that have the same inlet conditions but different injectors. It can be seen that the maximum temperature is lower for the shortest injector (S2). Also, the cooling of products is not so efficient as in S1. Results show that even far from reactor's ceiling, the flow regime generates a recirculation area at injector outlet, allowing the formation and stabilization of the flame, as shown on Figure 4 (b), and the flame is not deformed.

Study of injector's diameter

The internal diameter of the injector has a direct influence on the flow velocity. That effect changes the heat transfer and can displace the hydrothermal flame. Comparing cases S1 and S3, the reduction on diameter does not produce changes at reaction zone, but makes worse the heat transfer. The temperature inside the injector remains practically constant and the products are hotter than in case S1. Results are not shown here.

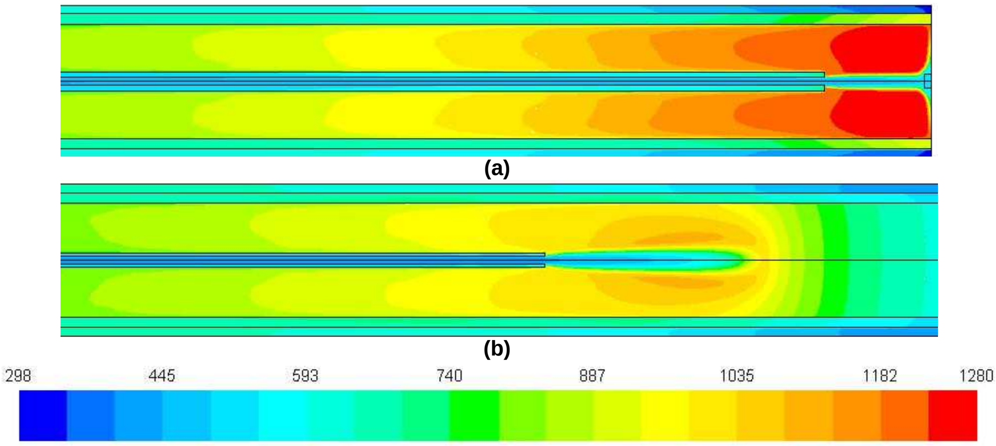

Figure 4- Contours of temperature (Kelvin): (a) Longer injector (case S1); (b) Shorter injector (case S2).

Influence of feed flow

Increasing the mass flow does not affect the heat transfer inside the injector, but it does at reaction chamber. Figure 5 shows that the reaction chamber remains at a temperature higher than in case of low flow, comparing temperature distribution for cases S2 and S5. This figure also indicates that, at higher mass flow, the flame is extended to the upper part of reactor.

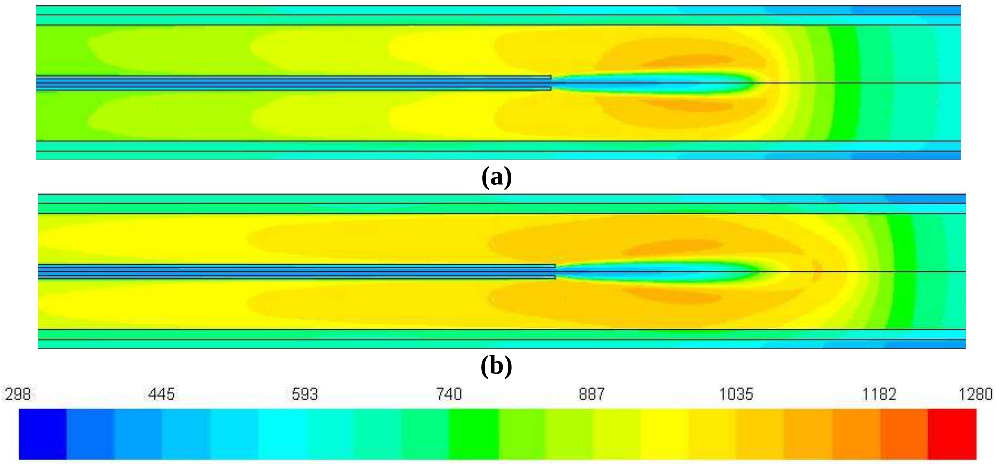

Figure 5 - Contours of temperature (K): (a) Lower mass flow (case S2); (b) Higher mass flow (case S5).

CONCLUSION

A CFD model for the cooled wall reactor developed by University of Valladolid was made. The model correctly predicts experimental temperature profiles and was applied to study the influence of operational and geometrical factors in the hydrodynamics of hydrothermal flame formation.

According to the model, the use of a long injector produces higher temperatures than the shorter one, but the hydrothermal flame is slightly deformed due the proximity to the reactor's ceiling. The short injector, on the other hand, produces a flame not deformed, and the reactor temperature reduces at upper and lower part.

Injector's diameter and feed flow have influence on fluid velocity. When injection velocity was increased the zone of maximum temperature in the reaction chamber was increased, indicating that the flame front was moving “pushed” by the flow. In the cases presented here, that effect was more dependent on feed flow than injector’s diameter.

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