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Comparison Between Hydrodynamic and Acoustic Cavitation in Microbial Cell Disruption

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Cavitation phenomena are associated with the formation, growth and the collapse of microbubbles and consequently, to the generation of very high pressures, shear stresses and temperatures, locally. Thanks to the cited features, the application of cavitation is a reliable tool for cell damage and hence disruption. In this paper a theoretical model for quantifying the mechanical effect of hydrodynamic cavitation (HC) and acoustic cavitation (AC) in killing micro-organism is reported. A physical model accounting for bubble dynamics, fluid turbulence, shear stress and pressure pulse generated from cavity collapse is developed, aimed at calculating the turbulent shear generated and the extent of microbial disinfection. The theoretical results are compared with the mechanical resistance of microbial cells in order to estimate the damaging effect.
Numerical results provide a practical tool for the estimation of process efficacy and parameter optimization, both for HC and AC devices. The effect of parameters is estimated and typical experiments from the pertinent literature are simulated in order to estimate the treatment efficiency. Results are in agreement with the related; moreover, from the energy efficiency point of view, it was observed that HC is almost an order of magnitude more energy efficient than AC.

1. Introduction

Cavitational devices are novel and promising multiphase reactors, based on the principle of release of large magnitude of energy due to the violent collapse of the cavities resulting in very high local energy densities (Gogate, 2007). Cavities can be generated by sound waves, usually ultrasounds (*Acoustic Cavitation*, AC) or by constrictions in the liquid flow (*Hydrodynamic Cavitation*, HC).
In the environmental field, cavitation is establishing itself as an energy-efficient tool for degrading persistent pollutants in waste liquid streams (Capocelli et al, 2012, 2013b). However, due to the generation of shear stresses, hot spots, highly reactive free radicals and turbulence associated with liquid circulation, cavitation process has been proven also to be a valid solution in the field of biochemical engineering. For the large-scale disruption of microorganisms, mechanical disintegrators such bead mills and high-pressure homogenizers are used, but with two main drawbacks: low energy efficiencies (5–10%) and high energy dissipation in the form of heat, which has to be efficiently removed (Gogate and Kabadi, 2009). This last feature is particularly relevant if the process is aimed at recovering intracellular components from micro-organisms, *i.e.* to protein release or intracellular enzyme extraction, to retain the integrity of these delicate bio-products.
As a matter of fact, microstreaming resulting from cavitation has been shown to produce shear stresses sufficient to disrupt cell membranes in water disinfection and biochemical downstream processes. The main mechanism is the onset of turbulence which creates vortices, shock waves and high shear stresses

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developed by viscous dissipative eddies, near which shear rates exist, higher than the shear rates throughout the bulk of the liquid (Doulah, 1977). Other cavitation effects, playing just a supporting role in the microbial disinfection, are chemical and heat consequence of bubble collapse (Mason et al., 2003).
Several experimental research studies have proven the effectiveness of cavitation in the field of disinfection and, more generally, in cell damage (Gogate, 2007; Mahulkar and Pandit, 2010, Gogate and Pandit, 2008; Jyoti and Pandit, 2001; Koval et al., 2011). Large scale applications of cavitation are mostly in the field of ballast water treatment (on-ship) thanks to its simplicity, durability, low maintenance and no need of chemicals (Gogate, 2007; Mahulkar and Pandit, 2010).
From the theoretical point of view, mathematical modelling of cavitating devices has made great steps forward during last ten years, allowing the simulation and prediction of bubble dynamics and conditions at the collapse stage, both for AC and HC techniques. Recently developed models are able to predict cavitation intensity in terms of pressure, temperature and radical species concentration (Toegel et al., 2000; Capocelli et al., 2012, 2013a-b; Krishnan et al., 2006). Nevertheless, there is still the need to develop predictive codes, correlations and theoretical models to help engineers in reactor design and process control (Hidalgo et al., 2012). Proper selection of the operating and geometric parameters decides the efficacy of the cavitational reactors in the desired application.
In this paper a theoretical model for quantifying the cavitationally generated turbulent shear and extent of microbial disinfection has been developed and applied to several kind of microorganisms (*e.g. zooplankton*, *phytoplankton* and *bacteria*). A physical mechanism accounting for bubble dynamics, cavitation event rate, fluid turbulence, shear stress and pressure pulse being generated from cavity collapse, is developed. The theoretical results are compared with the mechanical resistance of several microbial cells in order to estimate the possible damaging effect. Numerical results provide a practical tool for the estimation of process efficacy and parameter optimization, both for HC and AC devices. The effect of parameters is estimated for process optimization and the results are compared with the pertinent literature in order to validate the model. From the energy efficiency point of view, HC is proved to be of almost an order of magnitude more energy efficient than AC.

2. Modelling of cavitation

Different kinds of reactor are currently utilized for cavitation experiments: ultrasonic cavitation can operate in a batch mode or in a continuous mode where multiple units with a plurality of low electrical and acoustic power (1–3 Wcm^{-2}) in a continuous or in a pulsed mode; hydrodynamic cavitation can simply be generated by using a constriction such as an orifice plate, a Venturi or a throttling valve in a liquid flow. Fundamental parameters for the description of HC treatment are the orifice to pipe ratio β, the inlet pressure p_{in} and the cavitation number C_v. The simulation of bubble dynamics in both cases is extensively studied in the pertinent literature.
In this paper a model derived from the work by Toegel et al. (2000) is used, based on the diffusion limited approach, for the simulation of the bubble behaviour in AC and HC. It consists of the bubble dynamics with energy and mass balance on the collapsing bubble.
Further details on the application of the model to AC and HC is given in the papers by Capocelli et al., (2012, 2013a), respectively. The main difference between the application to HC and AC consists in writing an equation which properly describes the bulk pressure p_t [kPa]. For the AC it can be written as:

$$p_t(t) = p_{atm} - \sqrt{2I\rho c}\,\sin(2\pi f t) \qquad (1)$$

Where ρ is the water density, c is the sound velocity in the medium and f is the ultrasonic frequency [kHz]. In the case of HC, Moholkar and Pandit (1997) suggested the calculation of the pressure variation through the Bernoulli equation, by assuming a local velocity corrected with a sinusoidal term for addressing the turbulent fluctuation. According to their model, the calculation is given in Eq. 2.

$$U(t) = u(t) + \bar{u}'(t)\sin(2\pi f_T t) \qquad (2)$$

where u is the mean flow velocity, u' the turbulent fluctuation velocity [ms^{-1}] and f_t its frequency [kHz]. For the determination of the turbulent shear stress for the prediction of microorganism extent of killing is described by Eq.3-5. According to the pertinent literature (Sawant et al., 2008; Mahulkar and Pandit. 2010, Mahulkar et al., 2009) the stress generated from cavity oscillation can be related to the turbulence energy dissipation rates (ε), as shown in Eq. 3. This last can be calculated from the estimation of eddy size and the turbulent kinetic energy per unit mass $k(t)$ [$kJ\ kg^{-1}$]. The model of single bubble dynamics allows the calculation of the instantaneous velocity of the liquid at distance R_{max} from the bubble for the determination of the turbulent kinetic energy per unit mass *k(t),* as reported in Eq. 4 (m^2s^2).

$$\Delta P_c = \sqrt{\rho\, \mu\, \bar{\varepsilon}} \tag{3}$$

$$k(t) = \frac{1}{2}\left(\frac{R(t)^2}{{R_{max}}^2}\frac{dR}{dt}(t)\right)^2 \tag{4}$$

The cavitation assisted cell disruption is assumed to occur only due to the stress generated by the cavity collapse (Eq.5). The adopted model suggests a reaction rate proportional to the number of collapse with sufficient energy to overcome the minimum (activation energy) required for cell damage, S_{cell}. [kPa]. K [s^{-1}] can be seen as the product of collision frequency and number of bubble per unit volume.

$$\frac{dN}{dt} = -N(t)\, K \exp\left(-\frac{S_{cell}}{\Delta P_c}\right) \tag{5}$$

where N is the number of microorganism per unit volume. The proposed equation has been successfully adopted in literature for interpreting experimental results (Mahulkar et al., 2009; Mahulkar and Pandit, 2010; Sawant et al., 2008). Therefore, a way to compare simulation results of AC and HC has been found in Eq. 6 where the calculation of the energy consumption (*EC*, kWm^3) is reported:

$$EC = \frac{P\, t}{V \ln(N_0/N)} \tag{6}$$

in which P is the mechanical power put into the system and V is the volume of solution to be treated. This term does not represent a comparison in terms of electrical energy consumption because of the consistent differences existing between AC and HC (electrical yield, reactor configuration, frequency of collision and cavity concentration) and the variability resulting from the real conditions (nuclei size distribution, dissolved gas content). Nevertheless, by adopting some simplifying assumptions, *EC* can be considered a practical way to compare the two applications in terms of energy required for a fixed treatment efficiency.

3. Results and discussion

The results of single bubble dynamics model are visible in Figures 1 and 2. The behaviour of a single pre-existent nucleus of initial radius R_0 is simulated for different AC and HC experimental configurations (the values of operating parameters are summarised in Table 1 and 2). Figure 1 represents the bubble history in an ultrasonic bath for different ultrasonic frequencies at I=0.2 W cm^{-2} (Fig.1a) and I=1 W cm^{-2} (Fig. 1b). An increase of frequency reduces the time of bubble growth, therefore decreasing the water vapour amount and the consequent collapse intensity. From the comparison of Fig. 1a and 1b it is possible to observe a greater R_{max} reached at I=1 W cm^{-2}. Figure 2 reports simulation results of HC treatments at different operating conditions: inlet pressure p_{in}=1.5, 3, 6 bar, respectively for HC I,HC III, HC VI (*see* Table 2). Operational parameters are taken from a classical Venturi device described in literature (Saharan et al., 2011). In Figure 2a the dimensionless radius is reported *vs.* the length of the recovery zone: higher p_{in} (lower C_v) decreases the bubble growth phase in terms of space (time) required for collapse and bubble size. Figure 2b reports the bubble wall velocity for the simulations of Figure 2a: in correspondence of the bubble collapse, higher R' values (with an inversion at the rebound) are observed.
From the reported simulation it is possible to calculate *k(t)*, $\bar{\varepsilon}$ and ΔP as previously discussed. Consequently, the extent of killing is calculated for three different kinds of microorganisms. Experimental values of S_{cell} are taken from the cited literature: S_{cell}=117, 198, 25 kPa respectively for zooplankton, phytoplankton and bacteria. In order to provide a theoretical comparison (setting aside experimental configuration) the constant K is assumed equal in HC and AC, K= 2 s^{-1} (it can be varied by modifying the reactor configuration, temperature and gas content). The energy consumption is calculated for the 12 different conditions of Tables 1-2, and the three microorganism kinds, assuming 1 m^3 of solution and an extent of killing of the 95%.
The energy consumption of HC is one order of magnitude lower than in case of AC; according to the higher cell resistance, the $EC_{95\%}$ follows the ranking: bacteria > zooplankton > phytoplankton. Results are perfectly comparable with the cited pertinent literature cited in this work.
Additionally, Figure 3 shows the relation between C_v and the two most important calculated variable: ΔP (linear regression, R^2=0.937) and *EC* (exponential regression, R^2=0.977). It could be said that, operating at low cavitation number, is positive for the efficiency of the treatment. Nevertheless, by decreasing C_v, bubble population phenomena become more important and not negligible in the phenomenological modelling.

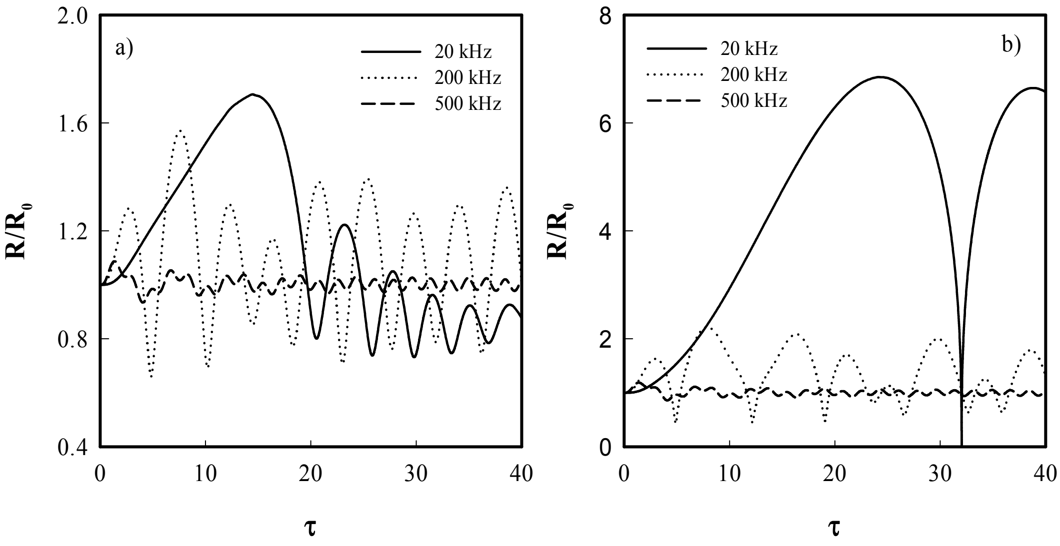

Figure 1a-b: Nondimensional bubble radius for AC in an ultrasonic bath in dependence of frequency. R_0=20μm. I= 0.2 Wcm^{-2} (a) I=1 Wcm^{-2} (b).

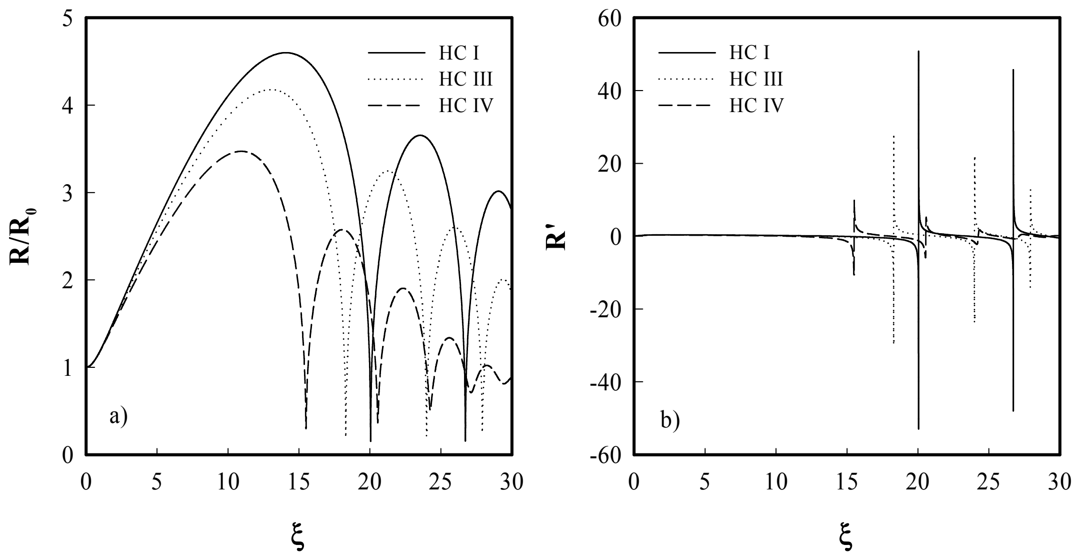

Figure 2a-b Simulation of bubble radius (a) and bubble wall velocity (b) for different HC experimental conditions (data are summarized in Table 2).

Table 1: Simulation of acoustic cavitation in microbial cell disruption

Case	*f* [kHz]	*I* [Wcm^{-2}]	*ε* [m^2s^{-3}]	*ΔP* [kNm^{-2}]	*$EC_{95\%}$* [$kWhm^{-3}$]	*$EC_{95\%}$* [$kWhm^{-3}$]	*$EC_{95\%}$* [$kWhm^{-3}$]
	frequency	*Energy intensity*	*Turbulence dissipation rate*	*Stress at R_{max}*	*Energy consumption (zooplanktons)*	*Energy consumption (phytoplanktons)*	*Energy consumption (bacteria: coliforms, streptococci)*
AC I	20	1	$3.2 \cdot 10^5$	1.85	1085.90	1132.64	1031.58
AC II	20	0.2	$3.4 \cdot 10^5$	1.78	204.93	205.83	203.83
AC III	200	1	$2.3 \cdot 10^5$	2.06	1078.83	1120.50	1030.18

AC IV	200	0.2	$4.2\cdot10^5$	1.51	220.33	231.97	206.94
AC V	500	1	$1.16\cdot10^4$	0.92	1159.08	1261.31	1045.69
AC VI	500	0.2	$8.51\cdot10^4$	0.34	289.67	364.35	219.08

Table 2: Simulation of hydrodynamic cavitation in microbial cell disruption

Case	p_{in} [bar]	v_0 [ms^{-1}]	C_v [-]	ε [m^{2}s^{-3}]	ΔP [kNm^{-2}]	$EC_{95\%}$ [kWhm^{-3}]	$EC_{95\%}$ [kWhm^{-3}]	$EC_{95\%}$ [kWhm^{-3}]
	Inlet pressure	*throat velocity*	*Cavitation number*	*Turbulence dissipation rate*	*Stress at R_{max}*	*Energy consumption (zooplanktons)*	*Energy consumption (phytoplanktons)*	*Energy consumption (bacteria, coliforms, streptococci)*
HC I	1.5	22.99	0.37	1.5·106	3.96	11.52	11.74	11.24
HC II	2	25.46	0.3	1.9·106	4.37	16.96	17.26	16.59
HC III	3	30.06	0.21	3.6·106	5.99	29.81	30.20	29.34
HC IV	4	33.16	0.18	4.6·106	6.80	43.73	44.24	43.13
HC V	5	36.3	0.15	5.8·106	7.59	59.66	60.27	58.92
HC VI	6	39.35	0.13	7.3·106	8.54	77.56	78.28	76.71

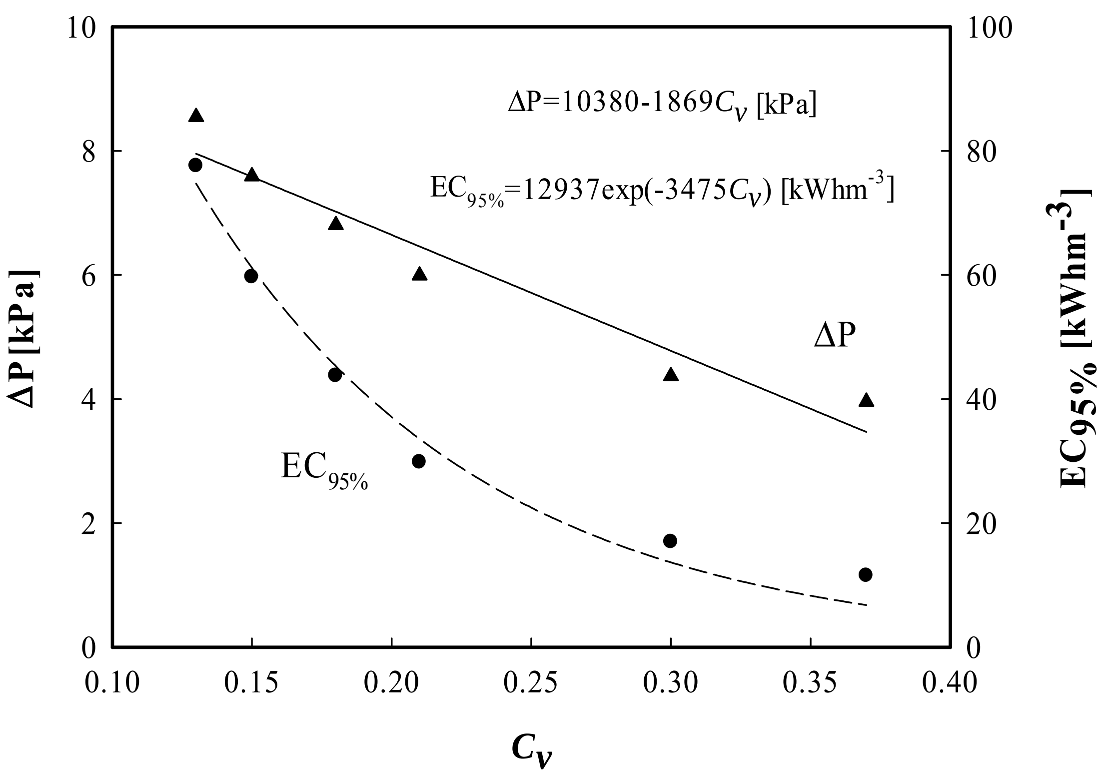

Figure 3: Stress on the cell ΔP and energy consumption EC versus C_v with regression curves (zooplankton, extent of killing 95%).

4. Conclusions

Simulation of single bubble dynamics has been used for quantifying the cavitationally generated turbulent shear and the extent of microbial disinfection. The calculated shear stress has been implemented in the estimation of disinfection efficacy for different cavitation reactors and micro-organisms (*zooplankton*, *phytoplankton* and *bacteria).* The effect of parameters is estimated for process optimization and the results are compared with the pertinent literature in order to validate the model. The simulations suggest to operate at higher p_{in} for HC and low *f* for AC: the lowest $EC_{95\%}$ has been found for the Venturi reactor operating at 1.5 bar and C_v = 0.37. From the energy efficiency point of view, HC is proved to be of almost an order of magnitude more energy efficient than AC, as extensively remarked in literature. A correlation between C_v and calculated variables has been proposed. Simulations can be extended to different experimental configurations; further model developments should take into account bubble population nucleation and interactions.

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