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Original Article

Theoretical Analysis on the Removal of Volatile Organic Compounds by Microwave Plasma

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Abstract:
Volatile Organic Compounds (VOCs) are a significant class of environmental pollutants with detrimental effects on human health and ecosystems. The development of efficient and reliable methods for VOC detection and degradation is crucial for environmental protection and industrial safety. Microwave plasma technology has emerged as a promising approach for VOC abatement due to its high energy efficiency, rapid reaction rates, and ability to operate at ambient conditions. Meanwhile, Density Functional Theory (DFT) has become an indispensable tool for understanding the molecular interactions and reaction mechanisms involved in VOC degradation processes. This study investigates the synergistic application of microwave plasma and DFT to enhance the understanding and optimization of acetone degradation. The results show that in the plasma field formed by microwave plasma, acetone can achieve direct degradation through the cleavage of covalent bonds, and can also undergo oxidation reactions with active free radicals to achieve indirect degradation. The theoretical calculation results are consistent with the experimental results, verifying the degradation of acetone via microwave plasma would be an efficient approach.

Keywords: VOC removal; acetone degradation; Degradation pathways; Microwave plasma; Density function theory (DFT)

Introduction

Volatile Organic Compounds (VOCs) are a diverse group of carbon-based chemicals that are widely emitted from industrial processes, transportation, and household products[1-3]. Due to their toxicity, carcinogenicity, and role in the formation of ground-level ozone and secondary organic aerosols, VOCs pose significant risks to human health and the environment[4-7]. As a result, stringent regulations have been imposed worldwide to limit VOC emissions, driving the need for innovative and efficient technologies for VOC detection and degradation.

Among the various methods for VOC abatement, plasma technology has gained considerable attention due to its unique advantages[8-12]. Microwave plasma generates highly reactive species, such as electrons, ions, and radicals, which can effectively break down VOCs into less harmful compounds, such as CO_2 and H_2O, even at room temperature and atmospheric pressure[13, 14]. The non-thermal nature of microwave plasma ensures high energy efficiency, making it a sustainable alternative to traditional thermal methods[15-19]. However, the complex chemical reactions and mechanisms involved in plasma-based VOC degradation require further investigation to optimize process parameters and improve performance.

Density Functional Theory (DFT) has proven to be a powerful computational tool for studying the molecular-level interactions and reaction pathways of VOCs[20-22]. By simulating the electronic structure and energy dynamics of VOC molecules and their interactions with plasma-generated species, DFT provides valuable insights into the decomposition mechanisms and intermediate products[23-25]. These theoretical findings can guide the design of experimental systems and enhance the efficiency of plasma-based VOC degradation.

This study aims to bridge the gap between experimental microwave plasma systems and theoretical DFT simulations to advance the understanding of VOC degradation processes. By combining the strengths of both approaches, we seek to elucidate the fundamental mechanisms of plasma-VOC interactions, optimize reaction conditions, and develop scalable solutions for environmental remediation. The integration of microwave plasma technology and DFT could contribute to the field of VOC abatement.

2. Descriptions and Theoretical Methods

2.1 Model Descriptions

The microwave plasma is applied to dissociate the VOCs in waste gas from chemical industries into CO_2 and H_2O, as shown in Fig. 1. The operating pressure is 1atm. The non-thermal plasma e*(electron), is produced via microwave-induced metal discharge, as we described in detail in our previous work[26, 27]. In Fig. 1, black, blue, and red sphere represent carbon atom, hydrogen atom, and oxygen atom, respectively. The waste gases containing organics enter into the electric field through the entrance. The degradation of organics occurred through homogeneous reactions and are classified into two types: (1) degradation under the effect of e*, for example, acetone undergoes a direct degradation reaction by the direct collision of e* (2) degradations under the effect of radicals ·OH, H· and O· produced by background gases H_2O and O_2, for example, as shown in Fig. 1. the radical O· is firstly produced by the collision of e* and O_2, and then the acetone is transformed into an acetoxy group and a methoxy group under the effect of O·. This paper would focus on the dissociation kinetics and mechanisms of acetone.

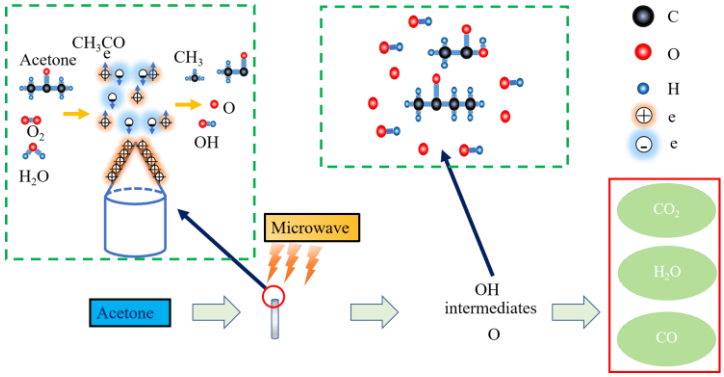


Figure 1. The schematic for acetone degradation by microwave plasma.

2.2 Theoretical Methods

The density functional theory (DFT), with which the single point energy, active energy, transition state, etc. of a chemical reaction can be derived, is performed to identify the degradation pathway of organics through using Gaussian16 software package. In this paper, the DFT calculation is carried out through two steps: (1) vibrational frequency calculation for acetone: species including reactants and products, are firstly established with the restricted Hartree-Fock (RHF) formulation in GaussView5.0, and then the geometry optimization for each specie is performed by using the LYP correction function (B3LYP) along with the split valence polarized basis set 6-311G(d,p). The optimized structure of each specie combined with coupled-cluster theory is also used to calculate the singlepoint energy. And the harmonic vibrational frequency calculations are adopted to confirm the energy minima for the structures of each specie based on B3LYP/6-311G(d,p); (2) pathway determination for each reaction: for the vibrational frequency calculation, the key step for pathway determination is to find out the transition state of each reaction, i.e., the stationary point. For each stationary point, additional energy calculation is executed by B3LYP with 6-311G(d,p) in conjunction with intrinsic reaction coordinate. Thus, the barrier energy and the pathway of each reaction can be derived.

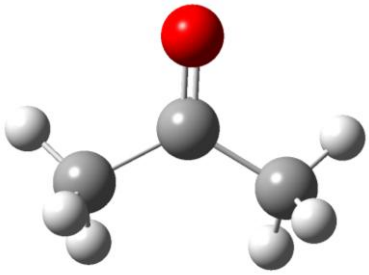


Figure 2. Acetone models for calculation. The red atom is oxygen atoms, the gray atoms are carbon atoms, and the white atoms are hydrogen atoms.

3. Results and Discussion

3.1. The Initial Step for Acetone Degradation

3.1.1. Direct Degradation Reaction of Acetone

In the microwave plasma field, acetone undergoes collisions with high energy electrons. Such collisions have the potential to induce the dissociation of covalent bonds, thereby triggering direct degradation. In the stable-state structure of acetone, three distinct types of covalent bonds are present. Their respective bond energies are 732.5 kJ/mol for the C=O bond, 347.5 kJ/mol for the C-C bond, and 406.1 kJ/mol for the C-H bond[28]. Evidently, the carbonyl C=O bond exhibits a relatively high bond energy. Conversely, the atoms within the methyl group are notably reactive, and the likelihood of the bond between the methyl group and the carbonyl group breaking is substantial. Consequently, the C-C bond in acetone is prioritized for investigation. This section is principally dedicated to the exploration of the C-C bond cleavage in acetone through DFT calculations. The corresponding calculation results are presented in Figure 3. The reaction mechanism is as follows: one methyl group in the acetone structure dissociates from the carbonyl group, while the other methyl group loses a hydrogen atom. After traversing the transition state (TS), ketene (CH2=C=O) and methane are produced. The potential energy barrier of this reaction amounts to 358.0 kJ/mol, absorbing heat energy of 48.6 kJ/mol.

From the above calculations, it is known that the dissociation process of acetone shows that the activation energy for the C-C bond cleavage reaction is 358.0 kJ/mol, which is slightly higher than the bond energy of the C-C bond, 347.5 kJ/mol. This indicates that the breaking of the C-C bond in acetone is determined by its bond energy. In the plasma formed by microwave plasma, there are a large number of high-energy electrons. These high-energy electrons collide with acetone, making the cleavage reaction of the C-C bond in the acetone structure easy to occur, thus causing the direct cleavage and degradation of acetone[29].

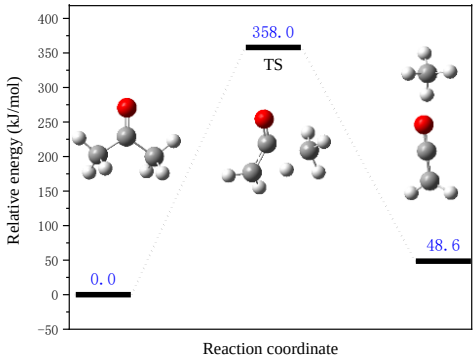


Figure 3. The pyrolysis reaction of acetone

To sum up, in the reaction of direct degradation of acetone by microwave plasma, acetone may generate methane. Although methane molecules do not appear in GCMS, this is because the

GCMS mass spectrometer can only detect molecules with a molecular weight greater than 30. In addition, methane is present in In a system with high temperature and rich oxygen free radicals, it is also very easy to be oxidized, and the existence time of methane molecules will be very short. This is consistent with literature reports that methane is generated in the acetone cracking reaction[29]. The theoretical calculation results are consistent with the experimental results, and the reaction path of direct degradation of acetone by microwave-induced metal discharge has been verified.

3.1.2 Indirect Degradation Reaction of Acetone

In addition to the direct cracking reaction, during the process of acetone degradation induced by microwave plasma, acetone may also undergo oxidation reactions with O_2 or other free radicals. Therefore, DFT calculations were further carried out for the reactions of acetone with O_2, hydroxyl radicals (OH·) and methyl radicals (·CH_3). The potential energy surface diagram of the reaction between acetone and O_2 is shown in Figure 4. From Figure 4, it can be seen that the reaction process involves acetone losing a methyl group and simultaneously attracting one O atom from O_2. After passing through the transition state TS, an acetoxy group and a methoxy group are formed. The potential energy barrier of this reaction is 140.1 kJ/mol, and the heat released is 225.1 kJ/mol.

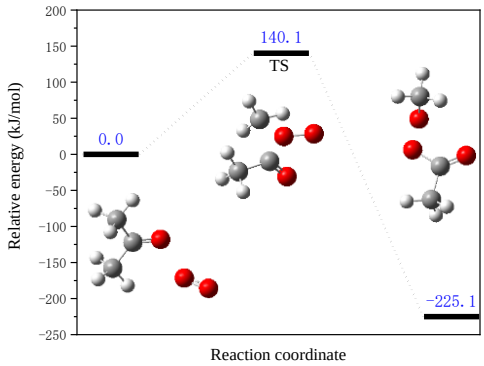
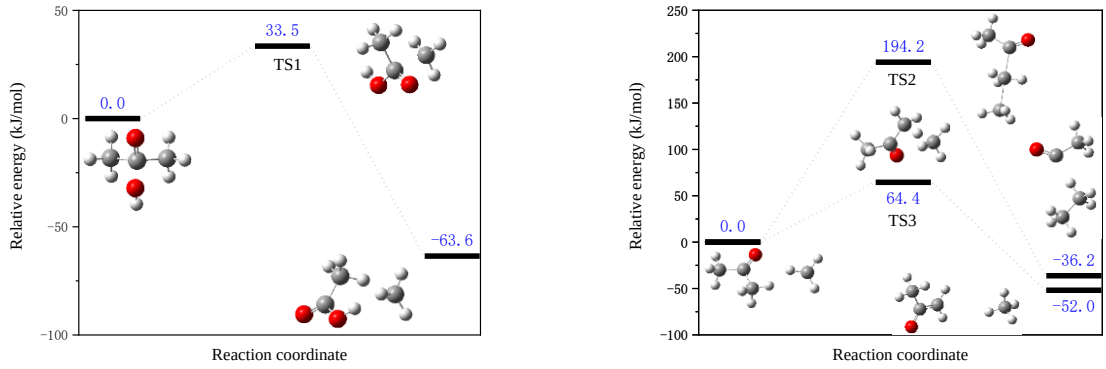


Figure 4 The Reaction of Acetone with O_2

Figure 5(a) is the potential energy surface diagram of the reaction between acetone and hydroxyl radicals (OH·). As can be seen from Figure 5, the reaction mechanism is that an OH group substitutes a methyl group in the acetone structure. After passing through the transition state TS1, acetic acid and methyl radicals are formed. The potential energy barrier of this reaction is 33.5 kJ/mol, and the heat released is 63.6 kJ/mol. From Figure 5(b), it can be known that the reaction between acetone and methyl radicals has two reaction pathways: (1) The methyl extraction reaction. Its reaction mechanism is that the methyl group in the acetone structure loses a hydrogen atom and connects with the methyl radical to form the transition state TS2 (butanone and hydrogen radicals). Then, the C-C bond between the ethyl group and the carbonyl carbon breaks and cleaves. The ethyl group attracts the hydrogen radical to form ethane, and the remaining part of butanone forms an acetyl radical. The potential energy barrier of this reaction is 194.2 kJ/mol, and the heat released is 36.2 kJ/mol. This reaction is equivalent to the methyl radical extracting one methyl group of acetone and combining to form ethane. (2) The hydrogen extraction reaction. Its reaction mechanism is that the methyl group in the acetone structure loses a hydrogen atom. After passing through the transition state TS3, methane and acetonyl radicals are formed. The potential energy barrier of this reaction is 64.4 kJ/mol, and the heat released is 52.0 kJ/mol. As can be seen from the above, compared with the methyl extraction reaction, the potential energy barrier of the hydrogen extraction reaction is 129.8 kJ/mol lower, and the heat released is 15.8 kJ/mol more. Therefore, from a thermodynamic perspective, the methyl extraction reaction is not easy to proceed, but this reaction cannot be completely excluded.

Based on the above analysis, acetone can react with free radicals to generate smaller free radicals

such as acetyl radicals, leading to the indirect degradation of acetone. Butanone is produced during the reaction, which is consistent with the experimental detection results, thus proving the reaction pathway of the indirect degradation of acetone at the atomic level. Theoretical calculation studies have found that the potential energy barriers of these reactions are relatively low. There are a large number of active free radicals in the microwave plasma field, making these reactions prone to occur. The theoretical calculation results are consistent with the experimental results, verifying the reaction pathway of the indirect degradation of acetone by microwave plasma.



(a) **(b)**

Figure 5. The Reaction of acetone with free radicals. (a) Reaction of acetone and OH radicals; (b) Reaction of acetone and methyl radicals.

3.2. **The Subsequent Degradation of Acetone**

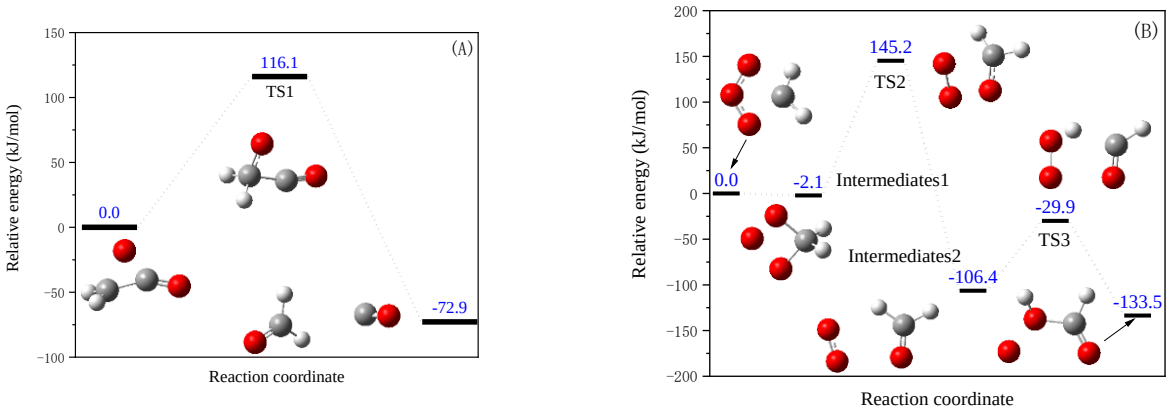
3.2.1 Free Radical Oxidation Reaction

As described previously, under the action of high-energy electrons, the acetone cracking reaction generates free radicals of smaller molecules. These free radicals can react with the active free radicals in the plasma field and eventually generate CO_2 and H_2O. In this section, DFT calculations are carried out for the reactions between the free radicals of smaller molecules and O and O_3 free radicals, including two reaction pathways: (1) the reaction between the acetyl radical and the O radical; (2) the reaction between the CH_2 radical and the O_3 radical.

Firstly, In the plasma field formed by microwave plasma, the acetyl group is easily bombarded by high-energy electrons, and its methyl group loses a hydrogen atom to generate ketene. Figure 6(a) is the potential energy surface diagram of the reaction between ketene and O radicals. It can be seen from Figure 6(a) that the reaction mechanism is that CH_2 in ketene attracts O radicals, and then the C-C bond is cleavage, passing through the transition state TS3, Formaldehyde and CO are generated. The potential energy barrier of this reaction is 116.1 kJ/mol, and the heat released is 72.9 kJ/mol.

Secondly, (2) In the plasma field formed by microwave plasma, methane collides with high-energy electrons, which can generate methylene (CH_2) radicals. Then, the CH_2 radicals react with active radicals. Figure 6(b) shows the potential energy surface diagram of the reaction between CH_2 radicals and O_3 radicals. As can be seen from Figure 6(b), the reaction is divided into three steps: (1) The combination reaction of CH_2 radicals and O_3 radicals. The C atom attracts two O atoms from O_3 to form Intermediate 1. There is no transition state in this reaction, and 2.1 kJ/mol of heat is released. (2) Intermediate 1 continues to react and is oxidized to Intermediate 2. The reaction mechanism is that one C-O bond in Intermediate 1 cleaves. The O atom separated from the C-O bond combines with an O radical, and the non-cleaved C-O bond forms a C=O bond. After passing through the transition state TS3, Intermediate 2, namely formaldehyde and O_2, is generated. The potential energy barrier of this reaction is 147.3 kJ/mol, and 104.3 kJ/mol of heat is released. (3) The oxidation reaction of formaldehyde. The reaction mechanism is that one

C-H bond in formaldehyde of Intermediate 2 cleaves to form a formyl radical and an H radical. Then, the H radical attracts one O atom from O_2 to form an OH radical. After passing through the transition state TS3, the formyl radical and the OH radical generate formic acid. The potential energy barrier of this reaction is 76.5 kJ/mol, and 27.1 kJ/mol of heat is released. From the above analysis, it can be known that the potential energy barrier of the reaction from Intermediate 2 to the product is relatively low, which means that the reaction of oxidizing formaldehyde to formic acid is relatively easy to occur.



(**a**) (**b**)

Figure 6. Free radical oxidation reaction. (a) Acetyl radical reacts with O; (b) CH_2 radical reacts with O_3.

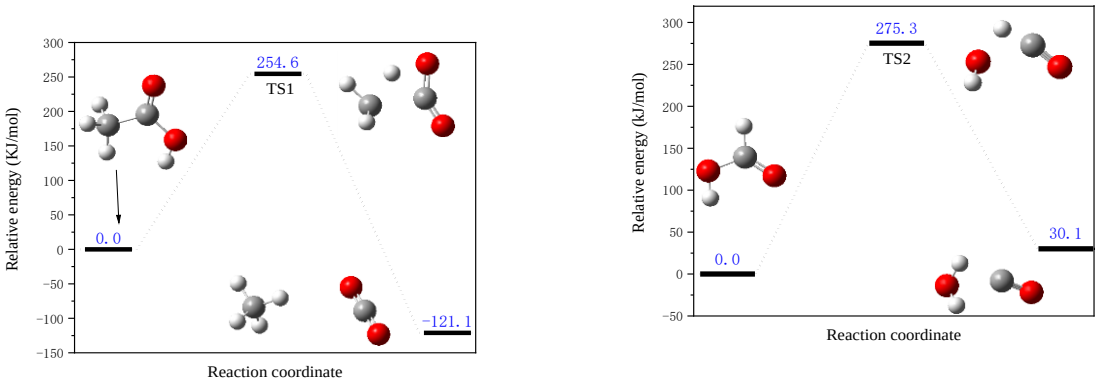
Based on the above analysis, the DFT calculation results show that the acetyl radical and CH_2 radical undergo oxidation reactions to form carboxylic acids. This is consistent with the organic products detected in the experiment, thus proving the reaction pathway of the indirect degradation of acetone at the atomic level. Since the background gas in the microwave plasma experiment is air, it means that there are a large number of oxygen-containing free radicals in the plasma formed by discharge, making the free - radical oxidation reaction prone to occur. The theoretical calculation results are consistent with the experimental results, and the reaction pathway of the indirect degradation of acetone by microwave plasma is verified.

3.2.2 Carboxylic Acid Decarboxylation Reaction

It is reported that the decarboxylation reaction is an important and frequently occurring reaction in organic chemistry[30, 31]. The decarboxylation of carboxylic acids is very likely to occur at high temperatures. As shown in the previous research, carboxylic acids, mainly formic acid and acetic acid, are generated in the reaction of acetone degradation by microwave plasma. Therefore, in this paper, DFT calculations were carried out for the decarboxylation reactions of acetic acid and formic acid respectively, and the calculation results are shown in Figure 7. As can be seen from Figure 7, acetic acid undergoes a cleavage reaction. The carboxyl group is cleaved from the alkyl group, and at the same time, the carboxyl group loses a hydrogen atom. After passing through the transition state TS1, methane and CO_2 are formed. The potential energy barrier of this reaction is 254.6 kJ/mol, and 121.1 kJ/mol of heat is released. The reaction mechanism of formic acid decarboxylation is that the carbon atom is cleaved from the hydroxyl group and the hydrogen atom. After passing through the transition state TS2, the carbonyl group turns into a C≡O triple bond to form CO, while the hydroxyl group and the hydrogen atom combine to form H_2O. The potential energy barrier of this reaction is 275.3 kJ/mol, and 30.1 kJ/mol of heat is absorbed.

As can be seen from the above analysis, through the DFT calculations of the decarboxylation reactions, it is found that formic acid and acetic acid produce CO and CO_2, which means that the final products of acetone after cleavage and oxidation reactions are CO_2 and CO. The

consistency between the theoretical calculation results and the experimental results indicates that the reaction pathway of the indirect degradation of acetone has been verified.



(**a**) (**b**)

Figure 7. Carboxylic acid decarboxylation reaction. (a) Acetic acid decarboxylation reaction; (b) Formic acid decarboxylation reaction.

3.3. The Reaction Pathway of Acetone Degradation by Microwave Plasma

Based on the above analysis, it was found through DFT calculations that acetone can not only collide with high-energy electrons, causing covalent bond rupture to achieve direct degradation, but can also undergo oxidation reactions with active free radicals to achieve indirect degradation. The main reaction path of direct degradation of acetone is: acetone directly collides with high-energy electrons, causing the covalent bond to break, forming methyl and acetyl free radicals; the acetyl group is easily bombarded by high-energy electrons, and its methyl group loses a hydrogen atom Ketone is generated; methane collides with high-energy electrons to generate methyl radicals; methyl radicals collide with high-energy electrons to generate methylene CH_2 radicals; formic acid and acetic acid undergo decarboxylation reactions to generate CO and CO_2. The reaction path of indirect degradation of acetone is mainly as follows: acetone reacts with free radicals such as O and OH to achieve indirect degradation of acetone. The main products are acetic acid and butanone; the acetyl radical undergoes an oxidation reaction to form formaldehyde and CO_2.

Through GC-MS analysis, it was found that some organic gases, such as butanone, acetic acid, etc., were generated during the degradation process. According to the infrared spectrum analysis, the main products were CO_2 and H_2O. Based on the analysis of these results, the reaction pathway of acetone degradation by microwave plasma can be preliminarily speculated, which also mainly includes two parts: (1) One is direct degradation, that is, acetone directly collides with high-energy electrons, and the covalent bonds are broken to form methyl and acetyl radicals [32]. The methyl and acetyl radicals can be further decomposed by high-energy electrons and free radicals, and then undergo a series of oxidation reactions with highly reactive free radicals such as O, OH, O_3, etc., and finally form CO, CO_2 and H_2O. (2) The other is indirect degradation, that is, acetone undergoes oxidation reactions with active free radicals in the plasma field, such as free radicals like O, OH, etc. or O_2, to generate acetic acid and methyl groups; the methyl group reacts with another acetone molecule to produce butanone, which is then further decomposed and oxidized into acetyl radicals and ethane; then the acetyl radicals undergo oxidation reactions to form formaldehyde and CO_2. Under the action of high-energy electrons and free radicals, methane continues to react and finally generates CO, CO_2 and H_2O. The process simulation is shown in Figure 8.

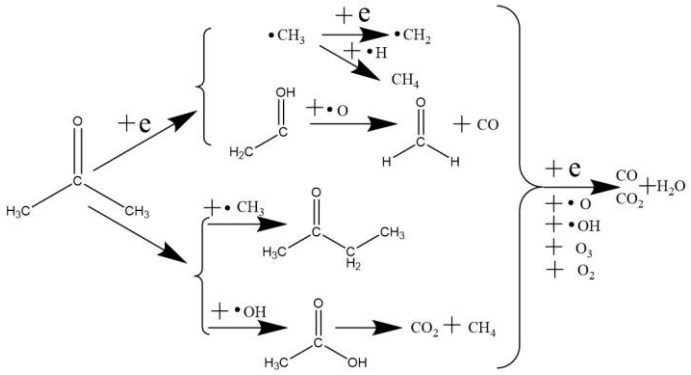


Figure 8. The network for degradation pathways of acetone by microwave plasma.

4 Conclusions

In this paper, for the acetone degradation reaction, appropriate model compounds were selected respectively. DFT calculations were used to analyze the geometric structures and reaction potential energy barriers. The effects of electrons and active free radicals on the VOC degradation reaction were studied at the atomic level, and the reaction mechanism of acetone degradation by microwave plasma was revealed. The main conclusions are as follows:

DFT calculations were employed to compute and analyze the degradation reaction pathways of acetone in microwave plasma, and the degradation mechanism of acetone was obtained. The results show that in the plasma field formed by microwave plasma, acetone can achieve direct degradation through the cleavage of covalent bonds, and can also undergo oxidation reactions with active free radicals to achieve indirect degradation. Reasonable intermediate transition states were found, and the scientific nature of the mechanism speculation was confirmed by theoretical calculations.

Through DFT calculations, it was found that the reaction pathway of acetone degradation by microwave plasma was further confirmed. Acetone directly collides with high-energy electrons, causing the cleavage of covalent bonds to form methane and ketene (CH_2=C=O), which can then be further decomposed by high - energy electrons or other free radicals. Subsequently, it undergoes a series of oxidation reactions with highly reactive free radicals such as O, OH, O_3, etc., ultimately forming CO, CO_2, and H_2O. In addition, acetone undergoes oxidation reactions with active free radicals in the plasma field, such as free radicals like O, OH, etc. or O_2, generating acetoxy groups, methoxy groups, acetic acid, methyl groups, acetonyl groups, and methane, etc. The methyl group reacts with another acetone molecule to produce butanone, which is then further decomposed and oxidized into acetyl radicals and ethane. Subsequently, the acetyl radicals undergo oxidation reactions to form formaldehyde and CO. Under the action of high - energy electrons and free radicals, methane continues to react and finally generates CO, CO_2, and H_2O. The theoretical calculation results are consistent with the experimental results, verifying the degradation of acetone via microwave plasma would be an efficient approach.

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