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FORMATION OF EXCITED MOLECULES FROM FRAGMENTS FORMED IN HETEROGENEOUS-HOMOGENEOUS PROCESSES IN THE NEAR-SURFACE LAYER AND THEIR IMPACT ON OXIDATION PROCESSES

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Abstract. This study focuses on the formation of excited molecules and their significant role in influencing dynamic regimes of low-temperature oxidation, particularly in the context of methane and acetaldehyde reactions. The investigation reveals how quantum resonance facilitates the formation of excited formaldehyde molecules, driving energy transfer processes that influence radical chain reactions and inhibit oxidation. These processes lead to the formation of weak shock waves, which emerge due to the interaction of water complexes with negative halogen ions and the self-decomposition of ozone. Using theoretical modeling, computer simulations, and spectroscopy, the study uncovers the role of quantum resonance in generating weak shock waves and establishing oscillatory regimes. These findings contribute to a deeper understanding of the mechanisms of low-temperature oxidation and the complex interactions of excited molecules, offering new applications in both scientific research and industry.

Keywords: shock waves; Hugoniot theory; resonance; relaxation; ion-molecular reactions.

1. Introduction

Processes occurring on material surfaces play a key role in shaping their properties and behaviour in various environments. One important aspect of such processes is the formation of excited molecules, which can arise from fragments ejected into the volume as a result of surface reactions. Excited molecules possess unique chemical and physical properties that can significantly influence subsequent reactions, including oxidation processes. The formation of excited molecules from fragments formed in surface processes, ejected into the volume, can significantly affect oxidation processes in several ways. Excited molecules in a higher energy state can more readily participate in oxidation reactions. The presence of unpaired electrons or higher energy in the excited state helps to overcome reaction barriers, facilitating oxidation reactions that may be kinetically hindered in the ground state, as Garrod *et al.*[1] noted in their study.

For instance, Klessinger and Pötter[2] highlighted that excited oxygen molecules (O_2) are more reactive towards organic compounds, leading to an increased oxidation rate. Besides, as Crim[3] noted, photochemically excited molecules can initiate oxidation reactions that otherwise proceed slowly or require higher temperatures. Westermayr and Marquetand[4] discuss that excited molecules can more easily undergo dissociation or ionization, generating active radicals or ions that can initiate or propagate chain oxidation reactions. For example, excited hydrocarbon fragments formed as a result of surface processes can dissociate to form reactive radicals, such as OH, which can oxidise other molecules. Furthermore, excited electronic states often have different potential energy surfaces, opening new oxidation pathways that are inaccessible from the ground state. This leads to the formation of oxidised products that are difficult to obtain through thermal oxidation alone. The new energetic landscape of excited states allows for reactions that do not occur in the ground state, expanding the range of possible oxidation products.

The study by Chen *et al.*[5] emphasises that the excess energy of excited molecules can be transferred to other particles through collisions, providing the activation energy required for oxidation reactions. This non-thermal excitation mechanism stimulates oxidation processes even at

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low bulk temperatures, increasing the overall reaction rate and efficiency. For example, ozone (O_3) containing excited oxygen atoms is used as an additive to examine the low-temperature oxidation of ethanol in the Liao *et al.*[6] study. Excited molecules can influence the formation of both gaseous and solid oxidation products.[7] In the case of Wang *et al.*,[8] coal oxidation involves the formation of oxygen-containing complexes on its surface and the release of gases such as CO and CO_2. However, the extent of these effects depends on the lifetime of the excited states, the concentration of excited particles, and their reactivity compared to ground-state oxidation pathways. Excited states are typically short-lived, and molecules must dissipate their excess energy through various pathways such as fluorescence, phosphorescence, or non-radiative decay, Rathnachalam[9] noted. Short-lived excited states may relax before participating in oxidation, whereas long-lived states can significantly impact the kinetics and mechanisms of oxidation.[10] For example, in the papers by Liu *et al.*[11] and Ibele *et al.*,[12] if excited states have a sufficiently long lifetime, they can markedly alter reaction dynamics, affecting the rates of formation and decay of intermediate products as well as the overall yield of final products. This is because they have higher energy content and potentially more favourable electronic configurations for certain types of reactions. Thus, examining excited molecules and their interactions in reaction systems is a crucial aspect for understanding and optimizing oxidation processes.

Despite considerable advancements in the analysis of low-temperature oxidation and the role of excited molecules, questions remain that require further investigation. One such issue is the detailed understanding of quantum resonance mechanisms. Although substantial research exists, the mechanisms of quantum resonance and recharging, particularly in low-temperature oxidation, remain inadequately explored. More data is needed on the specific conditions under which these processes are most effective. Understanding how excited states affect the kinetics and mechanisms of reactions under real conditions is important. Additional studies on the lifetime of excited states and their impact on long-term oxidation processes will help determine how the duration of these states influences overall reaction kinetics. Another critical aspect, the interaction of excited molecules with various radicals, especially in the presence of different catalysts, requires a deeper understanding. Conducting these studies will provide a deeper understanding of the fundamental mechanisms underlying oxidation processes and help develop new methods for their optimization on an industrial scale. The purpose of the study is to explore the possibility of the occurrence of weak shock waves during low-temperature oxidation.

2. Materials and Methods

In this study, various methods are applied to investigate the formation of excited molecules from fragments formed in surface processes, ejected into the bulk, and their impact on oxidation processes.

The Hugoniot theory was used to describe oxidation reactions and the formation of ozone molecules from intermediate products such as hydrogen peroxide (H_2O_2). This approach considers transitional processes and quantum effects, such as quantum resonance, which facilitates recharging and the formation of excited molecules. The study involves theoretical modelling of processes involving complexes of water molecules with negative chlorine ions anchored on the reactor surface. This allowed for the prediction of the likelihood of ozone molecule formation and the calculation of possible resonance transitions. For a detailed analysis of the mechanisms of formation and reactions, software packages such as Gaussian G09W and GaussianView 05 were used. These programmes enabled quantum-chemical calculations, including calculations of energy barriers, reaction probabilities, and energy diagrams of state transitions. Particular attention is paid to examining surface processes and the interaction of complexes at the phase boundary, which includes analyzing the adsorption and desorption of molecules on the surface, their impact on reaction kinetics, and the formation of active sites. Based on the data obtained, kinetic models describing the dynamics of oxidation processes in the presence of excited molecules were developed.

Kinetic models were developed in detail to describe the formation of excited formaldehyde (CH_2O) molecules, which consider resonant processes affecting the rate and efficiency of radical destruction. Initially, a surface model where adsorption processes occur was created. Computational methods were used to determine stable geometric configurations and the energetic characteristics of molecules adsorbed on the surface. Next, the energy barriers and thermal effects of radical adsorption on the surface were calculated. The mechanisms of molecule activation during their adsorption on the surface were determined, which is a crucial step in the process of forming excited molecules. Subsequently, the interactions between CH_3CO_3 radicals and adsorbed OH molecules were calculated. Pathways for the formation of excited CH molecules as a result of these interactions were identified. Computer modelling revealed the most probable mechanisms and conditions under which these processes occur. The decomposition of CH_3CO_3 radicals upon interaction with excited CH_2O molecules was then modeled. The impact of resonance processes on the rate and efficiency of radical decomposition was determined. This allowed for an understanding of how resonance energy transfer between particles can accelerate certain elementary acts and inhibit reactions by breaking the leading radical chains.

The models considered reaction probabilities, the rates of formation and decomposition of intermediate products, and the influence of thermal and non-thermal activation mechanisms. Both classical and quantum effects were accounted for in the calculations, providing an accurate description of the processes at the molecular level. For more precise evaluation, Monte Carlo and molecular dynamics methods were used, enabling the simulation of particle behaviour at the atomic level and considering the influence of various factors. To calculate the energy exchange between the particles of interest, an expression was used to compute the probability of photon emission or absorption by excited particles per unit time in a given solid angle[3]. The calculations detailed the influence of quantum resonance on recharging and the formation of excited molecules.

These methods and approaches collectively facilitated a comprehensive analysis of the processes related to the formation of excited molecules and their influence on oxidation reactions, which is a substantial step towards further understanding and optimizing industrial chemical processes.

3. Results and Discussion

The study investigated two main aspects: the formation of excited molecules from surface reactions and their role in the generation of weak shock waves, as well as the influence of these phenomena on reactor dynamics. The study explored the formation of slow shock waves in the reactor as a result of surface reactions, confirming the potential for generating such waves under feedback conditions. In the reactor's near-surface layer, the formation of excited formaldehyde molecules from the leading chain of CH_3CO_3 radicals was observed. By transferring energy, these molecules activated CH_3CO_3's decomposition, leading to the establishment of an oscillatory reaction regime within the system.

In the first instance, the study was based on the concept of a chain of elementary reactions involving complexes of water molecules with negative chlorine ions, fixed on the reactor's surface. These complexes interacted with intermediate products of the oxidation reactions of organic compounds, such as H_2O_2, as illustrated in examples (Eq. 1-5). The essence of this process lies in quantum resonance, which results in the conversion of H_2O_2 molecules into ozone molecules. This mechanism is based on the ability of water molecules and chlorine ion complexes on the reactor surface to create specific conditions that facilitate energy exchange between molecules and activate reactions. Consequently, a quantum resonance phenomenon occurs, accelerating the transition from H_2O_2 to ozone, thereby initiating processes that lead to the generation of slow shock waves in the reactor.

$$\mathrm{H_2O * Cl^- + H_2O_2 \rightarrow H_2O * Cl + H_2O * O^-}, \quad (1)$$

$$\mathrm{H_2O * O^- + O_2 \rightarrow H_2O + O_3^-}, \quad (2)$$

$$\mathrm{O_3^- + H_2O * Cl \rightarrow O_3 + H_2O * Cl^-}, \quad (3)$$

$$\mathrm{O_3 + M \rightarrow reaction\ channel}, \quad (4)$$

$$\mathrm{O_3 \rightarrow O + O_2}. \quad (5)$$

The reaction scheme illustrates the process leading to the onset of sharp pulsations in the reaction system during the initial stages of low-temperature oxidation of organic compounds. In the first stage, complexes of H_2O*Cl^- and H_2O_2 interact, creating a quantum resonance that facilitates the conversion of H_2O_2 into ozone molecules, denoted as H_2O*O^-. This process is accompanied by the release of a significant amount of energy, particularly in a narrow layer near the region of active reaction centres. In the third stage, quantum resonance occurs in the reaction between molecules O_3^- and H_2O*Cl, resulting in the formation of ozone (O_3) and the regeneration of H_2O*Cl^-. The self-decomposition of ozone molecules at high temperatures (600-700K) occurs very rapidly, within the range of 10^{-2} to 10^{-3} seconds, leading to a substantial release of energy in a narrow zone near the active reaction centres. Thus, the presence of quantum resonance in these elementary steps (the first and third) plays a crucial role in the dynamics of the reaction system, promoting the emergence of sharp pulsations and oscillations during the low-temperature oxidation of organic compounds.

Charge transfer from a negative ion to another particle is possible only if its electron affinity is higher than that of the neutral particle involved in the collision. In this context, the electron affinity of a chlorine atom (3.62 eV) exceeds that of a hydrogen peroxide molecule (3.02 eV), making such a process impossible at low collision energies. However, water can dissociate the negative chlorine ion and excite an additional electron to a level up to 0.6 eV, sufficient to induce resonance with the H_2O_2 molecule. This phenomenon plays a significant role in the reaction mechanisms under consideration. The self-decomposition of ozone, an exothermic process, leads to the formation of weak shock waves.[13] This study also examined the weak shock wave formation during the oxidation of methane.

Under certain conditions, such as the presence of a catalyst or at high temperature and pressure, the oxidation process is accompanied by the formation of shock waves. Shock waves arise due to the rapid release of energy in the form of heat and gases, leading to a sharp change in the pressure and density of the medium. During methane oxidation, intermediate high-energy radicals and molecules are formed, which enter into further reactions, releasing a significant amount of energy. Using the system parameters

$CH_4+O_2 \rightarrow$reaction products and applying the formulas of Hugoniot theory, as presented by Baker for ideal gases, the process can be described by Eqs. (6-7):

$$T = V - V^2, \quad (6)$$

$$T = 0.158(V-1)^2 + 0.37\beta, \quad (7)$$

where T is the temperature in dimensionless units; V is the volume in dimensionless units; β is the flux constant, which, at V=1, equals the energy flux.

For ideal gas mixtures, $CH_4+O_2 \rightarrow$reaction products β0=0.577 and β=0.43 are related through the equations of state. Based on the analysis presented in Fig. 1, weak shock waves will be generated in the system. This is confirmed by the intersection of the Hugoniot adiabat curves.

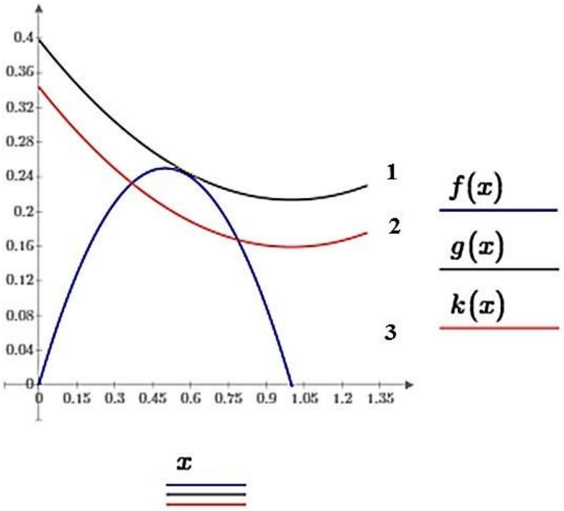

Fig. 1. The placement of the Hugoniot adiabats on the temperature-volume phase plane:

$$f(x) = x - x2, \quad (8)$$

$$g(x) = 0.185(x-1)2 + 0.577 * 0.37, \quad (9)$$

$$k(x) = 0.155(x-1)2 + 0.43 * 0.37. \quad (10)$$

Note: x denotes the dimensionless volume V, β_0 and curve 3 characterises the infinitely weak shock wave in the system.
Source: compiled by the authors.

Under β=0.43 in the methane oxidation system, the formation of ozone molecules in quantities of about 10^{18} per cm^3 near the "water molecule + negative chlorine ion" complex will lead to the appearance of a weak shock wave. Under conditions of quantum resonance, processes may occur where transitions between quantum states of methane and oxygen are associated with minimal energy losses, potentially causing a sudden change in the energy state of the system.[14] During the reaction, electrons are redistributed between methane and oxygen molecules, which can lead to an instantaneous release of energy capable of creating a shock wave. Shock waves arise from a sharp increase in pressure and temperature in the reaction zone.[15] Under quantum resonance and charge transfer, an instantaneous jump in the system's energy state may occur, leading to the formation of weak shock waves. These waves propagate through the medium, causing local changes in pressure and density. A weak shock wave can repeatedly reflect off the reactor walls without significant energy loss, allowing it to be recorded over an extended period.

In chemical reaction systems, energy exchange between particles plays a crucial role in establishing oscillatory dynamic regimes.[16] In such systems, excited particles, possessing significant internal energy, can substantially accelerate the elementary steps of chain processes and break weakly bonded particles by transferring energy to them. This process is particularly important under conditions of quantum resonance. The low-temperature oxidation of acetaldehyde, an intermediate product in the oxidation of many organic compounds, can serve as an illustration of energy exchange processes and their influence on the dynamic regimes of the reaction system.

Under conditions of quantum resonance, transitions between the energy levels of particles occur with minimal energy loss, facilitating the efficient transfer of energy between excited particles and surrounding molecules. Excited particles transfer their energy to other molecules, causing their dissociation or ionization. This process is particularly important in chain reactions, where such energy transfers can initiate or accelerate subsequent reactions. High-energy particles cause fluctuations in the concentrations of reactants and products, leading to unstable and oscillatory regimes.[17] These regimes are characteristic of many chain reactions, where energy is transferred along a sequence of reactions at varying rates.

In the low-temperature oxidation of acetaldehyde, the following key stages and processes are observed, represented by reaction Eqs. (11-14):

1. Initiation:

$$CH_3CHO + O_2 \rightarrow CH_3CO^{\bullet} + HO_2^{\bullet} \quad (11)$$

2. Propagation:

$$CH_3CO^{\bullet} + O_2 \rightarrow CH_3CO_3^{\bullet}, \quad (12)$$

$$CH_3CO_3^{\bullet} + CH_3CHO \rightarrow CH_3CO_3H + CH_3CO^{\bullet}. \quad (13)$$

3. Termination:

$$CH_3CO_3^{\bullet} + RH \rightarrow CH_3CO_3H + R^{\bullet}. \quad (14)$$

The termination of chain reactions with the formation of stable molecules. Oscillatory regimes in reaction systems, such as the low-temperature oxidation of acetaldehyde, arise due to the complex interactions between radicals and molecules within the system. Excited particles and quantum resonance lead to the rapid release of energy, creating conditions for oscillatory regimes. For instance, periodic oscillations in concentrations arise from cyclic changes in the rates of radical formation and destruction. Autocatalytic oscillations are caused by positive feedback in chain reactions, where the product of one stage accelerates the next. Thermal oscillations can occur due to the uneven distribution of heat within the reaction mixture, affecting the rate of chemical reactions. Energy exchange between particles in reaction mixtures through processes of quantum resonance and charge transfer plays a crucial role in establishing oscillatory dynamic regimes in chain reactions. The example of low-temperature oxidation of acetaldehyde shows that such processes can lead to complex and unstable dynamic regimes, influencing the concentrations of reactants and products and the distribution of energy within the system.

Resonant energy transfer between molecules is a crucial mechanism influencing the dynamics of reactions.[18] Two key factors contribute to this transfer: the redistribution of internal energy among different states of the molecules and the conversion of kinetic collision energy into internal molecular energy. Internal molecular energy encompasses several forms of energy, including electronic energy (associated with the electrons within the molecule), vibrational energy (the energy of atomic vibrations within the molecule), and rotational energy (the energy of molecular rotation). The mechanisms for redistributing internal energy include electronic transitions, vibrational transitions, and rotational transitions.[19] Excited electrons can move between energy levels, altering the molecule's energetic state. Molecules can transition between different vibrational levels, which changes their internal energy. Changes in rotational states can also contribute to energy redistribution. Kinetic collision energy can be converted into the internal energy of molecules. This occurs when the energy from collisions is transferred to excite the vibrational or rotational states of molecules. Energy transfer mechanisms during collisions include inelastic collisions and resonant collisions.[20] Inelastic collisions allow molecules to exchange energy, leading to changes in their internal energy. These collisions often result in the excitation of molecules, increasing their internal energy. In resonant collisions, energy is transferred particularly efficiently if the energy levels of the molecules are in resonance, meaning the energy required for a transition from one level to another in one molecule matches the energy transition in another molecule.

For resonant energy transfer to occur, the energy levels of the two interacting molecules must coincide or be close in energy. This condition allows energy to be transferred with minimal loss. The frequency and nature of molecular collisions also influence the likelihood of resonant energy transfer. Higher temperatures and pressures increase the frequency of collisions, which enhances the probability of resonant interactions. The occurrence of oscillatory phenomena due to quantum resonance during acetaldehyde oxidation is explained by the significant role of resonant energy transfer processes in chemical kinetics, which greatly affect reaction dynamics. In the CO_2 (667.3 cm^{-1}) and C_2H_4O (704 cm^{-1}) mixture, there is an intense vibrational-vibrational energy exchange, despite the resonance defect $\Delta v=36.7$ cm^{-1}. Energy exchange between CH_4 and CO also occurs almost resonantly, with a resonance defect of 617 cm^{-1}. To calculate the probability of photon emission or absorption by excited particles, expression (Eq. 15) is used:

$$dP_{f\ell}^{(+)} = \frac{\omega^3(n_{Qa}+1)\left|\vec{e}_a\vec{d}_{f\ell}\right|^2 d\Omega}{2\pi c^3\hbar}, \tag{15}$$

where $\vec{e}_a$ is the vector perpendicular to the direction of light propagation Q; n_{Qa} is the photon density; $\vec{d}_{f\ell}$ is the matrix element of the transition dipole moment from state f to state ℓ.

After integrating (Eq. 15), the simplified expression (Eq. 16) is obtained:

$$P_{f\ell} = \frac{2\omega^3}{3c^3\hbar}|d_{f\ell}|^2. \tag{16}$$

For spontaneous emission from a CO dipole with a friction coefficient $\omega=3.31*10^{14}$ c^{-1} and a dipole moment of 2.2 D, the probability of spontaneous emission of a single quantum is $P_{f\ell}=4127103$ c^{-1}. The absorption time (the inverse of the probability) is $\tau_{abs}=2423*10^{-4}$ s. Energy transfer between scattering particles under exact resonance can be described by Eq. (17):

$$P_{0-1}^{1-0} = \frac{1}{3^2}(V_{0.1})_1^2(V_{0.1})_2^2\frac{8\mu\ell^2}{\hbar^2}e^{\frac{\varepsilon}{kT}}, \tag{17}$$

where $\left(V_{0,1}\right)_1^2(V_{0.1})_2^2$ are the matrix elements of the interaction potential during the transition; ℓ is the characteristic range of the interaction potential; μ is the reduced mass; ħ is the Planck constant; ε is the depth of the potential well.

With values of $\ell=0.18$ Å; $kT=8.28*10^{-14}$ erg (corresponding to a temperature of 600 K) and $\varepsilon=8.056*10^3$ for dipole-dipole interaction at a distance of r=2.35 A°, the probability of vibrational-vibrational energy exchange during a collision between excited formaldehyde and CH_3CO_3 radicals is significant. This means that energy exchange occurs with each collision. In experiments on energy exchange between CO_2 and N_2 molecules during V-V exchange, energy is transferred almost with every collision. Thus, the presence of resonant energy transfer processes increases the likelihood of oscillatory phenomena in reaction systems. During acetaldehyde oxidation, excited formaldehyde molecules can transfer their energy to CH_3CO_3 radicals, leading to their destruction and reaction inhibition. The presence of feedback causes oscillatory behaviour, confirming the complexity and multifaceted nature of the processes involved.

The redistribution of molecular excitation energy and the conversion of collision kinetic energy into the internal energy of molecules are key factors facilitating the resonant transfer of energy between molecules. For instance, during the low-temperature oxidation of acetaldehyde, intermediate radicals efficiently transfer energy to each other through resonant collisions, accelerating chain reactions. In reactions where free radicals are formed, resonant energy transfer can significantly expedite the process by enabling effective energy exchange between radicals and molecules. These processes play a crucial role in the dynamics of chemical reactions, particularly in chain reactions, where effective energy transfer can markedly accelerate the reaction and influence its course. Based on the aforementioned**,** the mechanism of excited formaldehyde CH_2 molecule formation in the near-surface layer and its impact on the resonant breakdown of CH_3CO_3 radicals was investigated. It was found that acetaldehyde molecules and hydroxyl radicals adsorb onto the surface, forming intermediate products. Acetaldehyde then interacts with OH radicals, leading to the formation of intermediate CH_3CO_3 radicals and excited formaldehyde CH_2O molecules. Collisions between CH_3CO_3 radicals and OH radicals on the surface result in the loss of a hydrogen atom, which facilitates the formation of excited CH_2O molecules. These excited CH_2O molecules then interact with CH_3CO_3 radicals, leading to their resonant breakdown. These processes create a standing wave field in the reactor, which influences the dynamics and efficiency of oxidation processes (Fig. 2).

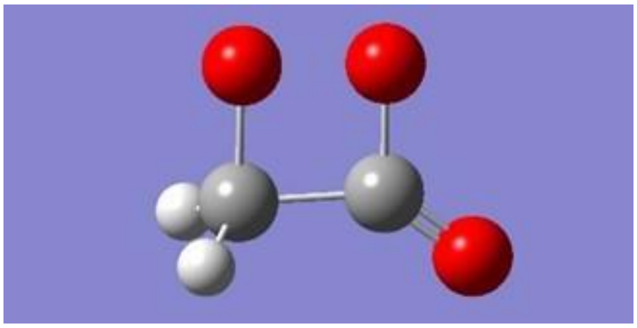

Fig. 2. Results of the collision of the terminal oxygen atom with a carbon atom, leading to self-dissociation {CH_2CO} within a time of τ=6.13/10^{-13} s

Note: material was created using Gaussian 09W and GaussView 5.0 software, employing the Energy and Optimization Minimization procedures within the Hartree-Fock method and the 3-21G basis set. The vibrational frequencies were calculated using the DFT method and the 6-31G basis set.
Source: compiled by the authors.

Formaldehyde molecules can inhibit the oxidation of acetaldehyde by affecting CH_3CO_3 radicals, which play a key role in chain reactions. Early studies suggested that formaldehyde inhibits this reaction, and this mechanism has been regarded as quite accurate. The role of formaldehyde excitation energy, which can act as an external factor, was analysed, and feedback mechanisms causing oscillatory behaviour in the reaction dynamics were discovered. Studies have shown that, in addition to standard reaction inhibition pathways, there exists a mechanism for resonant energy transfer from excited formaldehyde CH_2O molecules to CH_3CO_3 radicals. This mechanism involves the transfer of both electronic and vibrational energy, which accelerates the breakdown of radicals and inhibits the oxidation reaction.

Acetaldehyde is often an intermediate product in the oxidation of organic compounds. The calculated emission frequencies of formaldehyde and acetaldehyde molecules are 1861.2 cm^{-1} and 1827.7 cm^{-1}, respectively. The small difference of 33.5 cm^{-1} between these values indicates an almost resonant energy exchange between particles. Formaldehyde molecules are formed in an electronically and vibrationally excited state, and upon the relaxation of electronic energy according to the Franck-Condon principle, high vibrational states arise. These states transfer energy to chain- carrying radicals during collisions, making the inhibition process prolonged, as the vibrational stabilisation of CO molecules takes about 1 second at a pressure of one atmosphere. It follows that there are two mechanisms for the breakdown of CH_3CO_3 radicals:

1. Resonant electronic energy transfer, leading to the immediate breakdown of CH_3CO_3 radicals.

2. Stepwise transfer of vibrational energy, which prevents the restoration of the steady-state concentration of CH_3CO_3 radicals for an extended period. At a concentration of excited formaldehyde particles on the order of 10^{14} particles/cm^3, the number of collisions of a single CH_3CO_3 radical with these particles is approximately 10^5 collisions per second, according to molecular kinetic theory.

The impact of energy exchange on dynamic regimes in gas-phase chain reactions can be explained by the breakdown of CH_3CO_3 radicals by excited formaldehyde molecules. This leads to oscillatory behaviour during the low-temperature oxidation of acetaldehyde, which is confirmed by the presence of feedback mechanisms. It follows that some cold flame regimes may be a consequence of energy exchange. The presence of a weakly bound peripheral oxygen atom contributes to the formation of excited formaldehyde molecules. These molecules transfer their energy to CH_3CO_3 radicals through quantum resonance, leading to their breakdown and the inhibition of the acetaldehyde oxidation reaction. The presence of feedback causes oscillatory behaviour in the system, confirming the complexity and multifaceted nature of the processes occurring during the oxidation of acetaldehyde.

The study established that the excitation of molecules and charge transfer processes can significantly impact the kinetics and mechanism of oxidation. The results indicate that quantum resonance contributes to the formation of weak shock waves, which, in turn, affect the dynamic regime of the reaction system. Specifically, it was observed that under certain conditions, the self-decomposition of ozone molecules in the near-surface layer leads to a significant release of energy, which accelerates the reaction and induces oscillatory regimes.

This study reveals how resonant energy transfer processes during acetaldehyde oxidation result in oscillatory behavior, primarily due to interactions between excited formaldehyde molecules and CH_3CO_3 radicals. Tanner *et al.*[21] analyzed energy transfer efficiency in different systems, noting the importance of resonance conditions similar to the nearly identical emission frequencies observed for formaldehyde and acetaldehyde in this study. These close frequencies facilitate efficient energy transfer between molecules, contributing to the observed oscillatory dynamics and validating the theory that resonant interactions can significantly alter reaction pathways. Witting[22] emphasized that molecular excitation impacts chemical reaction rates, a concept central to this study's observation that excited formaldehyde molecules can alter the course of acetaldehyde oxidation. This aligns with the finding that such excitation can inhibit reactions by destabilizing CH_3CO_3 radicals through resonant collisions. Similar to how molecular excitation reshapes photochemical processes, this study confirms that excitation energy plays a crucial role in altering reaction dynamics.

The complexity of radical interactions found in this study reflects the findings of Stuhr *et al.*,[23] who highlighted the diverse behavior of oxygen-containing radicals in chemical systems. The observed inhibition of acetaldehyde oxidation, driven by excited formaldehyde, mirrors the multifaceted interactions of reactive species in other oxidation processes. The study supports the idea that energy transfer between radicals can control the stability and reactivity of a system, which is a core principle in oxygen reactivity studies. In line with Al-Nu'airat *et al.*,[24] this research indicates that resonant energy transfer can facilitate or hinder oxidation reactions, much like the influence of singlet oxygen on organic substrates. The precise energy alignment between formaldehyde and acetaldehyde molecules in this study is comparable to the conditions required for effective energy transfer in other systems, suggesting a universal behavior in radical-driven reactions.

Lee *et al.*[25] investigated low-temperature oxidation in organic systems, emphasizing how surface interactions impact reactivity. This resonates with the findings of this study, where the adsorption of acetaldehyde and radicals on the surface played a crucial role in forming reactive intermediates. The breakdown of CH_3CO_3 radicals in the presence of excited formaldehyde supports the idea that surface processes can significantly alter chemical kinetics, mirroring the sensitivity of oxidation processes to adsorbed species. May and Kühn[26] discussed the role of charge and energy transfer in chemical systems, highlighting the influence of surface-active centers. This concept directly correlates with the resonant breakdown of CH_3CO_3 radicals observed in this study, where energy transfer dynamics are closely tied to surface interactions. The presence of intermediate radicals on surfaces emphasizes the importance of localized energy exchange in determining reaction pathways. Sargsyan *et al.*[27] explored the formation of weak shock waves due to energy redistribution, an idea that parallels the resonant energy transfer processes observed in this study. The breakdown of radicals and formation of oscillatory regimes in acetaldehyde oxidation suggest that localized energy changes can impact overall reaction dynamics, similar to the influence of weak shock waves in other oxidation processes.

Cassani *et al.*[28] and Pribus *et al.*[29] both explored feedback mechanisms and non-linear behavior in chemical systems. This study's identification of oscillatory patterns due to resonant energy transfer aligns with their findings, as the inhibition of acetaldehyde oxidation suggests that energy feedback can create complex behavior, similar to the Belousov-Zhabotinsky type reactions. The presence of feedback loops confirms that resonant interactions can stabilize or destabilize reactive systems, affecting the reaction's progression. The current findings also resonate with the observations of Yuan *et al.*,[30] who demonstrated how subtle changes in autocatalytic systems can lead to oscillatory patterns. In this study, the interaction between excited formaldehyde and CH_3CO_3 radicals produced similar oscillatory behavior, driven by energy feedback mechanisms. This emphasizes the sensitivity of such systems to minor fluctuations in energy transfer.

Zhou *et al.*[31] discussed how specific oscillating systems react to variations in energy exchange, mirroring the behavior observed in this study. The impact of excited formaldehyde on acetaldehyde oxidation, leading to prolonged inhibition, highlights how delicate shifts in energy dynamics can significantly influence reaction pathways. The study's results support the idea that chemical oscillators are highly sensitive to resonant energy transfer processes. Rizvi *et al.*[32] and Yang *et al.*[33] both examined the importance of energy dissipation and its effects on chemical systems, reinforcing the findings of this study. The prolonged inhibition of acetaldehyde oxidation by formaldehyde suggests that energy transfer and dissipation play a key role in maintaining reaction stability, supporting the concept that oscillatory systems rely on continuous energy exchange. Gentili *et al.*[34] and Jiménez *et al.*[35] explored feedback-driven systems, both in chemical and biological contexts. The feedback loops identified in this study, which lead to oscillatory behavior during acetaldehyde oxidation, underscore the universality of feedback mechanisms in controlling system dynamics. The impact of energy feedback on acetaldehyde oxidation parallels the principles found in natural and synthetic oscillating systems.

The study's findings align with Zhang *et al.*,[36] who emphasized the significance of Förster resonance energy transfer in molecular interactions. In this case, the nearly resonant energy states between formaldehyde and acetaldehyde underscore the importance of precise energy matching for effective reaction control. The electronic and vibrational states of formaldehyde play a crucial role in dictating the stability of CH_3CO_3 radicals, highlighting the necessity of resonant conditions. Zheng *et al.*[37] discussed the Dexter-type energy transfer mechanisms, which are similar to the stepwise vibrational energy transfer observed in this study. The findings suggest that electronic and vibrational states interact to create prolonged effects on reaction dynamics, akin to how Dexter transfer processes influence chemical behavior. This parallel suggests that the detailed dynamics of radical interactions in acetaldehyde oxidation are governed by similar principles.

Lindsey *et al*.[38] highlighted how resonance conditions impact energy transfer efficiency, a concept central to this study's observation of oscillatory inhibition in acetaldehyde oxidation. The near-resonance between formaldehyde and acetaldehyde facilitates energy transfer that prolongs the reaction's inhibitory phase. Zimmerman and George[39] specifically discussed quantum resonance effects in molecular collisions, directly reflecting the resonant breakdown of CH_3CO_3 radicals observed in this study. Their discussion underscores how quantum effects can significantly impact reaction kinetics, validating the current study's findings on the crucial role of resonant energy transfer in chemical systems. This study's results demonstrate that the oscillatory behavior in acetaldehyde oxidation is driven by resonant energy transfer processes, supported by a wide range of previous studies that underscore the significance of resonance, feedback mechanisms, and energy dynamics in complex chemical systems.[40,41]

The unique properties of excited molecules, such as increased reactivity, different potential energy surfaces, and altered geometry, play a decisive role in influencing oxidation processes. These properties provide faster reaction rates, the formation of reactive intermediates, non-thermal activation, and the generation of unique oxidation products. The results obtained demonstrate that quantum resonance and the formation of excited molecules play a vital role in oxidation processes and can significantly impact the dynamics of the reaction system. These findings complement and extend existing knowledge of oxidation mechanisms and can be utilised to optimise industrial processes.

4. Conclusions

The study established that the presence of quantum resonance in a chain system can lead to the conversion of intermediate oxidation products of organic compounds, such as H_2O_2, into ozone molecules. The study demonstrated that if water complexes with negative halogen ions are near the reactor surface, quantum resonance facilitates the generation of weak shock waves. The generation of weak shock waves is associated with ozone molecule formation and decomposition, and the products of recharging and ion-molecular reactions near the surface layer, as exemplified by methane oxidation. It was established that in the presence of excited particles in the reaction mixture, there is a high probability of accelerating some elementary acts due to the resonant energy transfer between particles. This can cause the decomposition of leading radical chains, which in turn slows down the reaction. In the presence of feedback in the reaction medium, concentration oscillation regimes can arise. This phenomenon is due to the interaction of excited molecules and radical chain reactions, resulting in the complex dynamics of oxidation processes. Ozone molecules formed as a result of self-decomposition can further heat the reaction mixtures and increase the reaction rate. Heating reaction mixtures due to ozone molecule decomposition significantly affects the dynamic regime of the reaction system.

Understanding this influence is a relevant task for further research. These findings contribute to a deeper understanding of the mechanisms affecting low-temperature methane oxidation and highlight the need for further research to manage these processes and improve their efficiency. Future research prospects include examining the mechanisms of quantum resonance and the dynamics of excited particles, developing models, and experimentally confirming these processes. However, the study is limited by the assumptions of the models and experimental conditions, which may not fully correspond to real industrial conditions. Moreover, the influence of external factors and technological limitations reduces the accuracy of the obtained results, requiring further investigation.

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Conflict of Interest

I declare that the authors have no competing interests.

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ФОРМУВАННЯ ЗБУДЖЕНИХ МОЛЕКУЛ З ФРАГМЕНТІВ ГЕТЕРОГЕННО-ОДНОРІДНИХ ПРОЦЕСІВ У ПРИПОВЕРХНЕВОМУ ШАРІ ТА ЇХ ВПЛИВ НА ПРОЦЕСИ ОКИСНЕННЯ

Анотація. *У дослідженні розглядається формування збуджених молекул і їхня ключова роль у впливі на динамічні режими низькотемпературного окиснення, зокрема в реакціях метану та ацетальдегіду. Виявлено, що квантовий резонанс сприяє утворенню збуджених молекул формальдегіду, які забезпечують процеси передачі енергії, впливають на радикальні ланцюгові реакції та гальмують окиснення. Ці процеси призводять до формування слабких ударних хвиль, які виникають унаслідок взаємодії комплексів води з негативними галогенними іонами та саморозпаду озону. Завдяки теоретичному моделюванню, комп'ютерним симуляціям і спектроскопії досліджено роль квантового резонансу у формуванні слабких ударних хвиль і встановленні осциляційних режимів. Отримані результати сприяють глибшому розумінню механізмів низькотемпературного окиснення та складної взаємодії збуджених молекул, відкриваючи нові перспективи для застосування в науці та промисловості.*

Ключові слова: *ударні хвилі, теорія Гюгоніо, резонанс, розслаблення, іонно-молекулярні реакції.*