Research Article

Numerical Simulation and Investigation of System Parameters of Sonochemical Process

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This paper presents the effects of various parameters that significantly affect the cavitation. In this study, three types of liquid mediums with different physicochemical properties were considered as the cavitation medium. The effects of various operating parameters such as temperature, pressure, initial bubble radius, dissolved gas content and so forth, were investigated in detail. The simulation results of cavitation bubble dynamics model showed a very interesting link among these parameters for production of oxidizing species. The formation of $\cdot\text{OH}$ radical and H_2O_2 is considered as the results of main effects of sonochemical process. Simulation results of radial motion of cavitation bubble dynamics revealed that bubble with small initial radius gives higher sonochemical effects. This is due to the bubble with small radius can undergo many acoustic cycles before reaching its critical radius when it collapses and produces higher temperature and pressure inside the bubble. On the other hand, due to the low surface tension and high vapor pressure, organic solvents are not suitable for sonochemical reactions.

1. Introduction

The sonochemistry concept is a well-established technique, and now it is considered as one of the most popular advanced oxidation processes. In the last few decades, sonochemical process became one of the most popular techniques for synthesis of catalysts as well as different types of materials [4–7], degradation of pollutants [8–12], synthesis of biodiesel [13, 14], and so forth. Numerous literatures on sonochemistry have already been published [15–18] which reported the various beneficial effects of sonochemistry. The principal phenomenon behind all of these effects is the cavitation. Cavitation is nothing but nucleation, growth, and implosive collapse of a bubble. Cavitation occurs through the formation of bubbles or cavities present in liquid medium. Each cavitating bubble contains gas or vapor or a mixture of gas-vapor. When bubble contains only gas, the expansion of bubble is mainly by diffusion, pressure reduction, or by rise in temperature. However, there are several parameters which are directly involved in transient cavitation. Transient cavitation is nothing but the growth of bubbles extensively over time scales of the order of the acoustic cycle and then

undergoes an implosive/energetic collapse resulting in either fragmentation, decaying oscillation, or a repeat performance [19]. Cavitation can also be the result of the enlargement of cavities that are already present in bulk liquid. Sometimes cavitation bubbles are suspended/trapped in tiny cracks in the interface of solid and liquid. These cavitation bubbles grow and collapse in the medium based on the pressure variation inside the bubble. On the basis of pressure variation, cavitation can be categorized into four subsections: (1) hydrodynamic cavitation, (2) acoustic cavitation, (3) optic cavitation, and (4) particle cavitation [20]. Hydrodynamic cavitation is the result of pressure variation in the liquid medium due to the flow variation of liquid through the medium, while acoustic cavitation is due to the passing of acoustic waves in the liquid medium. Generally, acoustic cavitation occurs in the frequency range of 20 kHz to 1 MHz, that is, high power low frequency [20]. In acoustic cavitation, very high temperature and pressure (~ 5000 K and ~ 500 bar) are produced inside the bubbles due to transient collapse of cavitation bubbles. The bubble collapse occurs within a small time as 50 ns, and it is almost adiabatic. During the collapse of the bubble, many species are formed such as H_2 , O_2 , H_2O_2 ,

O_3 , $\cdot OH$, $\cdot H$, $\cdot O$, and $HO_2\cdot$. Among these species $\cdot OH$ radical is the most predominant radical species [21, 22] having an oxidizing potential of 2.33 V [9, 23]. For greater details in cavitation concepts, we would like to refer the readers to see the state of art reviews by Xu et al. [4], Apfel [24], Gong and Hart [25], Suslick et al. [26], and Gogate and Pandit [27].

2. Cavitation Bubble Dynamics Model

In order to investigate the various effects of cavitation, we have considered a model for a single cavitation bubble to simulate the radial motion of cavitation bubble. Although the single bubble analysis for radial motion of cavitation bubble does not give the entire phenomenon of the sonochemical process, but it can give a qualitative physical insight into the mechanism. The resultant effect of sonochemical reaction is the collective oscillations and collapse of cavitation bubbles, with strong interaction between them. For simulation of radial motion, the single bubble model is the most popular model to present the effects of cavitation, namely, physical and chemical effect. The physical and chemical effects induced by ultrasound and cavitation bubbles in the system can be determined using diffusion limited ordinary differential equation (ODE) model. This model is basically based on the boundary layer approximation proposed by Toegel et al. [28]. This radial motion of cavitation bubble model is derived from the partial differential equation (PDE) model of Storey and Szeri [29], which showed that water vapor entrapment in the cavitation bubble is mainly a diffusion limited process and not the condensation limited process. The main components of the radial motion of cavitation bubble dynamics are: (1) Keller-Miksis equation for the radial motion of the bubble [30], (2) equation for the diffusive flux of water vapor and heat conduction through bubble wall. The overall diffusion coefficient in ternary mixture (e.g. N_2 - O_2 - H_2O in case of air bubbles) or binary mixture (e.g., N_2 - H_2O or O_2 - H_2O or Ar - H_2O) has been determined using Blanc's law [31], (3) equation for heat conduction through cavitation bubble wall, and (4) overall energy balance treating the cavitation bubble as an open system. The set of 4 ODEs are also given below.

(1) Radial motion of the cavitation bubble:

$$\begin{aligned} & \left(1 - \frac{dR/dt}{c_L}\right) R \frac{d^2 R}{dt^2} + \frac{3}{2} \left(1 - \frac{dR/dt}{3c_L}\right) \left(\frac{dR}{dt}\right)^2 \\ &= \frac{1}{\rho_L} \left(1 + \frac{dR/dt}{c_L}\right) (P_i - P_t) \\ &+ \frac{R}{\rho_L c_L} \frac{dP_i}{dt} - 4\nu \frac{dR/dt}{R} - \frac{2\sigma}{\rho_L R}. \end{aligned} \quad (1)$$

Internal pressure in the bubble: $P_i = N_{tot}(t)kT/[4\pi(R^3(t) - h^3)/3]$.

Pressure in bulk liquid medium: $P_t = P_0 - P_A \sin(2\pi ft)$.

(2) Diffusive flux of water molecules: $dN_W/dt = 4\pi R^2 D_W(\partial C_W/\partial r)|_{r=R} \approx 4\pi R^2 D_W((C_{W,R} - C_W)/l_{diff})$.

Instantaneous diffusive penetration depth: $l_{diff} = \min(\sqrt{(RD_w)/|dR/dt|}, R/\pi)$.

(3) Heat conduction across bubble wall: $dQ/dt = 4\pi R^2 \lambda (\partial T/\partial r)|_{r=R} \approx 4\pi R^2 \lambda ((T_0 - T)/l_{th})$.

Thermal diffusion length: $l_{th} = \min(\sqrt{R\kappa/|dR/dt|}, R/\pi)$.

(4) Overall energy balance: $C_{V,mix} dT/dt = dQ/dt - P_i dV/dt + (h_w - U_w) dN_W/dt$.

Mixture heat capacity: $C_{V,mix} = \sum C_{V,i} N_i$ (where, $i = N_2/O_2/H_2O$).

Molecular properties of water: Enthalpy: $h_w = 4kT_o$.

Internal energy: $U_w = N_w kT(3 + \sum_{i=1}^3 ((\theta_i/T)/(\exp(\theta_i/T) - 1)))$.

Heat capacity of various species ($i = N_2/O_2/H_2O$):

$$C_{V,i} = N_i k \left(\frac{f_i}{2} + \sum \left(\frac{(\theta_i/T)^2 \exp(\theta_i/T)}{(\exp(\theta_i/T) - 1)^2} \right) \right). \quad (2)$$

The initial conditions of the ordinary differential equations are taken as: at $t = 0$, $R = R_o$, $dR/dt = 0$, $N_w = 0$, $Q = 0$, and $T = T_o$. Thermodynamic data for various species and physicochemical properties of various solvents, that is, cavitation medium, are given in Tables 1 and 2. The thermal conductivity and diffusion coefficient (transport parameters for the heat and mass transfer) are estimated using Chapman-Enskog theory using Lennard-Jones 12-6 potential at the bulk temperature of the liquid medium [1-3, 31]. This model ignores the diffusion of gas across bubble interface, because the time scale for the diffusion of gases is much higher than the time scale of cavitation bubble model. The ODEs in the bubble dynamics model have been solved simultaneously using Runge-Kutta 4th- and 5th-order adaptive step size method [32]. Various parameters used in the numerical solution of radial motion of cavitation bubble dynamics and their numerical values are given in Tables 1 and 2. The other parameters are as follows: ultrasound frequency (f) = 20 kHz, ultrasound pressure amplitude (P_A) = 150 kPa, initial bubble radius (R_o) = 5 μm , sound velocity in water (c_w) = 1481 m/s, sound velocity in toluene (c_T) = 1275 m/s, and sound velocity in n-hexane (c_H) = 1203 m/s. All these parameters remain unchanged unless otherwise stated.

Physical Effect of Ultrasound. Ultrasound propagates through the medium in the form of longitudinal wave with series of compression and rarefaction and causes rapid oscillatory motion of fluid elements called microstreaming. This motion gives rise to intense micromixing in the medium. The magnitude of the microstreaming velocity is given by $u = P_A/\rho c$. Substituting values of P_A as 1.5×10^5 Pa (or 1.5 bar), $\rho_w = 1000$ kg/m³, and $c_w = 1481$ m/s gives $u_w = 0.101$ m/s.

Sonochemical Effect of Cavitation Bubbles. The numerical solution of bubble dynamics model predicts the temperature,

TABLE 1: Thermodynamic data for various species (data taken from [1–3]).

Species	Degrees of freedom (translational + rotational) (f_i)	Lennard-Jones force constants		Characteristic vibrational temperatures θ (K)
		σ (10^{-10} m)	ϵ/k (K)	
N ₂	5	3.68	92	3350
O ₂	5	3.43	113	2273
Ar	3	3.42	124	—
H ₂ O	6	2.65	380	2295, 5255, 5400
C ₆ H ₁₂	6	5.75	386.4	1036, 1932, 1987, 2104, 4193
C ₆ H ₅ -CH ₃	6	5.82	451	1004, 1056, 2112, 2153, 2326, 4224, 4375

TABLE 2: Physicochemical properties of various solvents as cavitation medium.

Solvent	Boiling point (K)	Density (kg/m ³)	Viscosity (Pa·s)	Surface tension (N/m)	Vapor pressure [#] (kPa)
Water	373	1000	1.0×10^{-6}	0.072	2.5
Toluene	384	867	6.8×10^{-7}	0.029	4.0
n-Hexane	341	658	5.0×10^{-7}	0.018	16.2

#: calculated using Antoine type correlations.

pressure, and the number of gas and solvent molecules in the bubble at transient collapse. At transient collapse, temperature and pressure reach extreme conditions, which result in dissociation of molecules to form various chemical species. To calculate the composition of the bubble at the time of collapse, we assume that thermodynamic equilibrium is attained [9]. The equilibrium mole fraction of different chemical species in the bubble at the peak conditions reached at transient collapse is estimated using Gibbs free-energy minimization technique [33]. The radial motion of cavitation bubbles generates intense convection in the medium through two phenomena.

(i) Microconvection [20]: $V_{\text{turb}}(r, t) = (R^2/r^2)(dR/dt)$.

(ii) Shock (or acoustic) waves [34, 35]: $P_{\text{AW}}(r, t) = (\rho_L/4\pi r)(d^2V_b/dt^2) = \rho_L(R/r)[2(dR/dt)^2 + R(d^2R/dt^2)]$,

where V_b is the volume of the bubble. A representative value of r is taken as 1 mm. In bubble dynamic model, direct estimation of initial bubble radius is very difficult. Several phenomena such as rectified diffusion and fragmentation of the bubble cause continuous change in this parameter. In a multibubble system, a large variation in this parameter may be expected. In order to investigate the influence of this parameter, two numerical values for this parameter, namely, 5 and 10 μm , are selected for this present study. The equilibrium composition of the bubble contents was determined using the FactSage online software [36], which is based on the free-energy minimization algorithm same as proposed by Eriksson [33].

3. Numerical Solution of Mathematical Model

The simulation results of radial motion of cavitation bubble dynamics are depicted in Figures 1, 2, 3, 4, and 5 and Tables 3, 4, 5, 6, and 7. Tables 3–7 present the temperature (T_{max}) and pressure (P_{max}) peaks reached at the moment of transient collapse of cavitation bubble, the number of water molecules in the bubble at collapse, and the equilibrium composition of

the various species resulting from dissociation of entrapped molecules in the bubble when the temperature and pressure reached to its extreme conditions during transient collapse of cavitation bubbles.

3.1. Initial Bubble Size in the Liquid Medium. Bubbles with different initial radius present in the liquid medium play an important role in cavitation. Kumar and Moholkar [37] have reported that the smaller bubble has higher Laplace pressure, which results in higher expansion and more intense collapse during the transient collapse. In this present study, a single bubble model with different initial radius has been chosen to present the effects of bubble radius in sonochemical process. From Table 3, it could be seen that the $\cdot\text{OH}$ radical formation during transient collapse of cavitation bubble is higher with the initial bubble radius of 5 μm followed by 25 μm . This is due to the bubble with small bubble radius can undergo many acoustic cycles before reaching its critical radius when it collapses, and as a result the highest temperature peak is reached at the moment of transient collapse of the cavitation bubble with 5 μm radius bubble as shown in Figure 1 and Table 3.

3.2. Static Pressure of the System. As stated earlier in the previous section, the cavitation is nothing but the nucleation, growth, and implosive collapse of bubbles, but the growth/expansion of the bubble depends on the system's static pressure. So, when the bubble contains vapor, cavitation may occur due to reduced static pressure sufficiently at constant temperature. To investigate the effects of pressure, five different static pressures ranging from 100–300 kPa have been chosen. The results showed that as the static pressure increases the radical formation decreases drastically; even it becomes zero at higher ambient static pressure. This is due to at elevated static pressure, the sonochemical effects get eliminated which directly affects the generation of radical formation, provided the applied pressure must be greater than or equal to the acoustic pressure amplitude ($P_o \geq P_{\text{AW}}$) [9, 38]. The highest $\cdot\text{OH}$ radical production was seen at nearly

FIGURE 1: Simulations of radial motion of 5 and 25 micron air bubble in water. $f = 20 \text{ kHz}$; $P_A = 150 \text{ kPa}$; and $P_o = 100 \text{ kPa}$. Time history of (a) radius of the bubble; (b) temperature inside the bubble; (c) water vapor evaporation in the bubble; (d) pressure inside the bubble; (e) microturbulence generated by the bubble; and (f) acoustic waves emitted by the bubble.

FIGURE 2: Simulations of radial motion of 5 micron air bubble in water at 120 kPa and 150 kPa. $f = 20$ kHz; $P_A = 150$ kPa; and $R_0 = 5 \mu\text{m}$. Time history of (a) radius of the bubble; (b) temperature inside the bubble; (c) water vapor evaporation in the bubble; (d) pressure inside the bubble; (e) microturbulence generated by the bubble; and (f) acoustic waves emitted by the bubble.

FIGURE 3: Simulations of radial motion of 5 micron air bubble in water at 283 K and 343 K. $f = 20$ kHz; $P_A = 150$ kPa; and $P_o = 100$ kPa. Time history of (a) radius of the bubble; (b) temperature inside the bubble; (c) water vapor evaporation in the bubble; (d) pressure inside the bubble; (e) microturbulence generated by the bubble; and (f) acoustic waves emitted by the bubble.

FIGURE 4: Simulations of radial motion of 5 micron air bubble in water with O_2 bubble and N_2 bubble. $f = 20$ kHz; $P_A = 150$ kPa; and $P_o = 100$ kPa. Time history of (a) radius of the bubble; (b) temperature inside the bubble; (c) water vapor evaporation in the bubble; (d) pressure inside the bubble; (e) microturbulence generated by the bubble; and (f) acoustic waves emitted by the bubble.

FIGURE 5: Simulations of radial motion of 5 micron air bubble in toluene and n-hexane as cavitation medium. $f = 35$ kHz; $P_A = 150$ kPa; and $P_o = 100$ kPa. Time history of (a) radius of the bubble; (b) temperature inside the bubble; (c) water vapor evaporation in the bubble; (d) pressure inside the bubble; (e) microturbulence generated by the bubble; and (f) acoustic waves emitted by the bubble.

TABLE 3: Simulation summary of initial bubble size (R_0) dependent sonochemical process.

Species	Conditions at the first collapse of the bubble				
	$R_0 = 5 \mu\text{m}$	$R_0 = 25 \mu\text{m}$	$R_0 = 50 \mu\text{m}$	$R_0 = 100 \mu\text{m}$	$R_0 = 200 \mu\text{m}$
	$T_{\max} = 3999 \text{ K}$	$T_{\max} = 1688 \text{ K}$	$T_{\max} = 778.5 \text{ K}$	$T_{\max} = 409 \text{ K}$	$T_{\max} = 329.9 \text{ K}$
	$P_{\max} = 696.7 \text{ MPa}$	$P_{\max} = 30.57 \text{ MPa}$	$P_{\max} = 2.56 \text{ MPa}$	$P_{\max} = 288 \text{ kPa}$	$P_{\max} = 136 \text{ kPa}$
	$V_{\text{turb}} = 0.36 \text{ m/s}$	$V_{\text{turb}} = 6.11 \text{ m/s}$	$V_{\text{turb}} = 6.2 \text{ m/s}$	$V_{\text{turb}} = 7.95 \text{ m/s}$	$V_{\text{turb}} = 11.2 \text{ m/s}$
	$P_{\text{AW}} = 24.04 \text{ MPa}$	$P_{\text{AW}} = 8.80 \text{ MPa}$	$P_{\text{AW}} = 0.63 \text{ MPa}$	$P_{\text{AW}} = 0.27 \text{ MPa}$	$P_{\text{AW}} = 0.35 \text{ kPa}$
	$N_{\text{N}_2} = 1.28 \times 10^{10}$	$N_{\text{N}_2} = 1.32 \times 10^{12}$	$N_{\text{N}_2} = 1.03 \times 10^{13}$	$N_{\text{N}_2} = 8.11 \times 10^{13}$	$N_{\text{N}_2} = 6.44 \times 10^{14}$
	$N_{\text{O}_2} = 3.41 \times 10^9$	$N_{\text{O}_2} = 3.51 \times 10^{11}$	$N_{\text{O}_2} = 2.73 \times 10^{12}$	$N_{\text{O}_2} = 2.16 \times 10^{13}$	$N_{\text{O}_2} = 1.71 \times 10^{14}$
	$N_{\text{W}} = 2.91 \times 10^9$	$N_{\text{W}} = 2.5 \times 10^{11}$	$N_{\text{W}} = 9.08 \times 10^{11}$	$N_{\text{W}} = 2.98 \times 10^{12}$	$N_{\text{W}} = 1.15 \times 10^{13}$
Species	Equilibrium composition of species in the bubble at collapse				
	$5 \mu\text{m}$	$25 \mu\text{m}$	$50 \mu\text{m}$	$100 \mu\text{m}$	$200 \mu\text{m}$
N_2	6.26×10^{-1}	6.86×10^{-1}	7.38×10^{-1}	7.68×10^{-1}	7.79×10^{-1}
O_2	1.28×10^{-1}	1.82×10^{-1}	1.96×10^{-1}	2.04×10^{-1}	2.07×10^{-1}
H_2O	1.41×10^{-2}	1.30×10^{-1}	6.50×10^{-2}	2.80×10^{-2}	1.40×10^{-2}
N	1.56×10^{-5}	—	—	—	—
O	5.95×10^{-3}	—	—	—	—
H	2.83×10^{-4}	—	—	—	—
O_3	1.70×10^{-5}	—	—	—	—
H_2	2.53×10^{-4}	—	—	—	—
OH	9.51×10^{-3}	9.03×10^{-5}	—	—	—
HO_2	5.59×10^{-4}	5.81×10^{-6}	—	—	—
H_2O_2	2.00×10^{-5}	—	—	—	—
NO	8.47×10^{-2}	2.58×10^{-3}	1.49×10^{-6}	—	—
NO_2	1.70×10^{-3}	1.27×10^{-4}	2.84×10^{-6}	—	—
N_2O	3.61×10^{-4}	2.18×10^{-6}	—	—	—
NH	1.70×10^{-6}	—	—	—	—
HNO	5.95×10^{-5}	—	—	—	—
HNO_2	1.75×10^{-4}	7.06×10^{-6}	—	—	—

Note: solvent = water, temperature (T) = 303 K, static pressure (P_0) = 100 kPa, dissolved gas = air, and frequency (f) = 20 kHz.

ambient static pressure (i.e., 100 kPa), and the production of $\cdot\text{OH}$ radical decreases as the static pressure approaches to the magnitude of acoustic pressure, that is, 150 kPa. The production of $\cdot\text{OH}$ radical at 100 kPa is typically 1.5 fold higher than the $\cdot\text{OH}$ radical production at 120 kPa, while at 150 kPa or higher static pressure no $\cdot\text{OH}$ radical formation was seen. This result can be attributed to the temperature peak reached at the moment of collapse of the bubble. At the time of transient collapse, the highest temperature peak (3999 K) was seen when the pressure was 100 kPa, while the lowest temperature peak ($\sim 313 \text{ K}$) was observed with elevated static pressure of 300 kPa.

3.3. System Operating Temperature. Another important factor that affects the transient cavitation is system temperature. To study the temperature effect on sonochemical process, the numerical simulations were run in the temperature range from 283 to 373 K (viz. 283, 303, 323, 343, and 373 K). The simulation results are depicted in Figure 3. As the temperature in the system increases the formation of oxidizing species due to transient cavitation of bubbles reduces drastically. This could be attributed to the effects of bubble radius as discussed in the earlier section. In this case, vapor bubbles grow

with increasing the temperature through the phenomenon of boiling [20]. So, the lower the temperature means the higher the cavitation effects in the system. Table 5 shows that the production of $\cdot\text{OH}$ radical is highest with the lowest temperature, that is, at 283 K, while at the boiling point of water no $\cdot\text{OH}$ radical formation has been observed. The overall trend of the $\cdot\text{OH}$ radical production under various operating temperature is $283 \text{ K} > 303 \text{ K} > 323 \text{ K} > 343 \text{ K}$.

3.4. Type of Dissolved Gas Content. The type of dissolved gas has an impact on bubble nucleation rate as described in the literatures [15, 37]. The simulation results for four gases are shown in Table 6 and Figure 4. The production of $\cdot\text{OH}$ radical as well as H_2O_2 is highest for O_2 bubble followed by air, Ar, and N_2 bubble. Also the generation of O_3 per bubble for oxygen bubble is one order of magnitude higher than the O_3 generation by air bubble. The radicals by air bubble are formed through the reactions (3)–(22), while (24) and (25) represent the radical formation by O_2 bubble [39]. The production of radicals is least with N_2 bubble as compared to other gas bubbles. This is due to the scavenging of radicals by N_2 molecules through the reactions (3)–(16). Moreover, there is no regeneration of $\cdot\text{OH}$ and $\text{O}^\cdot$ radicals by O_2 when the

TABLE 4: Simulation summary of sonochemical process under various static pressures (P_o).

Conditions at the first collapse of the bubble					
	$P_o = 100$ kPa	$P_o = 120$ kPa	$P_o = 150$ kPa	$P_o = 200$ kPa	$P_o = 300$ kPa
$T_{\max}$	3999 K	3024 K	977.3 K	353.4 K	312.7 K
$P_{\max}$	696.7 MPa	286.3 MPa	4.62 MPa	416 kPa	477 kPa
V_{turb}	0.36 m/s	0.21 m/s	0.07 m/s	0.008 m/s	0.002 m/s
P_{AW}	24.04 MPa	5.43 MPa	120 kPa	2 kPa	0.6 kPa
N_{N_2}	1.28×10^{10}	1.48×10^{10}	1.78×10^{10}	2.28×10^{10}	3.28×10^{10}
N_{O_2}	3.41×10^9	3.95×10^9	4.74×10^9	6.07×10^9	8.73×10^9
N_{W}	2.91×10^9	1.81×10^9	8.86×10^8	8.19×10^{10}	3.81×10^8
Equilibrium composition of species in the bubble at collapse					
Species	1 bar	1.2 bar	1.5 bar	2 bar	3 bar
N_2	6.26×10^{-1}	6.99×10^{-1}	7.60×10^{-1}	7.68×10^{-1}	7.83×10^{-1}
O_2	1.28×10^{-1}	1.67×10^{-1}	2.02×10^{-1}	2.04×10^{-1}	2.08×10^{-1}
H_2O	1.41×10^{-2}	7.45×10^{-2}	3.80×10^{-2}	2.80×10^{-2}	9.00×10^{-3}
N	1.56×10^{-5}	—	—	—	—
O	5.95×10^{-3}	9.35×10^{-4}	—	—	—
H	2.83×10^{-4}	4.09×10^{-5}	—	—	—
O_3	1.70×10^{-5}	3.71×10^{-6}	—	—	—
H_2	2.53×10^{-4}	1.67×10^{-4}	—	—	—
OH	9.51×10^{-3}	6.33×10^{-3}	—	—	—
HO_2	5.59×10^{-4}	3.60×10^{-4}	—	—	—
H_2O_2	2.00×10^{-5}	2.74×10^{-5}	—	—	—
NO	8.47×10^{-2}	4.30×10^{-2}	2.64×10^{-5}	—	—
NO_2	1.70×10^{-3}	1.03×10^{-3}	1.09×10^{-5}	—	—
N_2O	3.61×10^{-4}	1.10×10^{-4}	—	—	—
NH	1.70×10^{-6}	—	—	—	—
HNO	5.95×10^{-5}	1.38×10^{-5}	—	—	—
HNO_2	1.75×10^{-4}	1.40×10^{-4}	—	—	—

Note: solvent = water, dissolved gas = air, initial bubble size (R_0) = 5 μm , temperature (T) = 303 K, and frequency (f) = 20 kHz.

bubble contents are N_2 gas. So the total number of radicals per bubble in N_2 bubbling is always lower than the other gas bubbles. The trend of production of $\cdot\text{OH}$ radical per bubble with various gases bubbling is as follows $\text{O}_2 > \text{Air} > \text{Ar} > \text{N}_2$.

TABLE 5: Simulation summary of system temperature (T_0) dependent sonochemical process.

Species	System temperature				
	$T = 283 \text{ K}$	$T = 303 \text{ K}$	$T = 323 \text{ K}$	$T = 343 \text{ K}$	$T = 373 \text{ K}$
	Conditions at the first collapse of the bubble				
	$T_{\max} = 3989 \text{ K}$	$T_{\max} = 3999 \text{ K}$	$T_{\max} = 3733 \text{ K}$	$T_{\max} = 2683 \text{ K}$	$T_{\max} = 811.7 \text{ K}$
	$P_{\max} = 681.5 \text{ MPa}$	$P_{\max} = 696.7 \text{ MPa}$	$P_{\max} = 623.9 \text{ MPa}$	$P_{\max} = 175.3 \text{ MPa}$	$P_{\max} = 1.79 \text{ MPa}$
	$V_{\text{turb}} = 0.35 \text{ m/s}$	$V_{\text{turb}} = 0.36 \text{ m/s}$	$V_{\text{turb}} = 0.45 \text{ m/s}$	$V_{\text{turb}} = 1.08 \text{ m/s}$	$V_{\text{turb}} = 4.63 \text{ m/s}$
	$P_{\text{AW}} = 24.75 \text{ MPa}$	$P_{\text{AW}} = 24.04 \text{ MPa}$	$P_{\text{AW}} = 21.56 \text{ MPa}$	$P_{\text{AW}} = 4.43 \text{ MPa}$	$P_{\text{AW}} = 220 \text{ kPa}$
	$N_{\text{N}_2} = 1.38 \times 10^{10}$	$N_{\text{N}_2} = 1.28 \times 10^{10}$	$N_{\text{N}_2} = 1.21 \times 10^{10}$	$N_{\text{N}_2} = 1.13 \times 10^{10}$	$N_{\text{N}_2} = 1.04 \times 10^{10}$
	$N_{\text{O}_2} = 3.66 \times 10^9$	$N_{\text{O}_2} = 3.41 \times 10^9$	$N_{\text{O}_2} = 3.20 \times 10^9$	$N_{\text{O}_2} = 3.02 \times 10^9$	$N_{\text{O}_2} = 2.77 \times 10^9$
	$N_{\text{W}} = 7.94 \times 10^8$	$N_{\text{W}} = 2.91 \times 10^9$	$N_{\text{W}} = 1.23 \times 10^{10}$	$N_{\text{W}} = 8.15 \times 10^{10}$	$N_{\text{W}} = 1.79 \times 10^{12}$
Species	Equilibrium composition of species in the bubble at collapse				
	283 K	303 K	323 K	343 K	373 K
N_2	7.07×10^{-1}	6.26×10^{-1}	4.13×10^{-1}	1.16×10^{-1}	6.00×10^{-3}
O_2	1.45×10^{-1}	1.28×10^{-1}	8.84×10^{-2}	2.83×10^{-2}	2.00×10^{-3}
H_2O	1.63×10^{-2}	1.41×10^{-2}	1.21×10^{-2}	2.80×10^{-2}	9.93×10^{-1}
N	1.72×10^{-5}	1.56×10^{-5}	3.84×10^{-6}	—	—
O	6.67×10^{-3}	5.95×10^{-3}	2.44×10^{-3}	5.69×10^{-5}	—
H	3.21×10^{-4}	2.83×10^{-4}	1.06×10^{-4}	2.57×10^{-6}	—
O_3	1.89×10^{-5}	1.70×10^{-5}	8.38×10^{-6}	2.28×10^{-7}	—
H_2	2.91×10^{-4}	2.53×10^{-4}	1.30×10^{-4}	2.29×10^{-5}	—
OH	1.08×10^{-2}	9.51×10^{-3}	5.27×10^{-3}	8.08×10^{-4}	—
HO_2	6.31×10^{-4}	5.59×10^{-4}	3.25×10^{-4}	4.22×10^{-5}	—
H_2O_2	2.28×10^{-5}	2.00×10^{-5}	1.36×10^{-5}	4.60×10^{-6}	—
NO	9.51×10^{-2}	8.47×10^{-2}	4.72×10^{-2}	4.57×10^{-3}	—
NO_2	1.90×10^{-3}	1.70×10^{-3}	1.04×10^{-3}	1.11×10^{-4}	—
N_2O	4.01×10^{-4}	3.61×10^{-4}	1.88×10^{-4}	8.69×10^{-6}	—
NH	1.89×10^{-6}	1.70×10^{-6}	—	—	—
HNO	6.67×10^{-5}	5.95×10^{-5}	2.74×10^{-5}	9.69×10^{-7}	—
HNO_2	1.96×10^{-4}	1.75×10^{-4}	1.12×10^{-4}	1.76×10^{-5}	—

Note: solvent = water, dissolved gas = air, initial bubble size (R_0) = 5 μm , static pressure (P_0) = 100 kPa, and frequency (f) = 20 kHz.

3.5. Type of Solvent or Cavitation Medium. The solvent or cavitation medium is another important factor that affects directly on the sonochemical process. In order to assess the suitability of solvent for cavitation, we have chosen three solvents with different physicochemical properties, namely, water, toluene, and n-hexane, as shown in Table 2. To address this issue, we have presented the numerical solution with various solvent as cavitation medium in Figure 5 and Table 7, which lists the temperature and pressure peak reached at the moment of collapse with various equilibrium compositions of species. The number of $\cdot\text{OH}$ radical production is highest when water is used as cavitation medium. This can be attributed to the lower surface tension and higher vapor pressure of the organic solvent. The production of $\cdot\text{OH}$ radical in water is typically two orders of magnitude higher than that in toluene. So, due to the low intensity of bubble collapse, organic solvents are not able to generate sufficient numbers of radical *in-situ* for sonochemical reactions.

4. Conclusions

The lower is the system temperature the higher is the cavitation effects, that is, when the system temperature is

moderately low the effect of cavitation is more. In this present study, the radical formation due to cavitation is highest when the system temperature is 283 K. So, the system with low operating temperature and cavitation medium contents with small initial bubble radius is always preferable for sonochemical reactions since this type of sonochemical reaction systems are able to generate large amount of highly oxidizing species. Due to the high vapor pressure and low surface tension, organic solvents cannot produce large amount of radicals in the reaction medium; thus, they are not suitable for sonochemical reactions. However, they could be good solvents for extraction or other processes using ultrasound. Moreover, depending on the process requirement one can choose the system with different gas bubbling and aqueous or organic solvents for conducting experiments.

Nomenclature

- $C_{V,i}$: Heat capacity at constant volume, J $\text{kg}^{-1} \text{K}^{-1}$
 c_L : Velocity of sound in liquid medium, m s^{-1}
 c_W : Velocity of sound in water, m s^{-1}

TABLE 6: Effect of dissolved gas content on sonochemical process.

Species	Conditions at the first collapse of the bubble			
	Air bubble	Nitrogen bubble	Oxygen bubble	Argon bubble
	$T_{\max} = 3999 \text{ K}$	$T_{\max} = 4379 \text{ K}$	$T_{\max} = 4155 \text{ K}$	$T_{\max} = 4551 \text{ K}$
	$P_{\max} = 696.7 \text{ MPa}$	$P_{\max} = 772.3 \text{ MPa}$	$P_{\max} = 758.2 \text{ MPa}$	$P_{\max} = 786.6 \text{ MPa}$
	$V_{\text{turb}} = 0.36 \text{ m/s}$	$V_{\text{turb}} = 0.37 \text{ m/s}$	$V_{\text{turb}} = 0.37 \text{ m/s}$	$V_{\text{turb}} = 0.37 \text{ m/s}$
	$P_{\text{AW}} = 24.04 \text{ MPa}$	$P_{\text{AW}} = 28.25 \text{ MPa}$	$P_{\text{AW}} = 30.78 \text{ MPa}$	$P_{\text{AW}} = 27.28 \text{ MPa}$
	$N_{\text{N}_2} = 1.28 \times 10^{10}$	$N_{\text{N}_2} = 1.63 \times 10^{10}$	$N_{\text{O}_2} = 1.63 \times 10^{10}$	$N_{\text{Ar}} = 1.63 \times 10^{10}$
	$N_{\text{O}_2} = 3.41 \times 10^9$	$N_{\text{W}} = 3.88 \times 10^9$	$N_{\text{W}} = 3.88 \times 10^9$	$N_{\text{W}} = 2.54 \times 10^9$
	$N_{\text{W}} = 2.91 \times 10^9$			
Species	Equilibrium composition of species in the bubble at collapse			
	Air bubble	Nitrogen bubble	Oxygen bubble	Argon bubble
N_2	6.26×10^{-1}	8.05×10^{-1}	—	—
O_2	1.28×10^{-1}	2.80×10^{-4}	7.93×10^{-1}	1.09×10^{-3}
Ar	—	—	—	8.65×10^{-1}
H_2O	1.41×10^{-2}	9.69×10^{-3}	1.13×10^{-2}	9.21×10^{-3}
N	1.56×10^{-5}	5.85×10^{-5}	—	—
O	5.95×10^{-3}	5.06×10^{-4}	1.87×10^{-2}	1.34×10^{-3}
H	2.83×10^{-4}	2.48×10^{-3}	2.21×10^{-4}	2.59×10^{-3}
N_3	—	1.45×10^{-6}	—	—
O_3	1.70×10^{-5}	—	3.28×10^{-4}	—
H_2	2.53×10^{-4}	6.73×10^{-3}	1.03×10^{-4}	4.31×10^{-3}
OH	9.51×10^{-3}	2.50×10^{-3}	1.57×10^{-2}	4.09×10^{-3}
HO_2	5.59×10^{-4}	6.77×10^{-6}	2.34×10^{-3}	2.07×10^{-5}
H_2O_2	2.00×10^{-5}	8.86×10^{-7}	4.75×10^{-5}	1.79×10^{-6}
NO	8.47×10^{-2}	5.65×10^{-3}	—	—
NO_2	1.70×10^{-3}	4.93×10^{-6}	—	—
N_2O	3.61×10^{-4}	3.02×10^{-5}	—	—
NH	1.70×10^{-6}	2.68×10^{-5}	—	—
NH_2	—	2.42×10^{-5}	—	—
NH_3	—	1.78×10^{-5}	—	—
HNO	5.95×10^{-5}	2.25×10^{-5}	—	—
HNO_2	1.75×10^{-4}	2.16×10^{-6}	—	—

Note: solvent = water, initial bubble size (R_0) = 5 μm , temperature (T) = 303 K, static pressure (P_0) = 100 kPa, and frequency (f) = 20 kHz. $\text{O}_2 > \text{air} > \text{Ar} > \text{N}_2$.

c_{T} : Velocity of sound in toluene, m s^{-1}
 c_{H} : Velocity of sound in n-hexane, m s^{-1}
 D_{w} : Diffusion coefficient of solvent vapor, $\text{m}^2 \text{s}^{-1}$
 f : Frequency of ultrasound wave, Hz
 f_i : Translational and rotational degrees of freedom
 h : Van der Waal's hard core radius, m
 $I_{\text{diff,w}}$: Instantaneous diffusive penetration depth for water molecules
 k : Boltzmann constant, J K^{-1}
 N_{W} : Number of water molecules trapped in the bubble
 N_{N_2} : Number of N_2 molecules in the bubble
 N_{O_2} : Number of oxygen molecules in the bubble
 N_{T} : Number of toluene molecules in the bubble
 N_{H} : Number of n-hexane molecules in the bubble

N_{Ar} : Number of Ar molecules in the bubble
 N_{tot} : Total number of molecules (gas + vapor) in the bubble
 P_o : Static pressure in the liquid medium, Pa
 $P_{\max}$: Pressure peak reached in the bubble at the time of first collapse, Pa
 P_{AW} : Pressure amplitude of the acoustic wave generated by the cavitation bubble, Pa
 Q : Heat conducted across bubble wall, J s^{-1}
 R : Radius of the bubble, m
 R_o : Initial radius of the cavitation bubble, m
 dR/dt : Bubble wall velocity, m s^{-1}
 t : Time, s
 T : Temperature of the bubble contents, K
 T_o : Ambient (or bulk liquid medium) temperature, K
 $T_{\max}$: Temperature peak reached in the bubble at the time of first collapse, K

TABLE 7: Simulation summary of sonochemical process with different solvent as cavitation medium.

	Conditions at the first collapse of the bubble		
	H ₂ O ₂	C ₆ H ₅ -CH ₃	C ₆ H ₁₂
$T_{\max}$	3179 K	4835 K	1151 K
$P_{\max}$	355 MPa	961.7 MPa	44.55 MPa
V_{turb}	0.25 m/s	0.15 m/s	0.005 m/s
P_{AW}	12.61 MPa	30.16 MPa	188 kPa
N_{N_2}	1.31×10^{10}	1.13×10^9	1.07×10^{10}
N_{O_2}	3.47×10^9	2.99×10^8	2.85×10^9
N_{W}	1.21×10^9	4.02×10^3	6.05×10^{10}
Species	Equilibrium composition of species in the bubble at collapse		
	H ₂ O ₂	C ₆ H ₅ -CH ₃	C ₆ H ₁₂
N ₂	7.09×10^{-1}	7.17×10^{-1}	1.40×10^{-1}
O ₂	1.66×10^{-1}	1.26×10^{-1}	—
H ₂ O	5.37×10^{-2}	—	6.28×10^{-2}
N	—	1.92×10^{-4}	—
O	1.38×10^{-3}	2.06×10^{-2}	—
H	5.90×10^{-5}	1.51×10^{-6}	—
N ₃	—	3.86×10^{-6}	—
O ₃	5.44×10^{-6}	3.84×10^{-5}	—
H ₂	1.77×10^{-4}	—	8.98×10^{-1}
OH	6.96×10^{-3}	1.95×10^{-5}	—
HO ₂	4.10×10^{-4}	1.04×10^{-6}	—
H ₂ O ₂	2.68×10^{-5}	—	—
NO	5.14×10^{-2}	1.42×10^{-1}	—
NO ₂	1.23×10^{-3}	2.29×10^{-3}	—
NO ₃	—	1.66×10^{-6}	—
N ₂ O	1.49×10^{-4}	7.48×10^{-4}	—
N ₂ O ₃	—	1.15×10^{-6}	—
HNO	1.91×10^{-5}	—	—
HNO ₂	1.57×10^{-4}	—	—
CO	—	7.10×10^{-6}	1.18×10^{-2}
CO ₂	—	1.26×10^{-5}	7.02×10^{-4}
NH ₃	—	—	9.90×10^{-3}
HCN	—	—	1.48×10^{-5}
CH ₄	—	—	2.37
C ₂ H ₄	—	—	1.11×10^{-4}
C ₂ H ₆	—	—	4.09×10^{-3}

Note: dissolved gas = air, initial bubble size (R_0) = 5 μm , temperature (T) = 303 K, static pressure (P_0) = 100 kPa, and frequency (f) = 35 kHz.

- V_{turb} : Average velocity of the microturbulence in the medium generated by ultrasound and cavitation in the medium (estimated at 1 mm distance from bubble center), m s^{-1}
- ρ_{L} : Density of the liquid, kg m^{-3}
- ν : Kinematic viscosity of liquid, $\text{m}^2 \text{s}^{-1}$
- σ : Surface tension of liquid, N m^{-1}
- κ : Thermal conductivity of bubble contents, $\text{W m}^{-1} \text{K}^{-1}$
- λ : Thermal diffusivity of bubble contents, $\text{m}^2 \text{s}^{-1}$

θ : Characteristic vibrational temperature(s) of the species, K.

Conflict of Interests

The authors of the paper do not have any direct financial relation that might lead to a conflict of interest for any of the authors.

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