

## EFFECT OF DIFFERENT CHEMICAL MECHANISMS IN SONOCHEMICAL MODELLING

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#### ABSTRACT

Quantitative modelling of chemical processes inside an acoustically driven gas bubble has been a keen interest in sonochemistry. Presumably the most difficult task of chemical modelling is that the rate of every single chemical reaction has to be calculated precisely. The complications originate from the fact that the reaction rates depend exponentially on the temperature. It follows that correct validation of the model parameters is essential in reaction kinetics.

In the present paper, a precisely validated, up-todate chemical mechanism is introduced for a single sonochemical bubble with initial content of pure oxygen and water vapour. The model properly includes specified third-body coefficients, pressuredependency, reaction duplication, and it works with up-to-date, validated Arrhenius-constants.

The chemical yield is compared to three other, widely applied chemical mechanisms in the literature. The results point out that apart from some moderately good agreement in some cases, the chemical yield can vary between several orders of magnitude amongst the various mechanisms in a wide parameter range. Additionally, qualitative validation is performed with  $H_2O_2$  measurements from the literature, as well.

As a consequence, we can certainly state that applying an up-to-date chemical mechanism is mandatory in order to make quantitatively correct conclusions about chemical activity.

Keywords: bubble dynamics, chemical modeling, chemical reactions, reaction mechanisms, sonochemistry

#### NOMENCLATURE

$\dot{Q}_{th}$	[W]	heat flux
ΣŻ	[W]	total heat
Α	$[m^2]$	bubble surface
$A_i$	[1]	pre-exponential factor of reac-
		tion <i>i</i>

$C_{v}$	[J/molK]	specific heat on constant
	2	volume
$E_i$	$[mol/cm^3s]$	activation energy of reaction <i>i</i>
Ι	[1]	number of chemical reactions
Κ	[1]	number of chemical species
М	$[mol/cm^3]$	total concentration
$P_{\infty}$	[bar]	ambient pressure
R	$[\mu m]$	bubble radius
$R_g$	[J/kgK]	universal gas constant
T	[K]	internal temperature
$T_{\infty}$	[K]	ambient temperature
V	$[m^3]$	bubble volume
$b_i$	[1]	temperature exponent of reac-
		tion <i>i</i>
$c_k$	$[mol/cm^3]$	concentration of species $k$
$c_L$	[m/s]	sound speed in liquid
f	[kHz]	ultrasound frequency
$k_f, k_b$	[1]	forward/backward reaction
$l_{th}$	[ <i>m</i> ]	rate constant thermal boundary layer thick-
n.	[mol]	ness total amount of substance
p	[bar]	internal pressure
r DA	[bar]	pressure amplitude
РА <i>(</i> ):	$[mol/cm^3s]$	net rate of reaction <i>i</i>
qi t	[s]	time
Ωι:	[1]	third-body efficiencies
$\alpha_{kl}$	$[m^2/s]$	thermal diffusivity
	[1]	chemical symbol of species $k$
	[1]	production rate
ر ک	[W/mK]	heat flux coefficient
	[Pas]	liquid dynamic viscosity
r L V	[1]	stochiometric coefficient
, 0,	$[k_0/m^3]$	liquid density
РL CT	[N/m]	surface tension
$\tau$	[1]	dimensionless time
•	L+J	

#### Subscripts and Superscripts

	_	_
L	liquid	
$\infty$	far-field	d value

*f*, *b* forward, backward

*i* reaction index

*k* component index

#### **1. INTRODUCTION**

In a liquid domain, excited by high intensity and high frequency ultrasound, the dissolved gas content forms bubble clusters that consist of millions of micron-sized bubbles [1, 2]. If the pressure amplitude exceeds Blake's critical threshold [3], the bubbles can grow even 100 times their equilibrium size in the negative pressure phase. This is followed by a rapid compression in the positive pressure phase due to the high inertia of the liquid (inertial cavitation). During the strong collapse, the peak pressure and temperature can reach up to hundreds of bar and thousand of Kelvins, respectively [4]. With these conditions, the bubbles act as tiny chemical reactors, as the gas components dissociate and several different molecules are created. The new species are later applied in various areas of engineering, i.e. polymer synthesis [5], producing nanoparticles [6], or degradation of wastewater [7, 8].

Quantitative modeling of chemical reactions inside oscillating bubbles has been studied continuously since the mid-1990s [9, 10, 11]. However, some major difficulties have emerged during the years. Presumably, the reason of the biggest challenge in sonochemical modelling is that the rates of most chemical reactions have *exponential* dependence on the temperature. This fact results in an extreme sensitivity on the model parameters and demands a precise and up-to-date validation process (e.g. for the Arrhenius constants). Most of the applied chemical mechanisms in the sonochemical literature tend to lack an advanced validation method, and the applied model parameters are often outdated.

Besides using up-to-date parameters in the reaction mechanism, there are other modelling issues which are usually neglected during the computation of a chemically active bubble. For example, the socalled three-body reactions are occasionally taken into account, but *enhanced* third-body efficiencies for specific molecules are rarely specified. In addition, pressure-dependence of reaction rates is seldom included in the mechanisms, although it can change the chemical rates significantly due to the high compression ratio inside a bubble. Finally, the rate constants of some specific reactions can have a more complex dependence on the temperature than exponential; this also needs a special care.

In the present study, *a precisely validated, up-to-date chemical mechanism* for a single, chemically active bubble is introduced [12], which takes into account all the mentioned modelling issues. It is compared numerically to 3 widely applied chemical mechanisms in the sonochemistry literature at various driving parameter (ultrasound amplitude and frequency) values.

#### 2. MATHEMATICAL MODEL

The mathematical model of a chemically active bubble is divided into two main parts: physical and chemical. The physical part of the model describes the temporal evolution of the bubble radius, temperature and pressure, while the chemical part focuses on the chemical processes and the rates of the chemical reactions. By this separation, the difference between the chemical mechanisms can be examined precisely, since the physical part of the model is kept the same during the simulations.

It is important to mention that in this article, most parameter values are not given, only the governing equations are presented. The interested reader is referred to our recent publication [13], where a detailed description can be found with all the necessary constants and model parameters.

#### 2.1. Physical model

In our model, the following assumptions are made. A single, spherically symmetric gas bubble is considered that initially contains non-condensable gas (oxygen) and water vapour. The gas content is treated as an ideal mixture of ideal gases. The concentrations of species, the pressure and the temperature are considered as spatially uniform except a thermal boundary layer, which is necessary to calculate heat fluxes with the bulk liquid. Non-equilibrium evaporation and condensation are also included.

The radial dynamics of an oscillating bubble is described by the modified Keller–Miksis equation [14] in the form of

$$\left(1 - \frac{\dot{R}}{c_L}\right) R\ddot{R} + \left(1 - \frac{\dot{R}}{3c_L}\right) \frac{3}{2} \dot{R}^2 = \left(1 + \frac{\dot{R}}{c_L} + \frac{R}{c_L} \frac{d}{dt}\right) \frac{(p_L - p_{\infty}(t))}{\rho_L}, \quad (1)$$

where R(t) is the radius of the bubble, t is the time,  $c_L$  is the sound speed in the liquid and  $\rho_L$  is the density of the liquid.  $p_L$  is the liquid pressure at the bubble wall which is related to the internal pressure (p) via the boundary condition

$$p = p_L + \frac{2\sigma}{R} + 4\mu_L \frac{\dot{R}}{R} \,. \tag{2}$$

Here,  $\sigma$  is the surface tension and  $\mu_L$  is the dynamic viscosity of the liquid. The dots stand for derivatives with respect to time. The far field pressure  $p_{\infty}$  contains the harmonic ultrasound excitation as

$$p_{\infty}(t) = P_{\infty} + p_A \sin\left(2\pi f t\right),\tag{3}$$

where  $P_{\infty}$  is the ambient pressure,  $p_A$  and f are the ultrasound pressure amplitude and frequency, respectively; these two are the driving parameters that will be investigated later.

For calculating the internal pressure p in Eq. (2), the ideal gas law is applied as

$$p = MR_gT, (4)$$

where M is the total concentration of the mixture,  $R_g$  is the universal gas constant and T is the internal temperature. It is calculated by solving the first law of thermodynamics in the time-dependent form of

$$\dot{T} = \frac{-p\dot{V} + \sum \dot{Q}}{n_t \overline{C}_v}, \qquad (5)$$

where  $V = 4R^3\pi/3$  is the volume of the bubble,  $\sum \dot{Q}$  is the sum of heat flux and reaction heats.  $n_t$ is the total amount of substance of the mixture in moles and  $\overline{C}_v$  is the average molar heat capacity of the mixture at constant volume. The heat capacities and other thermodynamic quantities are approximated with polynomials via the NASA chemical equilibrium code [15]. Again, see Ref. [13] for details.

Heat conduction between the fluid and the bubble interior is modelled with the approach used by several authors in the past [16, 17]. In a thermal boundary layer, the temperature changes linearly from the bubble mean temperature T to the ambient liquid temperature  $T_{\infty}$ , which is kept constant. In this approach, the amount of heat transfer is approximated as

$$\dot{Q}_{th} = A\overline{\lambda} \left. \frac{\partial T}{\partial r} \right|_{r=R} \approx A\overline{\lambda} \left. \frac{T_{\infty} - T}{l_{\text{th}}} \right|_{r=R}$$
(6)

where A is the area of the bubble surface,  $\overline{\lambda}$  is the averaged thermal conductivity of the mixture and  $l_{th}$  is the thickness of the thermal boundary layer calculated as

$$l_{\rm th} = \min\left(\sqrt{\frac{R\overline{\chi}}{\dot{R}}}, \frac{R}{\pi}\right),\tag{7}$$

where  $\overline{\chi}$  is the averaged thermal diffusivity of the mixture. Non-equilibrium evaporation and condensation of water are considered here as a net substance flow rate into the liquid, with the method of Fujikawa [18].

As a summary, the physical part of the model results in a set of ordinary differential equations: the Keller–Miksis equation (1) is of second order for the bubble radius R(t), and Eq. (5) is of first order for the internal temperature T(t). The internal pressure is obtained form Eq. (4) as and algebraic equation.

#### 2.2. Chemical model

The chemical part of the model focuses on calculating the rate of chemical reactions and temporal evolution of the molecule numbers of each chemical species. First, let us consider the following reversible chemical reactions involving K chemical species in the general form of

$$\sum_{k=1}^{K} v_{ki}^{f} \chi_{k} \Leftrightarrow \sum_{k=1}^{K} v_{ki}^{b} \chi_{k} \qquad (i = 1, ..., I),$$
(8)

where  $v_{ki}$  are the stoichiometric coefficients,  $\chi_k$  is the chemical symbol for the *k*th species, and *I* is the total number of reactions. The superscripts *f* and *b* indicate forward and backward directions, respectively.

The net rate of reaction  $i(q_i)$  is calculated as the difference of forward and backward rates as

$$q_{i} = k_{f_{i}} \prod_{k=1}^{K} c_{k}^{\nu_{ki}^{f}} - k_{b_{i}} \prod_{k=1}^{K} c_{k}^{\nu_{ki}^{b}}, \qquad (9)$$

where  $c_k$  is the concentration of species k,  $k_{f_i}$  and  $k_{b_i}$  are the forward and backward reaction rate constants of reaction *i*, respectively (defined later). The basic equation for calculating the forward reaction rate constants is the modified Arrhenius-equation in the form of

$$k_{f_i} = A_i T^{b_i} \exp\left(\frac{-E_i}{R_g T}\right),\tag{10}$$

where  $A_i$  is the pre-exponential factor,  $b_i$  is the temperature exponent, and  $E_i$  is the activation energy. The backward rate constants  $k_{b_i}$  are calculated via proper thermodynamic conditions, see [13] for details. With all  $q_i$  values, the production rate of each species is expressed as

$$\dot{\omega}_k = \sum_{i=1}^{l} v_{ki} q_i, \qquad (k = 1, ..., K),$$
 (11)

where  $v_{ki} = v_{ki}^b - v_{ki}^f$ .  $\dot{\omega}_k$  represents the rate of change of  $c_k$  due to chemical reactions. The complete system of ordinary differential equations is completed as

$$\dot{c}_k = \dot{\omega}_k - c_k \frac{V}{V} \,, \tag{12}$$

with the amount of water vapour being adjusted with the net evaporation rate.

In our presented model, the above described method is complemented with possible third-body efficiency and pressure-dependency of certain reactions. In the former case,  $q_i$  in Eq. (9) is modified as  $q'_i = q_i[M]$ , where [M] is the effective total concentration of the third-body species, expressed as  $[M] = \sum_{k=1}^{K} \alpha_{ki}c_k$ . Here,  $\alpha_{ki}$  is the matrix of the third-body efficiencies. Usually, most  $\alpha_{ki}$  is assumed to be 1, and only those that differ from 1 are highlighted in

A detailed explanation of reaction rates in the case of pressure-dependent reactions is omitted here. Nonetheless, in a state-of-the-art chemical mechanism, they play an essential role, especially if the pressure varies by orders of magnitude. The forward rate constant of a pressure-dependent reaction is shown at constant temperature in Figure 1. It is apparent that the reaction rate changes multiple orders of magnitude in the pressure interval that emerges during strong bubble collapses (from one to around hundreds of bars). This implies the necessity of taking into account pressure dependency. It should be noted here that depending on the model parameters, the trend of pressure-dependency can be highly different for each reaction.

[13].



Figure 1. Forward rate constant of a pressuredependent reaction  $H + O_2 (+M) \Leftrightarrow HO_2 (+M)$  as a function of pressure, at T = 2000 K.

#### **3. METHOD OF COMPARISON**

The main aim of the present study is to show the importance of appropriate chemical mechanism in sonochemical calculations. As a process, we make numerical simulations with 3 different, widely applied chemical mechanisms in sonochemistry, and compare the results with our newly introduced mechanism. All of the models have been used for bubbles containing initially only  $O_2$  and water vapour. Our mechanism will be labeled as ELTE/HDS2022, and it will be considered as the most precise one.

The three other mechanisms are labeled in this paper as KAMATH1993 [19, 20], YASUI2003 [21] and MEROUANI2014 [22]. The names and years refer to the first appearance in sonochemical simulations. These mechanisms tend to work with outdated Arrhenius coefficients, and the backward rate constants  $k_{b_i}$  are calculated by prescribed backward Arrhenius coefficients, rather then precise thermodynamic equilibrium conditions. Some third-body efficiencies are occasionally indicated, but pressuredependency is not taken into account in either model. The exact values of the applied Arrhenius coefficients can be found in the aforementioned papers; however, it can be observed that some of these constants can vary even by multiple orders of magnitudes. Conceivably, this may result in remarkably different results, see later sections.

In our work, we perform numerical simulations at different driving parameters (pressure amplitude and frequency). For each parameter combination, the *chemical yield* is defined, see Sec. 4.1. The simulations are made with all 4 different mechanisms at the whole examined parameter regime, with the physical part of the model being kept the same. The models are compared by the chemical yields of some specific chemical species.

#### 4. RESULTS

#### 4.1. Definition of chemical yield

After solving the complete system of ordinary differential equations at a given parameter combin-

ation numerically, one would get the time curves of bubble radius R(t), internal temperature T(t), and concentration profile  $c_k(t)$  for each species. The convergent part of the result is shown on Figure 2 at  $p_A = 1.6$  bar, f = 50 kHz and  $R_E = 4 \mu m$ . Note that the time axes are in dimensionless form of  $\tau = t \cdot f$ , which means that  $\tau = 1$  belongs to one excitation cycle.



Figure 2. Time curves at  $p_A = 1.6$  bar, f = 50 kHz and  $R_E = 4 \,\mu \text{m}$  with the ELTE/HDS2022 model. The bubble radius (blue) and temperature (red) curves are on the top chart, the amount of substance of each species are on the bottom chart (on logarithmic scale).

Chemical yield is the numerical metric that quantifies the chemical activity of the bubble. In our work, it is defined for each chemical species as the amount of substance at the maximum bubble radius. In Fig. 2, the vertical dashed lines represent the maximum radius, and the chemical yields for some components are marked with arrows. During further evaluation, the chemical yields of hydrogenperoxide ( $H_2O_2$ ) and OH radical will be compared as two of the important molecules in sonochemical applications [23, 24].

#### 4.2. Difference among the chemical mechanisms

Our strategy to compare the examined mechanisms is to perform the numerical simulations at different driving parameters with the four model, and examine the chemical yields. In Figure 3, the yields of H<sub>2</sub>O<sub>2</sub> are show as a function of pressure amplitude (between 1 and 2 bars) at  $R_E = 4 \mu m$  at four different driving frequencies with the 4 models. The vertical axes are on logarithmic scales.

It is apparent from the charts that large variance emerges between all four models, in almost all the amplitude domain. For example, the yield



Figure 3. The chemical yield of  $H_2O_2$  as a function of pressure amplitude at  $R_E = 4 \,\mu\text{m}$  at four different driving frequencies with the 4 models.

of  $H_2O_2$  with KAMATH1993 is the largest, by more then one order of magnitude then the others. Especially at lower frequencies, there is an immense amount of difference between the results. Considering ELTE/HDS2022 as the best chemical mechanism, MEROUANI2014 (red lines) shows the closest yield values, but the numerical values can differ by a factor of 3-5. The model of YASUI2003 behaves even qualitatively differently than the other three; it shows a visible peak of  $H_2O_2$  yield at lower pressure amplitude values for all driving frequencies, followed by a steep decrease as  $p_A$  increases (except for f = 200 kHz). This can lead to the identification of false optimal operating conditions.

Similar conclusions can be taken in the case of OH radical, see Figure 4. Here, the chemical yield of OH is plotted at the same parameter domain as of  $H_2O_2$ . It can be observed that even the trends with YASUI2003 and KAMATH1993 are rather different from the others, especially on lower frequencies. MEROUANI2014 is at least qualitatively similar to ELTE/HDS2022, but the 3 to 5 times differences are appear here, as well.

As a consequence, it is clear that the calculated chemical yields usually differ by several orders of magnitudes; thus, the *proper modelling of the chemical reactions is mandatory* for drawing meaningful conclusions.

# 4.3. Qualitative validation of the chemical mechanism

Due to the complex behaviour of chemical reactions, the validation of different chemical mechanisms are possibly the most difficult task in the topic. As a qualitative validation, we compare the results to the measurements of Brotchie et al. [25], where they



Figure 4. The chemical yield of OH as a function of pressure amplitude at  $R_E = 4 \,\mu\text{m}$  at four different driving frequencies with the 4 models.

measured the chemical output of  $H_2O_2$  as a function of driving frequency. Their results showed that there exist an optimal driving frequency (regarding  $H_2O_2$ outcome) at around  $f \approx 200 - 300$  kHz.

We performed numerical simulations at constant  $R_E = 8 \,\mu\text{m}$  and  $p_A = 2 \,\text{bar}$ , on various driving frequencies between 20 and 350 kHz with all four examined mechanisms. The chemical yields of H<sub>2</sub>O<sub>2</sub> are show on Figure 5, with logarithmic yield axis. The maximum yield values are marked with circles for each mechanism. It can be observed that only ELTE/HDS2022 model predicts the maximum yield correctly over the domain of [25]. The other three ones underestimate the optimal frequency by even 100 - 200 kHz. This result also confirms our presupposition that our up-to-date chemical mechanism is the most precise one – at least regarding H<sub>2</sub>O<sub>2</sub> outcome.

#### 5. SUMMARY

The present paper focuses on the chemical modelling of an ultrasound driven gas bubble. An up-todate chemical mechanism is presented for a bubble initially containing only oxygen and water vapour. The model includes accurately validated Arrheniuscoefficients and third-body efficiency factors, takes into account pressure-dependent reactions, and calculates the backward rate constants from accurate equilibrium equations.

The mechanism is compared to three other chemical models that are widely used in sonochemistry with the physical part of the models kept the same. The analysis is made via a well-defined chemical yield. The results showed that there are orders of magnitude differences between the yields of  $H_2O_2$  and OH as calculated from the various chem-



Figure 5. The chemical yield of  $H_2O_2$  as a function of frequency at  $R_E = 8 \mu m$  and  $p_A = 2$  bar with the 4 models. The maximum yield values are marked with circles for each mechanism.

ical models in a wide parameter range. In addition, the trends of the yield as a function of control parameters can have different characteristics; thus, one can identify false optimal operating conditions.

Additionally, the models were compared to the  $H_2O_2$  measurements of Brothcie et al. [25]. It turned out that only ELTE/HDS2022 mechanism estimates the optimal driving frequency range properly.

The presented results imply that in order to make qualitatively and quantitatively correct conclusions about the chemical activity, *it is essential to employ a state-of-the-art, properly validated chemical mechanism* for a given sonochemical task.

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