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Modeling hydroxyl radical control process in hydrodynamic cavitation reactors

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Key words: Component, Hydrodynamic cavitation, Radical, Collapsing pressure, Temperature, Cell decomposition, PID controller.

Abstract

Cavitations phenomenon is resulted from elevated temperature and pressure and production of free radicals. This technology can be employed to disinfect drinking water and waste water. What is important in cavitations reactors is the production of hydroxyl radicals, which plays a significant role in removing coliforms. So, it was attempted to control radical production through controlling the input pressure. It was examined by placing a PID controller. The presented control algorithm is carried out based on trial and error. Flow diagram of hydroxyl radical control model was also designed using pressure. The relationship between design in term of cavitational intensity (according to collapsing pressure and temperature) and cavitational efficiency (according to radical) will be based on operational parameters regarding the hydrodynamic cavitations in order to perceive the design information concerning cavitational intensity and radical efficiency.

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Introduction

In concomitance with population growth in the world and development in different industries, contamination of drinking water has turned out to one of major global issues. Results of studies show that today underground water tables have numerous problems especially in large and populated cities of the world emanated from the permeation of industrials waste, presence of abruption wells of human waste disposal, excessive use of chemical washers and pickles, chemical and organic fertilizers permeation deep into the ground. Most of these contaminants dissolve in water and removing them from water requires a complicated and expensive technology such as reverse osmosis the use of which is not cost effective for any government in large-scale refinements of high volume water. Cause of abnormal effects in hop spots production terms, reactive oxygen species, and turbulent with liquid circulation; cavitation is an appropriate tool for water treatment. Notwithstanding, hydrodynamic cavitation reactors are more effective and suitable comparing to acoustic cavitation reactors. The advent of such reactors regarding microbial treatment has been done in recent years. Among the factors effective in the cavitations reactors are: the tension produced by cavity, cell wall resistance, dissolved gas concentration, acoustic current produced by ultrasound. The important matter is to control further hydrodynamic cavitations on operating parameters and the cavitations intensity. Here, it has been attempted that a small part of it is covered. The process of microbial cell dissolution occurs in several ultrasound operations such as water, waste treatment operation and the like. Although th studies done on ultrasound regarding the microbial cells decomposition have been successful in laboratory scale, its application in industrial scale will be limited cause of the lack of sufficient knowledge considering cell decomposition mechanism, absence of kinetic equation for anticipating cell decomposition rate and lack of scale increase strategy. The analysis of a kinetic model for cell decomposition on one hand and the importance of the dissolved gases one the other are required for proper anticipation of the cell decomposition. But our information regarding the kinetics is very limited and our best knowledge for cell decomposition model is presented in the articles.

The aim of this study is modeling hydroxyl radical control process in hydrodynamic cavitation reactors and study relationship between design in term of cavitational intensity and cavitational efficiency will be based on operational parameters regarding the hydrodynamic cavitations in order to perceive the design information concerning cavitational intensity and radical efficiency.

Methodology

Effective factors in the cavitations reactors

The reasons to use cavitations are as follow: 1. Reaction time decrease 2. Reaction return increase 3. Using a variety of pressures and temperatures comparing to conventional methods. 4. Decrease in reaction induction period 5. The possibility of replacing the path as a result of reactivity increase 6. Initiation of the chemical reaction as a result of high reactivity production of hydroxyl radicals (Parag *et al*, 2004). Among the factors effective in the cavitations reactors are: the tension produced by cavity, cell wall resistance, dissolved gas concentration, acoustic current produced by ultrasound. The important matter is to control further hydrodynamic cavitations on operating parameters and the cavitations intensity. Here, it has been attempted that a small part of it is covered. The process of microbial cell dissolution occurs in several ultrasound operations such as water, waste treatment operation and the like. Although the studies done on ultrasound regarding the microbial cells decomposition have been successful in laboratory scale, its application in industrial scale will be limited cause of the lack of sufficient knowledge considering cell decomposition mechanism, absence of kinetic equation for anticipating cell decomposition rate and lack of scale increase strategy. The analysis of a kinetic model for cell decomposition on one hand and the importance of the dissolved gases one the other are required for proper anticipation of the cell decomposition. But our information regarding the kinetics is very limited and our best knowledge for cell decomposition model is presented in the articles.

Software for modeling

What is important is the production of hydroxyl radicals laying a significant role in eliminating conforms. So, it was attempted to control radical production through controlling entry pressure. It was examined by placing a PID controller. The modeling is carried out using MATLAB software.

Result and discussions

Hydrodynamic Cavitations

Cause of the capability of the hydrodynamic cavitation to improve energy return and above all the capability of the method to work in a larger scale, it is possible to be replaced with acoustic cavitation. The greatest attempt to exploit the statement is via experiments and experiences. However, a brief history of hydrodynamic cavitation has not had a basic guideline for understanding the method. From engineering point of view, cavitation must be carried out aiming at saving energy and dissolving materials in water (Donka and Milcho, 2004).

Different types of the reactor include: high pressure hemogenizer, high velocity hemogenizer, plate orifice. Hydrodynamic cavitation is produced simply by plate orifice, regulating vent or valve. The relationship between fluid pressure-velocity is derived by Bernoulli equation. Using the equation, significant performance effects can be gained (Arrojo and Benito, 2008).

Maintaining the Integrity of the Specifications Reactive Effect Mechanism of Hydrodynamic Cavitation in Water

Employing cavitations process on water leads to separation of its molecules. Under tough conditions and using X ray, it is possible to observe chemical reactions and biological effects. Through certain experiments, we can observe bubble resonant frequencies occurring under different conditions. Physical and chemical changes were shown by experiment (Anan'in *et al.*, 1975). Firstly, it is the concentration of OH^- and H^+ that changes, but in this case production of compounds like H2 and H_2O_2 are not present. Hydroxyl reactive oxygen species kinetics is when water is subjected to the impact of the waves. Chemical changes in water during the operation using hydrodynamic cavitation reactors will comprise change in PH and Hydrogen peroxide composition. When there is no correct data on the amount of hydrogen peroxide composed and reactive oxygen species produced in cavitation, such an image of the chemical changes in water is inappropriate. Luminsans intensity value is compatible with the amplitude of hydrogen peroxide concentration composed when oxygen is present. The information demonstrates that the effective factors on hydrodynamic cavitation contact on the water cannot be expressed by the presence of the chemical changes during cavitation (Anan'in *et al.*, 1975).

According to some researchers, if it is exposed to hydrodynamic cavitation conditions, hydrogen binds will be released and complexes of a water molecule will be decomposed, and finally water will be dissolved. So, applying hydrodynamic cavitation to water under atmospheric pressure leads to the production of OH^- , H°, H_2O_2, H^+, H_2O, and OH°. The concentration of radicals is determined by consuming oxalic acid which only reacts with hydroxyl radicals. Oxalic acid is oxidized by radical OH. Oxalic acid is also measured via titration with potassium permanganate at 80. One of the oxalic acid products is hydrogen peroxide titrated by permanganate. To determine its concentration, potassium iodide solution can be added released by titrating iodine through sodium thiosulfate. Resulting information shows that a decrease in bubble size can be along with an increase in the amount of energy inlet. Composition and collapse of the cavitation bubbles are the results of change in density, electrical conduction and temperature degree. The effects of electron contact in water and in cavitation bubbles will be in accordance with Marguls theory:

$$H_20 \xrightarrow{US} H_20^*$$
$$H_20 \xrightarrow{US} H_20^* + e^- \qquad (1)$$
$$H_20 \xrightarrow{US} H^\bullet + OH^- + e^-$$
$$H_20 \xrightarrow{US} H^+ + OH^- + e^-$$

Each of these processes occurs between two particles and in 10-14s. The reaction of radicals' composition will happen in presence of suitable amounts of oxygen or hydrogen in a cavitation bubble. Presence of H° and OH°. in water is proved by researchers. There is a probability of a three-time impact increase as pressure in a bubble. These impacts establish a channel for a chemical reaction (Anan'in *et al.*, 1975).

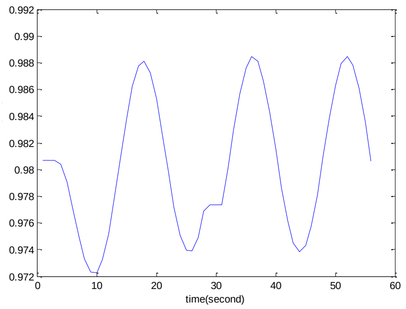

Fig. 1. Variation of out pressure controller with out time.

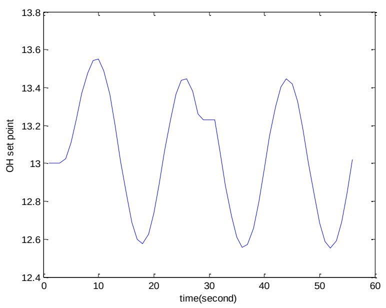

Fig. 2. Variation of inlet OH radicals with time at setpoint.

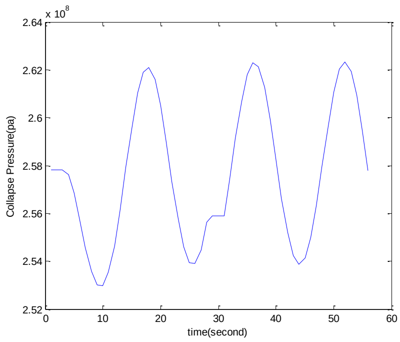

Fig. 3. Variation of collapse pressure with time at out flow diagram.

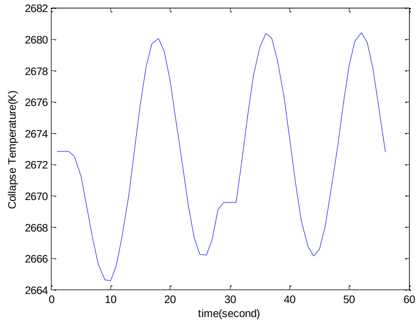

Fig. 4. Variation of collapsetemorature with time at out flow diagram.

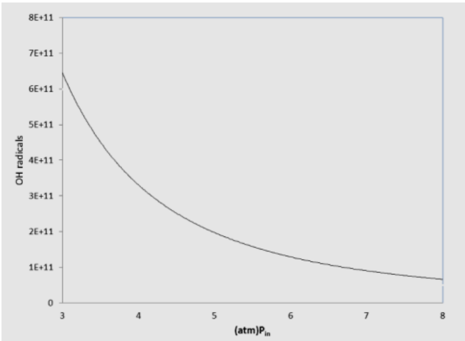

Fig. 5. The amount of OH• varying with inlet pressure. Ro =1μm; temperature= 298 K; dia orifice/dia pipe = 0.1; dia pipe = 5 cm; cavitation number = 0.6.[20].

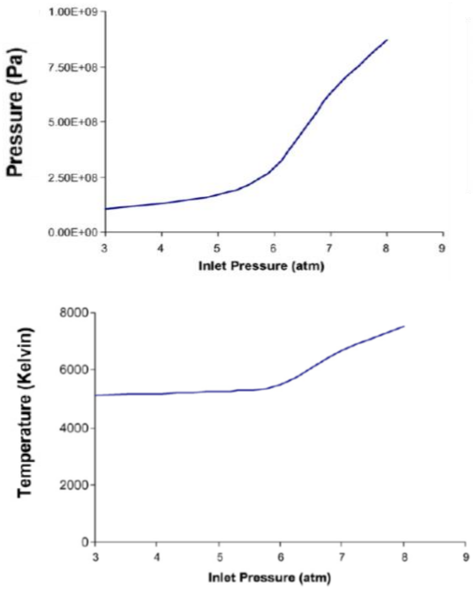

Fig. 6. Variation of collapse pressure and temperature with inlet pressure.

Ro =1μm; temperature = 298 K; dia orifice/dia pipe = 0.1; dia pipe=5cm; cavitation number = 0.6.[20].

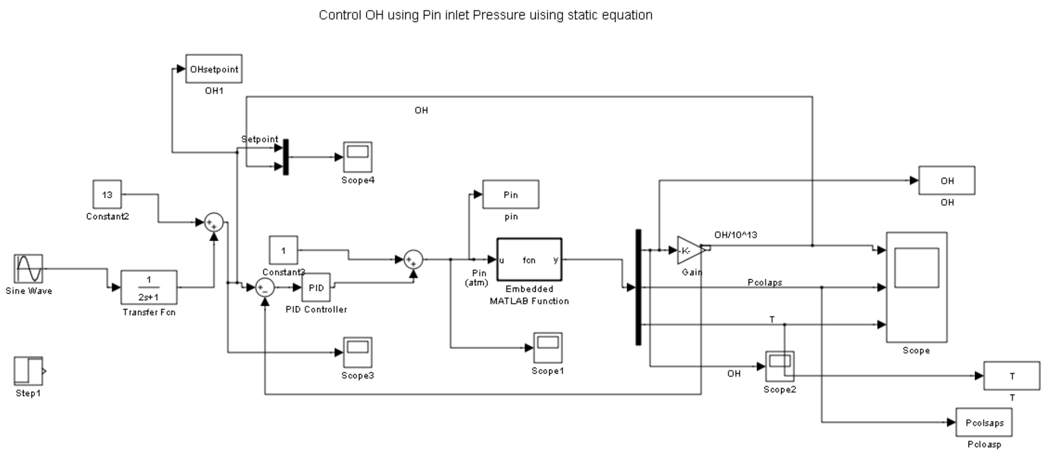

Fig. 7. Flow diagram of the hydroxyl radicals control model using pressure.

Controlling Hydroxyl Radicals and Process Modeling

A chemical process is practically a rational and engineering arrangement of the processing units such as reactors, heat exchangers, absorption and concentration towers, pumps and evaporators. The objective and reason of the process is the transformation of a series of raw and basic materials inlet into high value-added products. During the operation, the objective must be accomplished under a series of requirements including the technical, economic, social as well as environmental disorders: (personnel) safety and equipments maintenance, desirable characteristics of the products, bioenvironmental rules, and cost effectiveness. Accordingly, it is obvious that we need to have both monitoring (observation) and control (protection). So, the first and most important control point is to indirectly change the desirable quantities. The second point is regarding the existence or presence of an accurate tool. For manual or automatic control, we have to understand in one way or another whether the desirable variable has been changed to need passivizing or not. The third point is in parallel with the first point so that which effective engineering variable such as current intensities we can choose to be our desirable effective and of course indirect influencing means on our affected quantity.

Hydrodynamic cavitation reactor return and also cavitational effects control are higher than the acoustic reactors. Accordingly, it was attempted that hydrodynamic cavitation reactors were modeled based on the chemical reactions. So, the important is the matter of hydroxyl radicals. The radicals permeate into water. Hydrogen peroxide is composed as a result of the radicals' combination out of cavitations bubble. Under such conditions, water molecules undergo the chemical breakdown resulted from hydroxyl radicals and hydrogen atoms. Since oxidation is the most important path of decomposition, the amount of hydroxyl radicals existing in the system directly depends on the decomposition return (Mahvi, 2009). Knowing about the existence of these radicals is of considerable significance, as a result, it is attempted to control the amount of radical OH by controlling entering pressure so as to enhance the return.

Designing the controller is aimed at choosing the type and calculating the best values of the controller parameters. Selecting the type of controller depends on the process requirements, desirable cost and the skill of the person. The best way is to start the control ring simulation (MATLAB software possesses special facilities such as Simulink to simulate control systems) and observe the system behavior against different controllers or various parameters of a specific controller (Woo *et al.*, 2000; Cohen and Coon, 1953).

There are two types of quantitative and qualitative expressions for modeling that the quantitative and analytical process model is of remarkable significance. The model includes static and dynamic modeling which if the simulation is aimed at designing that we consider it as a combination of two subsequent formulation and solution phases, then static and dynamic modeling are not different, but solution and characterization will be more challenging with dynamic state (Cohen and Coon, 1953; Netushil, 1978). The biggest problem with the model is that the dynamic model does not exist in the control simulation. So, the static model must be used. In fact, we have changed the inlet is that we can reach desirable concentration using the controller, namely, we have a certain concentration of the hydroxyl radicals at the outlet then what inlet must the controller enter the system so as to reach the desirable concentration. First, we must have an explanatory model on the control algorithm. Choosing the type of controller is the important thing in the model. Firstly, cause of simplicity and secondly the absence of consistent error or offset, Proportional -Integral-Derivative Controllers or PID controllers are used. This controller is the most widely used industrial controller in the industries with noise-free outlet measurements. However, it must be remembered that in the system there will be no need to filter for noise removal cause of utilizing hydrodynamic cavitation, since these types of reactors are more stable than the others. In addition to memory and feedback error history, the derivative of the controller is also used here. It must be noted that the practice of integral and derivative are carried out in the controller (algorithm) itself. The algorithm (mathematical - calculation) and also its transmission function are as follow (Astrom *et al.*, 1995):

$$\bar{u}(t) = K_C e(t) + \frac{K_C}{\tau_I}\int_0^t e(\zeta)d\zeta + K_C\tau_D \frac{de(t)}{dt} = K_C e(t) + K_I\int_0^t e(\zeta)d\zeta + K_D\frac{de(t)}{dt} \qquad (2)$$

$$\bar{u}(s) = K_C e(s) + \frac{K_C}{\tau_I}\frac{1}{s}e(s) + K_C\tau_D s e(s) \quad , K_I \overset{\Delta}{=} \frac{K_C}{\tau_I} \quad , K_D \overset{\Delta}{=} K_C\tau_D$$

$$G(s) = \frac{\bar{u}(s)}{e(s)} = K_C + \frac{K_C}{\tau_I}\frac{1}{s} + K_C\tau_D s = K_C + K_I\frac{1}{s} + K_D s$$

Finally, PID controller has the transformation function as follow (Datta *et al*, 2000):

$$\frac{M(s)}{e(s)} = k_c\left(1 + \frac{1}{\tau_I(s)} + \tau_D(s)\right) \qquad (3)$$

Where k_c and τ_1 (integral time constant), τ_D (derivative time constant) depend on the process dynamic, measurement element, final element of the controller and needs of the system and must be optimized. Major advantage of using the derivative practice is the acceleration of the outlet response or controlled variable (change in determined amount or eliminating the disorder) and has somehow the property of anticipation. The system is stable; that is, for all the amounts of the inlet with limited domain, its outl*et al*so remains stable. The parameter in control part is the control return or kc (Kevin, 2002). The return increase shows that little error is observed and the outlet takes a larger value; it is as if the process is slow (the process changes ratio), but we want to accelerate it using the process response controller. Reversely, if k_c is small, it means that the process is fast and we want to make the response dynamics slow. The values of kc and k_I equal unity.

Keller-Miksis equation (Amit *et al*, 2008) (Equation 4) is used in the model which is as follow:

$$OH = C_3\left\{R_0^{0.2428} \times P_{in}^{-4.6457} \times \left(\frac{d_o}{d_p}\right)^{-0.4732}\right\} \qquad (4)$$

Collapse pressure and temperature is a function of different operational parameters (inlet pressure, orifice cavity diameter, initial radial) which itself can depend on the return of hydroxyl radicals during the cavity collapse and the number of water molecules. It is supposed that argon; nitrogen, oxygen, and water molecules permeate into bubble during the reaction and will compose solubility products during concentration and collapse. So, initial products of chemical reactions in the bubbles will include hydroxyl radicals expected. Hydroxyl radicals' return is estimated under different conditions and we can offer a relationship between OH radicals and collapse pressure and temperature by inlet pressure. Orifice cavities diameter and initial radial of the nucleus can be in relation with the chemical products composed. The changes in collapse pressure and temperature are in relation with initial cavity radial, basic pressure and orifice cavity diameter to pipe diameter ratio as follow:

$$P_{collapse} = C_1 \left\{ R_0^{-1.2402} \times P_{in}^{2.2949} \times \left(\frac{d_o}{d_p} \right)^{-0.4732} \right\} \qquad (5)$$

$$T_{collapse} = C_2 \left\{ R_0^{-0.2877} \times P_{in}^{0.3579} \times \left(\frac{d_o}{d_p} \right)^{-0.1303} \right\}$$

Where $P_{collapse}$ is the collapse final pressure in Pascal, R_o is the initial radial in μm, P_{in} is the inlet pressure in atm, and d_o/d_p is the ratio of orifice diameter to the pipe diameter. Initial diameter of the cavity is 1 μm and the ratio of orifice diameter to the pipe diameter is 0.1. The values of are respectively $4*10^{13}$,3633.3, and $8*10^8$ through mathematical relationships and via empirical tests (Amit *et al*, 2008).

Effect of inlet pressure

First, we will have outlet pressure changes of PID controller (Flow Diagram 7). The changes will be time-proportionate. Pressure is as an inlet to the process that is the controller outlet. By passing through PID controller and as time passes by, we will see decrease and increase in pressure so that we will observe step-by-step changes with time (10s). In the next step, we will have hydroxyl radical changes with time at the set point. The changes have reverse ratio with the inlet pressure. As the inlet pressure increases, the number of hydroxyl radicals at the set point decreases.

Effect of Collapse pressure and Temperature

The process outlet comprises collapse temperature and pressure and the number of hydroxyl radicals. Diagram OH is as an outlet which must be controlled. As respectively shown in Diagrams 2, 3, and 4; the number of hydroxyl radicals, pressure and temperature of collapse in proportion to time. Based on the results, it can evidently be observed that as the inlet pressure decreases, the number of radical OH increases, and vice versa. If we have a review of the empirical results from Pandit *et al*'s (Amit *et al.*, 2008) experiments (as shown in Fig. (Mahvi, 2009), when the inlet pressure increases, the number of hydroxyl radicals decreases which is obviously observed in the control diagram represented.

With a glance at the empirical results shown in Fig. (6) regarding collapse temperature and pressure, it is possible to clearly observe the collapse temperature and pressure. Of course, it must be noted that there is no exact control empirical information for accurate comparison. Now, we will address the diagrams derived from modeling. Diagram 3 and Diagram 4 show the increase of collapse pressure and temperature with time. Comparing to inlet pressure, we find that as the inlet pressure increases, $C_1 C_2 C_3$ the collapse pressure and temperature increase and as the inlet pressure decreases, the collapse pressure and temperature also decrease. In all diagrams and cause of a change in the set point in 30s, it takes a while for being updated and for frequencies to get started.

Conclusions

It seems that hydrodynamic cavitation is a new and appropriate method for water treatment. According to the researchers, among different hydrodynamic cavitation reactors, plate orifice will be suitable cause of its flexibility in controlling the cavitation intensity. Hydrodynamic cavitation reactors have higher energy return in treating and decomposing microbial cells comparing to acoustic reactors. The number of hydroxyl radicals is significant in cavitation reactors and water treatment. So, it is possible to control the number of the radicals by developing a suitable control model. Here, a static model was developed which controlled the amount of hydroxyl radicals' production for enhancing reactor return.

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