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# Control of Process in Reactor for the Treatment of Phenol, Computational Fluid Dynamics and Phytotoxicity tests in Sweet Pepper Seeds

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***Abstract***— This research showed an Direct Contact Thermal Treatment (DiCTT) with the possibility of oxidizing phenolic compounds. Optimal conditions were identified for complete phenol degradation (>98%) and Total Organic Carbon (TOC) conversion (>35%). A comparative study of the combustion mechanism of methane and natural gas was carried out to compare the observed calculations of a model using Computational Fluid Dynamics (CFD) to the experimental data. Thus, the natural gas flow rate ($Q_{GN}$=1 $m^3 \cdot h^{-1}$) and the equivalent ratio ($\phi$=1) were used based on the evaluation of the best operating conditions of the flame. We use the techniques for determining phytotoxicity with sweet pepper seeds, and thus, identify the class of pollutants in the liquid effluent. The tests were carried out for phytotoxicity in sweet pepper seeds with phenol application, in the analyzed values of Root Growth Indexes (RGI), and Germination Indexes (GI), which showed the nongrowth of these seeds.

***Index Terms***—Control of Process, DiCTT, CFD, Phytotoxicity.

## I. INTRODUCTION

Recently, from the development of scientific studies in learning technology, several research scientists have reported advances in computational modeling [1], making it possible to compare the observed calculations of a model using Computational Fluid Dynamics (CFD) to the experimental data analyzed in laboratory research. The use of fluid dynamics has greatly developed in the field of engineering, mainly from the areas of oil and natural gas generation, in *offshore* platforms [2]. The CFD has been employed as an extremely necessary technique, along with theory and experimentation methods of analysis, design, optimization and resolution of complex problems of nonisothermal flow [3]–[5].

Computational modeling has been employed in complex situations, allowing an approximation of obtained experimental values [6].

Brandão [7] showed models with high accuracy in the prediction of contaminant degradation, such as phenol. Thus, some research has revealed that several organic and hazardous substances, such as phenol and its aromatic intermediates, among other halogenated or volatile organic components, frequently contaminate industrial effluent streams [8]. However, the presence of phenols in the aquatic environment has been a priority factor and of great relevance by the USEPA (US Environmental Protection Agency) [9].

The resolution No. 430 of the National Council for the Environment (CONAMA) was announced by legislation on May 13, 2011, which defines for the presence of total phenols, the maximum limit of 0.5 $mg.L^{-1}$, as a discharge standard for industrial effluents [9].

Data reported in the literature have shown methods for degrading effluents contaminated by phenolic compounds [10]. Thus, an unconventional Advanced Oxidation Processes (AOPs) called Direct Contact Thermal Treatment (DiCTT) has been developed [2, 11]. The DiCTT is based on direct contact between the contaminated liquid effluent stream and the flame produced by a natural gas combustor containing free radicals, such as: •OH, •H, $\cdot CH_3$ and •CH [9].

The evaluation of phytotoxicity in certain seeds has shown the characteristics of some effluents containing chemical substances, considering the class of pollutant effluent [12, 13]. The Root Growth Index (RGI) and the Germination Index (GI) have been fundamental and widely used in the calculations, after the data obtained in the analyses, being an effective, sensitive, and acceptable method as a biological marker capable of measuring the phytotoxicity present in the medium [14].

This study aims to obtain information on the thermal tests, which analyzed the natural gas flow rate ($Q_{GN}$, 2–4 $m^3 \cdot h^{-1}$) from the effect of air excess (*E, 10%*), recycling rate of the combustion gases ($Q_{RG}$, 50%), liquid phase flow rate ($Q_L$, 170 $L \cdot h^{-1}$), molar ratio of stoichiometric phenol to hydrogen peroxide ($R_{PH}$, *50%*), and the initial phenol concentration ($C_{Ph0}$, 500 $mg \cdot L^{-1}$) on the energy efficiency of the process. This research presentes showed a DiCTT method that use of natural

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gas as an energy source and production of hydroxyl radicals (•OH), the possibility of oxidizing phenolic compounds at low temperatures and the use of atmospheric pressure. The analytical technique adopted to analyze the residual concentration of phenol, and to identify intermediates formed during the reaction, was High Performance Liquid Chromatography (HPLC) and to evaluate the reduction of the organic load contained in the liquid phase we use the Total Organic Carbon (TOC) analyzer. The variation in effluent acidity was determined by measuring the hydrogen potential, pH-meter. The research work studied also allows collaboration for a more accurate theoretical-computational analysis of the process by the DiCTT reactor, using the Computational Fluid Dynamics (CFD) modeling method. Thus, we use the natural gas flow rate ($Q_{GN}$=1 $m^3 \cdot h^{-1}$) and the equivalent ratio ($\phi$=1), based on the evaluation of the best operating conditions of the flame, aiming at the validation and optimization of the operational conditions of the process. This research also aims to identify the effects of phenolic effluent on phytotoxicity in sweet pepper seeds, analyzing the RGI and GI of each seed, at different concentrations of phenol, being a sensitive method.

## II. MATERIALS AND METHODS

### A. *Reagents*

In the experimental tests were prepared a synthetic solution containing phenol (99% PA, Dynamic) and hydrogen peroxide, $H_2O_2$, analytical grade (35% PA, Vetec) in order to assist in the oxidation stage of the liquid phase. The methanol used in the High Performance Liquid Chromatography (HPLC) analysis was UV/HPLC (99.9% PA, Vetec), and phosphoric acid, $H_3PO_4$ (25% PA, Vetec) we use in the TOC analysis [2, 6].

### B. *Description of the DiCTT Pilot Plant*

The pilot plant used in the experiments was composed of a vertical, stainless-steel reactor and a gas–liquid separator. The DiCTT process is a technique appropriate for *off-shore* oil drilling platforms, where natural gas is available and space is limited [2]. Free radicals are generated from the combustion of natural gas (methane) according to the reaction mechanism described, as in

$$\begin{aligned} & X \rightarrow \bullet Y + \bullet Z \\ & \bullet Y + O_2 \rightarrow W + \bullet U \\ & \bullet U + X \rightarrow \bullet Y + H_2 O \\ & \bullet U + X \rightarrow \bullet T + \bullet U + \frac{3}{2} H_2 \end{aligned} \qquad (1)$$

where: X=($CH_4$-Methane); •Y=(•$CH_3$-Methyl Radical); •Z=(•H-Hidrogen Radical); •U=(•OH-Hidroxyl Radical); W= ($CH_2O$-Methanal); $O_2$=Molecular Oxygen; $H_2O$=Water; •T= (•CH- Methylidyne Radical); $H_2$=Molecular Hidrogen.

Initially, after heating the water to almost $70^0$C, a sample of 250 mL of treated water (white) was collected, and soon after, a synthetic phenol solution was prepared and added in Tank 1 of the DiCTT reactor with a 250-L volume. Then, the synthetic effluent was transferred from Tank 2, where the entire solution was recirculated. Hydrogen peroxide was also added to the recirculation Tank 2 to react stoichiometrically with the phenol, initiating oxidation in the aqueous phase at a molar ratio stoichiometric of Phenol/Hydrogen Peroxide, $R_{P/H}$. The effluent was injected into the vertical reactor through a positive displacement pump to produce a helical flow on its inner walls and increase the contact of the liquid effluent with the flame produced by the combustion of natural gas inside the DiCTT reactor.

A fraction of the combustion gases were recycled to more quickly heat the solution in tank 2, and thus dissolve a part of the residual oxygen from the combustion in the reaction liquid, thus inducing the thermochemical oxidation of the phenolic compounds. In the experimental tests, samples of 250 mL of the phenolic solution were collected in duplicate, according to the process time (t, 0–220min), in amber plastic bottles, and then were refrigerated.

In the DiCTT process was used atmospheric pressure. Its operation was done manually, with the assistance of a Supervisory Software for monitoring and controlling the process variables. The temperature data, generated by the combustion gases were obtained through the use of thermocouples axially distributed along the reactor wall. Fig. 1 shows the software for monitoring and controlling of the process variables.

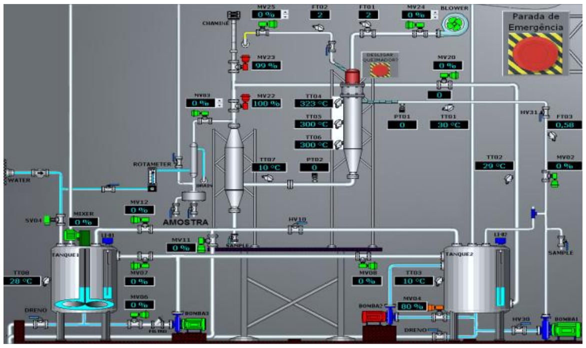

Fig. 1. Screen of the Supervisory Software for Monitoring and Control of the Process variables.

### C. *Analytical Techniques*

The concentrations of phenol was monitored using High-Performance Liquid Chromatography (HPLC), Shimadzu, model LC-20AT, with UV detector, and a CLC-ODS column M/C-18/Shimadzu with 250 mm in length and 4.6 mm in diameter. An isocratic elution mode was used. The oven temperature was 35°C; the flow rate of the mobile phase, 0.75 $mL \cdot min^{-1}$; injection volume of 20 $\mu$L; mobile phase consisting of 10% methanol and 90% phosphoric acid with pH adjusted to 2.2; and UV detector wavelength, 270 nm to detect phenol [15].

Analytical techniques using Total Organic Carbon (TOC) analyzer was measured, *TOC*Vcsh model, Shimadzu, to analyse phenolic mineralisation quantitatively. TOC analyzer is able to quantify the total organic carbon and total nitrogen indices simultaneously. *TOC* is the difference between the Total Carbon (TC) and the Inorganic Carbon (IC) content [16].

### D. *Measured and Calculated Parameters*

A molar ratio stoichiometric of Phenol/Hydrogen Peroxide, $R_{P/H}$, corresponds to the number of moles of hydrogen peroxide needed to completely convert 1 mole of phenol into carbon dioxide and water described [6], as in

$$C_6H_5OH + 14\,H_2O_2 \rightarrow 6\,CO_2 + 17\,H_2O \qquad (2)$$

The percentage division of Phenol Degradation ($P_h$) [6] was calculated by using (3), as in

$$P_h = \left(\frac{Q_L.C_{Ph0} - Q_L.C_{Ph} - F_G.C_{Phv}}{Q_L.C_{Ph0}}\right).100 \qquad (3)$$

where: $Q_L$ is the volumetric liquid flow rate, $C_{Ph0}$ is the initial phenol concentration, $C_{Ph}$ is the phenol concentration at a given time, $F_G$ is the mass flow rate of dry air and $C_{Phv}$ is the phenol concentration in the condensate at a given time.

The percent *TOC* conversion (*TOC*) [6] was calculated by using (4), as in

$$TOC = \left(\frac{Q_L.TOC_0 - Q_L.TOC - F_G.TOC_v}{Q_L.(TOC_0 - TOC_B)}\right).100, \qquad (4)$$

where: $TOC_0$ is the initial total organic carbono concentration, TOC and $TOC_V$ is the total organic carbono and the total organic carbon in the condensate, respectively, at a time point t of the process and $TOC_B$ is the total organic carbon in the blank.

### E. Theoretical-Computacional Studies by CFD

The mathematical modeling with computational studies of natural gas combustion was achieved with Fluent$^{TM}$ software. According to the burner geometry, a model based on nonpremixed combustion was used based on the elementary equations of mass, energy and quantity of motion balances, which characterize the important values of fluid dynamics [17].

Thus, the $CH_4$-Skel mechanisms were developed by the Sandia Laboratory for methane combustion, and the GRI 3.0 system was established by scientists from the Department of Mechanical Engineering at the Berkeley University [18].

The combustion of methane and natural gas was evaluated to investigate the effect of the nature of the fuel, as shown in Table I [17].

The natural gas flow rate ($Q_{GN}$=1 $m^3 \cdot h^{-1}$) and the equivalent ratio ($\phi$=1) was used based on the evaluation of the best operating conditions of the flame, which is capable of promoting the greatest performance of the DiCTT process.

TABLE I: COMPOSITION OF NATURAL GAS

| Component | Molar fraction (%) |
|---|---|
| Methane | 89.0 |
| Ethane | 8.0 |
| Propane | 0.3 |
| Nitrogen | 1.5 |
| $CO_2$ | 1.2 |

The mixture fraction (*f*) was used to define the flame boundaries since it is related to the equivalent ratio ($\phi$), as in

$$f = \frac{\phi}{\left(\frac{A}{F}\right) + \phi} \qquad (5)$$

where: A/F is the air-fuel ratio and $\phi$ is the equivalent ratio.

The flame boundary was defined by the location where the mixture fraction assumed the stoichiometric value, as in

$$f = \frac{1}{\left(\frac{A}{F}\right)_{\text{stoich.}} + 1} \qquad (6)$$

where: (A/F) is the stoichiometric air-fuel ratio, whose values depend on the nature of the fuel, as shown in Table II.

TABLE II: COMPOSITION OF NATURAL GAS

| Fuel | Ratio $(A/F)_{\text{stoichiometric}}$ on a volumetric basis | Ratio $(A/F)_{\text{stoichiometric}}$ on a mass basis |
|---|---|---|
| Methane | 9.53 | 17.20 |
| Ethane | 16.68 | 15.90 |
| Propane | 23.82 | 15.25 |
| Butane | 30.97 | 14.98 |
| Natural Gas* | 9.88 | 16.09 |

*Calculated from the composition presented in Table I.

### F. Phytotoxicity Tests

Phytotoxicity tests were carried from the sweet pepper seeds. The concentrations of phenol ($C_{Ph}$) used in this research were 5; 10; 40; 120; 140 and 160 $mg \cdot L^{-1}$ and the hydrogen potential (pH) of 3; 6 and 9. The results analyzed were related to the Root Growth Index (RGI), and Germination Index (GI) (%) of the samples, respectively. The positive control that did not germinate was performed with a zinc sulfate ($ZnSO_4$) solution, while the negative control that germinate was obtained with deionized water (white) [12].

The sample temperature was measured with a digital thermometer, being constant at 20.7°C. The variation of pH values was obtained in acid and basic media, respectively, from the solutions of phosphoric acid ($H_3PO_4$) and sodium hydroxide (NaOH) using the pH-meter [12].

The samples in Petri dishes were incubated with alternating luminosity to simulate the natural growth of the seeds. Thus, 10 seeds were placed in each petri dish, adding 2.5 mL of the solution, according to the defined $C_{Ph0}$ (%) and pH (-). Then, the plates were sealed with PVC film and placed in an incubator at a temperature of 20.7°C. After 5 days, the sweet pepper seeds were evaluated by the germination index. When germination occurs, the ideal standard defined for each seed is the measurement in 5 mm ideal for the size of the radicle, which should be measured with a caliper. Therefore, in the sweet pepper seeds, the Root Growth Index (RGI) and the Germination Index (GI) were observed [13].

## III. RESULTS AND DISCUSSION

### A. Study of Phenol Degradation and TOC Conversion

Fig. 12a, and 12b show the phenol degradation and TOC conversion profiles, respectively, as a function of time using different $Q_{GN}$ of 2, 3, and 4 $m^3 \cdot h^{-1}$. The liquid phase flow rate ($Q_L$) was 170 $L \cdot h^{-1}$, the initial phenol concentration ($C_{Ph0}$) was in the range of 500 $mg \cdot L^{-1}$, the air excess (E) was 10% and the molar ratio of stoichiometric phenol to hydrogen peroxide ($R_{PH}$) was 50%.

Fig. 12a, and 12b show, respectively, that for $Q_{GN}$ of 2, 3, and 4 $m^3 \cdot h^{-1}$, the phenol degradation was almost completely achieved and a greater mineralization (>30%) of the liquid phase was obtained in the range 160-210 min of operation. The highest phenol degradation and TOC conversion, i.e., above 98% and 35%, respectively, were observed for $Q_{GN}$ of 4 $m^3 \cdot h^{-1}$. The first stage of the reaction, called the induction period, did not present a significant effect on phenol degradation and TOC conversion, respectively, at a time of approximately 80 min. However, after the induction period, the reaction velocity became more pronounced, reaching phenol degradation values above 98% and Total Organic Carbon (TOC) conversion (>35%). Thus, a mixture from the combustion of natural gas/air excess under the same reaction conditions can growth the amounts of radical propagation reactions, thereby increasing the profile of phenol degradation and TOC conversion.

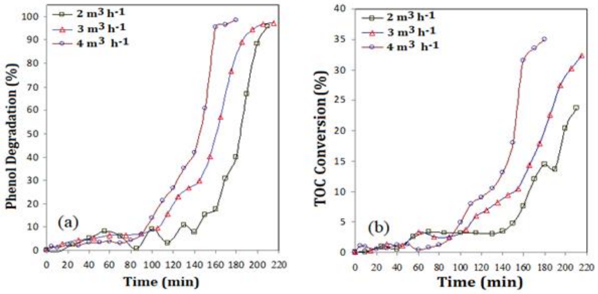

Fig. 2. a) Profile of phenol degradation; b) Evolution of TOC conversion. $C_{Ph0}$=500 $mg \cdot L^{-1}$; E= 10%, $R_{PH}$= 50%, $Q_L$= 170 L·h-1, $Q_{GN}$= 2, 3, and 4 $m^3 \cdot h^{-1}$.

Hydrogen peroxide can be used as an oxidant, and also induces the formation of more free radicals (•OH), that existent in the thermochemical oxidation of phenol act as reaction accelerators.

Brandão *et al*. [9] showed the effect of initial phenol concentration ($C_{Ph0}$) of 500, 1000 and 1500 $mg \cdot L^{-1}$, the molar stoichiometric ratio of Phenol/Hydrogen peroxide ($R_{P/H}$) of 25, 50 and 75 % and time (t) of 30, 90 and 150 min on the oxidation of phenolic effluents by DiCTT. The organic pollutant was degraded with a conversion higher than 99% and a Total Organic Carbon (TOC) mineralization exceeding 40%, to a ($R_{P/H}$) of 75%, independent of the $C_{Ph0}$.

### *B. Modeling and Simulation of the DiCTT Method by CFD*

In this work, a comparative study of the combustion mechanism of methane and natural gas was carried out, with the system working in nonadiabatic mode, where a simplified combustion mechanism was used.

The effects of the mechanisms of thermal exchange by radiation and convection were not evaluated, aiming to predict the values of the temperature of the gases, the rate of generation of free radicals •OH of the process, and the length of the combustion flame.

Initially, a first mechanism was used in the simulation of combustion, where the fuel was entirely composed of methane. Soon after, a second mechanism was proposed, where the fuel was natural gas, according to the composition shown in Table I.

*- Nonadiabatic reactor, stoichiometric combustion of methane and natural gas* ($\phi$=1)*, and flow rate* ($Q_{GN}$=1 $m^3 \cdot h^{-1}$)

Fig. 3 shows the influence of the gas properties on the temperature distribution in the DiCTT reactor, noting that there was not much variation by the nature of the fuel gas.

Fig. 4 shows a comparison of the temperatures obtained at the reactor wall for the two fuels. Thus, we observed that the nature of the fuel, methane or natural gas, has no significant influence on the temperature profile under the conditions studied.

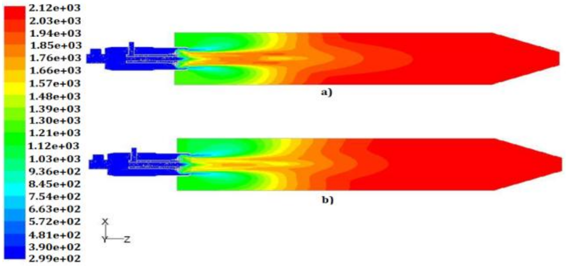

Fig. 3. Temperature contour for nonadiabatic wall condition, without considering the effects of thermal exchange mechanisms by radiation and convection ($Q_{GN}=1\ m^3 \cdot h^{-1}$ and $\phi$= 1);
a) Methane fuel; b) Natural gas fuel.

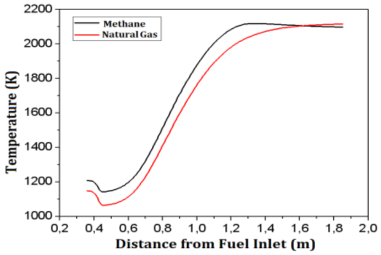

Fig. 4. Comparison of temperature profiles for nonadiabatic wall condition, without considering the effects of thermal exchange mechanisms by radiation and convection ($Q_{GN}=1\ m^3 \cdot h^{-1}$ and $\phi$= 1).

Table I shows that natural gas is made up of 89% methane, so the Theoretical Adiabatic Combustion Temperature (TACT) for these two fuels, methane and natural gas is around 2310K. Therefore, the study proved that in the tests via CFD, the flue gas temperature reached its maximum value in the final half of the reactor, with values of 2200K. This same order of magnitude and the small difference in temperature can be caused by thermal exchanges, due to advective flow, since it is a nonadiabatic operation.

Fig. 5 presents the results of the fuel characteristics on the mass fraction contour of the •OH species produced.

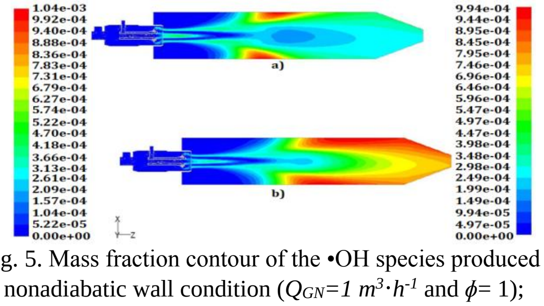

Fig. 5. Mass fraction contour of the •OH species produced for nonadiabatic wall condition ($Q_{GN}=1\ m^3 \cdot h^{-1}$ and $\phi$= 1);
a) Methane fuel; b) Natural gas fuel.

Fig. 6 shows a comparison of the mass fraction contour of the •OH. We evidenced that in the natural gas combustion the concentration of the •OH species was slightly lower with a value of $0.994 \times 10^{-3}$, while in the methane combustion it was $1.04 \times 10^{-3}$. Thus, the distribution of •OH species using natural gas was more elongated, with a high concentration of •OH near the wall, in the final half of the DiCTT reactor.

Fig. 6 also shows that before the value of z = 0.70 m, no hydroxyl radical formation was observed, but when methane combustion was used, the concentration of •OH reached a maximum value of z = 1.2 m, and then continuously reduces less than half of the maximum observed value, probably due to recombination reactions. However, when natural gas combustion was employed, the maximum concentration of •OH was reached at a value of z = 1.4 m with the concentration of •OH practically unchanged until the end of the reactor length. Therefore, the rate of generation of free radicals •OH, inside the reactor is a variable that is difficult to quantify experimentally, due to the complexity of the measurement technique, making its mapping by CFD fundamental for the studies of advanced oxidation processes.

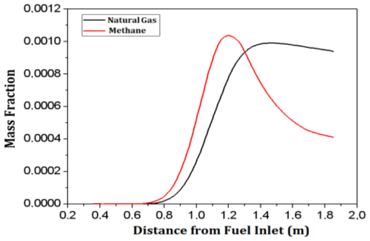

Fig. 6. Comparison of the mass fraction contour of the •OH for nonadiabatic wall condition ($Q_{GN}=1\ m^3\cdot h^{-1}$ and $\phi= 1$).

Fig. 7 shows the flame length for the combustion of methane and natural gas, respectively. The results obtained reveal that the fuel characteristic has a significant effect on the kinetics of the reaction, in view of the different mechanisms used for each fuel, and consequently on the distribution of the hydroxyl radicals generated, and on the elongation of the combustion flame length. Thus, natural gas was used in this research, due to the greater generation of hydroxyl radicals to facilitate the degradation of organic compounds through advanced oxidation processes, contributes to the control of the emission of industrial chemical pollutants to the environment, the great availability of this gas in several natural reserves of oilfields on the planet, and the low cost compared to other fuels.

Brandão *et al*. [2] showed the mathematical modeling of natural gas combustion with Fluent$^{TM}$ software, adopting Computational Fluid Dynamics (CFD) as a research tool and from the combustor geometry, a model based on nonpremixed combustion was used. Thus, the effect of the air excess (*E*) and natural gas flow rate ($Q_{GN}$) was estimated. The CFD modeling for $Q_{GN} = 4\ m^3\cdot h^{-1}$, E = 10%, and ($Q_L$) of 170 $L\cdot h^{-1}$ showed an increase in the region and in the emission of the combustion flame within the reactor, to Z>1.0 m, favoring a more distributed formation of •OH.

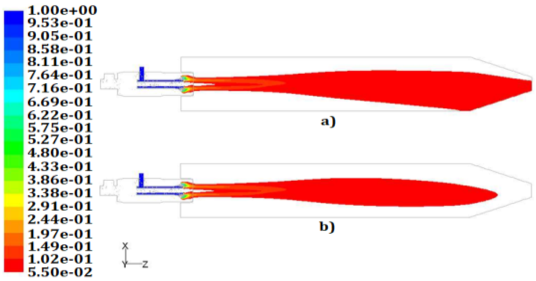

Fig. 7. Flame length for nonadiabatic wall conditions ($Q_{GN}=1\ m^3\cdot h^{-1}$ and $\phi= 1$); a) Methane fuel; b) Natural gas fuel.

## C. *Phytotoxicity Tests*

Fig. 8a to 8f show the photographic results of the phytotoxicity tests, at phenol concentrations of 5; 10; 40; 120; 140; and, 160 $mg\cdot L^{-1}$, and pH values of 3, 6 and 9, respectively, in sweet pepper seeds.

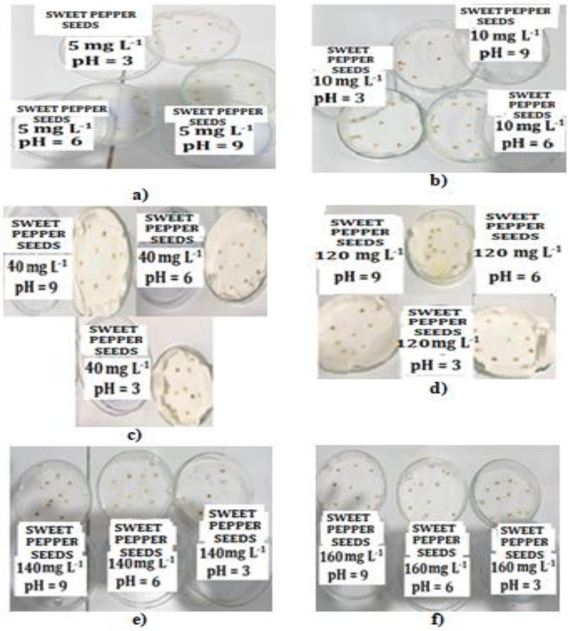

Fig. 8. Phytotoxicity tests for $C_{Ph0}$: 5; 10; 40; 120; 140 and 160 $mg\cdot L^{-1}$ and the hydrogen potential (pH) of 3; 6 and 9.

Fig. 8a-8f demonstration that the Root Growth Index (RGI), and the Germination Index (GI) were not quantified in the sweet pepper seeds. These results show that phenol is quite toxic, according to various concentrations analyzed for this type of seed, and this bioindicator technique is a very sensitive method, due to the characteristics of each effluent analyzed [13].

## IV. CONCLUSION

The thermochemical oxidation of phenol adopting the Direct Contact Thermal Treatment (DiCTT) technique proved to be effective reaching phenol degradation values above 98%. However, the Total Organic Carbon (TOC) conversion (>35%) requires even more operational time. The study of the effect of the natural gas flow rate ($Q_{GN}$, 2–4 $m^3\cdot h^{-1}$) showed that for a $Q_{GN}$ of 4 $m^3\cdot h^{-1}$, the highest values of phenol degradation and TOC conversion were achieved in a shorter operational process time. The results obtained in the simulation studies of non-premixed combustion using Computational Fluid Dynamics (CFD) applying the commercial software Fluent$^{TM}$, it was possible to conclude that the nature of the gas (natural gas or methane) does not have a significant effect on the definition of the flue gas temperature profile obtained from the conditions studied. The distribution of the •OH species in the case of natural gas combustion is better compared to methane gas, with a high concentration near the wall in the final half of the reactor (z=0.70m). The flame length for the combustion of methane and natural gas reveal that the fuel characteristic has a significant effect on the kinetics of the reaction, and consequently on the distribution of the hydroxyl radicals generated, and on the elongation of the combustion flame length. The evaluation of phytotoxicity in sweet pepper seeds from synthetic water samples containing phenol was investigated and showed their characteristics according to the bioindicator method. The 18 experimental assays related to phytotoxicity studied showed that the Root Growth Index (RGI) and the Germination Index (GI) were not quantified in the sweet pepper seeds. Therefore, this bioindicator technique using seeds becomes of paramount importance, due to the efficiency it has demonstrated according to the characteristics of each effluent analyzed. In this process, both the integument and the endosperm of the bioindicator allow some toxic organisms to be able to act on the effluent, according to the resistance to germination in the environment in which they are present. Although, in the sweet pepper seeds for all concentrations of phenol studied at different pH values no seed was able to germinate. Thus, the presence of phenols in the aquatic environment has been a priority factor and of great relevance for the whole society, in addition to being reported by several scientific researches around the world.

## ACKNOWLEDGMENT

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