

Investigation on the Pyrolysis Mechanism of Epoxy Resin from Decommissioned Wind Turbine Blades via Experiments and Molecular Simulation[#]

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ABSTRACT

The efficient resource recovery of decommissioned wind turbine blades is a key challenge for the sustainable development of the wind power industry. Pyrolysis technology, as a promising recycling method, relies fundamentally on understanding the pyrolysis mechanism of the epoxy resin matrix. This study aims to reveal the pyrolysis behavior and reaction mechanisms of epoxy resin from decommissioned blades through a multi-scale approach integrating macro- and micro-scale investigations. Thermogravimetry–Fourier transform infrared spectroscopy (TG-FTIR) was employed to experimentally study the powdered blade material, obtaining macroscopic pyrolysis characteristics, kinetic parameters, and the evolution of gaseous products. Meanwhile, ReaxFF reactive force field molecular dynamics simulations were applied to construct an epoxy resin model and simulate its pyrolysis process, tracking bond breaking, generation of small molecular products, and reaction pathways at the atomic scale. The TG-FTIR results showed that the pyrolysis of epoxy resin mainly occurs in two stages, with the maximum mass loss peak at 428°C; the main gaseous products included CO, CO₂, H₂O, phenol, and various hydrocarbons. The molecular simulation results were highly consistent with the macroscopic experiments, not only reproducing the mass loss trend and main product categories but, more importantly, revealing that the initial pyrolysis reactions start with the cleavage of ether (C–O) and C–N bonds, and visually demonstrating the formation pathways of key products such as CO, CO₂, and H₂O. Through mutual validation and complementation between experiments and simulations, this study clarifies, for the first time from a multi-scale perspective, the pyrolysis mechanism of epoxy resin from decommissioned wind turbine blades, identifying initial reaction pathways and key weak bond sites. The research outcomes provide an important theoretical basis and data support for optimizing the pyrolysis process parameters of

decommissioned blades and achieving directed conversion and high-value recovery.

Keywords: Epoxy resin; Pyrolysis mechanism; ReaxFF molecular dynamics; TG-FTIR

1. INTRODUCTION

The global shift towards renewable energy has driven unprecedented growth in the wind power sector. As a result, a wave of first-generation wind turbines is now being decommissioned, leading to an urgent waste management crisis centered on end-of-life (EOL) turbine blades [1]. These blades are primarily manufactured from composite materials consisting of glass or carbon fibers reinforced with a thermosetting epoxy resin matrix. The highly cross-linked, stable molecular structure of these polymers renders them resistant to degradation and extremely challenging to recycle through conventional means [2]. Consequently, the long-term sustainability and circularity of the wind energy industry are critically dependent on developing advanced recycling strategies for these complex waste streams.

Pyrolysis, a thermochemical conversion process, presents a promising pathway for the resource recovery of EOL blade materials. It offers the potential to generate valuable energy products (syngas, oils) and recover reinforcing fibers, thereby supporting a circular economy model [3]. However, the optimization and scale-up of pyrolysis technology for epoxy-based composites are hindered by an insufficient fundamental understanding of their decomposition mechanisms. The precise pathways of bond cleavage, the evolution of volatile species, and the influence of the complex, formulated resin chemistry on these processes remain poorly elucidated. Macroscopic experimental techniques, notably thermogravimetric analysis coupled with Fourier transform infrared spectroscopy (TG-FTIR), are routinely employed to probe pyrolysis behavior [4]. These

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methods provide critical data on global mass loss trends, apparent kinetics, and the qualitative identification of gaseous products. Despite their utility, they offer limited atomic-scale insight into the initial reaction triggers, specific bond-breaking sequences, and the detailed formation pathways of key products [5].

To overcome these limitations, reactive force field molecular dynamics (ReaxFF MD) simulations have emerged as a powerful computational tool [6]. This method enables the investigation of complex reaction networks in large, realistic molecular systems without pre-defined pathways, allowing for the direct observation of chemical events at the atomic level. The true strength of this approach is realized when simulation predictions are rigorously validated against experimental data, creating a multi-scale framework that offers a more complete and mechanistically sound understanding than either technique can achieve independently. While previous research has investigated epoxy pyrolysis, existing studies often rely on isolated experimental or computational approaches and frequently utilize simplified model compounds [7]. A significant knowledge gap exists in applying an integrated multi-scale methodology to the actual, complex epoxy resins sourced from real-world EOL wind turbine blades. A detailed understanding of the synergistic decomposition mechanisms—particularly the identification of the key weak linkages that initiate pyrolysis and govern product distribution—is lacking and requires validation across different scales [8].

To bridge this gap, this study employs a coupled experimental and simulation approach to fundamentally elucidate the pyrolysis mechanism of epoxy resin from decommissioned wind turbine blades. Macroscopic experiments using TG-FTIR are conducted to determine comprehensive pyrolysis characteristics, kinetic parameters, and real-time gas evolution profiles. Concurrently, a representative molecular model of the industrial epoxy system is constructed for ReaxFF MD simulations, enabling atomic-scale tracking of the pyrolysis initiation, bond dissociation, and reaction pathways leading to fragment and gas formation. The specific objectives are to experimentally characterize the thermal degradation behavior and product release; simulate the pyrolysis process to uncover initial decomposition steps and key weak bonds; and achieve mutual validation between simulation and experiment to establish a conclusive multi-scale reaction mechanism. The findings from this work provide critical fundamental insights necessary for optimizing pyrolysis process parameters to enhance product yield and quality,

ultimately advancing the sustainable and high-value recycling of EOL wind turbine blades.

2. MATERIALS AND METHODS

2.1 Sample preparation and characterization



Fig. 1 Cutting parts used in pyrolysis experiments

The raw materials for retired wind turbine blades used in the experiment were taken from the main beam of retired blades in a certain wind power plant. The resin matrix in the leaf is bisphenol A-type epoxy resin with a content of about 24%, and the reinforcing material is boron free E-type glass fiber with a content of about 76%. The raw materials used in the experiment are blade blocks cut from retired blade main beams, with a size of 1cmx1cmx4cm, as shown in Fig. 1.

2.2 Experimental methods

The pyrolysis characteristics of the Epoxy Resin sample were evaluated using TG-FTIR and TG-GC/MS. Each test sample weighed approximately 10 mg. Pyrolysis temperatures ranged from 303.15 to 1,173.15 K. As the carrier gas, the argon had a constant flowrate of 50 ml/min during the pyrolysis, and the heating rate was set as 10 K/min.

2.3 Simulation methods

The molecular weight of Epoxy Resin typically ranges from 100,000 to 500,000. Due to computational limitations, it is essential to select an appropriate degree of polymerization as a model for PE in simulation studies. Previous research by Xuan et al. [9] investigated various degrees of polymerization ($n = 25, 50, 100, 250$) for PE under identical conditions, revealing that $n = 25$ was sufficiently representative. In this study, we selected a degree of polymerization of 100 for our model compound, as illustrated in Fig. 2.

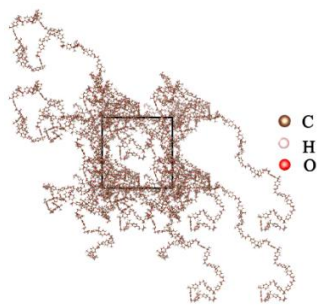


Fig. 2 Epoxy Resin model simulated by ReaxFF-MD

3. RESULTS AND DISCUSSION

3.1 Experimental Analysis of Pyrolysis Characteristics via TG-FTIR

3.1.1. Pyrolysis Behavior and Mass Loss

The thermal decomposition behavior of the epoxy resin from decommissioned wind turbine blades was investigated through thermogravimetric analysis (TGA). The TG and DTG curves (Fig. 3) reveal that the pyrolysis process occurs primarily in two distinct stages. The first minor mass loss stage, observed between approximately 473.15–623.15 K, is attributed to the release of adsorbed water, residual solvents, and the initial breakage of the weakest chemical linkages. The second and major decomposition stage occurs within the temperature range of 623.15–823.15 K, with the maximum mass loss rate peak centered at 701.15 K. This stage is associated with the extensive cleavage of the polymer backbone and the primary release of volatile species, accounting for most of the mass loss.

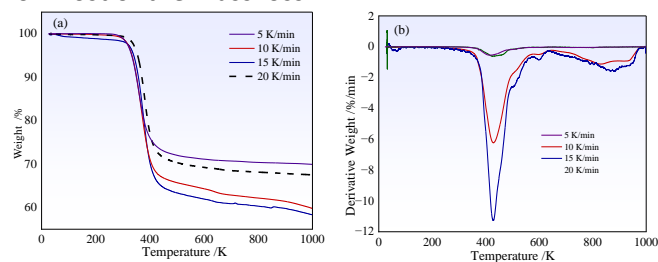


Fig. 3 Thermogravimetric analysis (TG) and DTG results of epoxy resin pyrolysis

3.1.2. Evolution of Gaseous Products

The identification and evolutionary profiles of the volatile products during pyrolysis were monitored online by FTIR spectroscopy. The 3D FTIR spectra and Gram-Schmidt curves (Fig. Y) indicate that the main gaseous products include CO, CO₂, H₂O, phenol, and various light hydrocarbons (e.g., CH₄, C₂H₄). The release profiles of these gases are highly temperature-dependent. CO and CO₂ evolve over a broad temperature range, starting from around 300 °C, with their release rates peaking near

the DTG maximum. The detection of phenol derivatives confirms the fragmentation of aromatic segments in the epoxy network. The generation of hydrocarbons suggests secondary cracking reactions of alkyl chains at higher temperatures.

3.1.3. Kinetic Analysis

The apparent activation energy (E_a) of the pyrolysis process was determined using isoconversional methods (Flynn-Wall-Ozawa and Kissinger-Akahira-Sunose). The calculated average apparent activation energy was found to be kJ/mol. The variation of E_a with conversion degree (α) suggests a complex multi-step reaction mechanism, as the value does not remain constant throughout the process. This complexity underscores the involvement of parallel and consecutive reactions during the thermal degradation of the cross-linked epoxy resin.

3.2 Atomic-Scale Reaction Mechanisms Unveiled by ReaxFF MD Simulations

3.2.1. Model Validation and Replication of Macro-Scale Trends

A large-scale molecular model of the representative epoxy resin network was constructed and subjected to ReaxFF molecular dynamics simulations at elevated temperatures (e.g., 2000–3000 K to accelerate reactions). The simulated mass loss profile as a function of temperature successfully reproduced the two-stage decomposition trend observed in the experimental TG curves. Furthermore, the simulation quantitatively predicted the major product classes (CO, CO₂, H₂O, phenols, hydrocarbons), demonstrating a remarkable consistency with the TG-FTIR results. This agreement validates the chosen molecular model and the ReaxFF force field for studying the pyrolysis chemistry of this system.

3.2.2. Influence of Heating Rate and Pyrolysis Temperature on the Reaction

To investigate the influence of heating rate on the pyrolysis process, the reaction system was heated from 0 K to 3000 K at rates of 5, 10, and 15 K/ps, respectively, to analyze its effect on the product distribution. Furthermore, ReaxFF molecular dynamics simulations were conducted at fixed temperatures of 2200, 2400, 2600, 2800, and 3000 K (with a system containing 5 target molecules) to isolate the effect of thermal energy on the reaction pathways and decomposition efficiency; the results are summarized in Fig. 5. The simulations revealed that the heating rate significantly influences the

observed pyrolysis products. Faster heating rates (15 K/ps) led to a higher abundance of intermediate radicals and larger molecular fragments due to the shorter residence time at intermediate temperatures, which limited the extent of secondary cracking reactions. In contrast, slower heating rates (5 K/ps) allowed more time for these primary fragments to undergo further decomposition, resulting in a higher final yield of small gaseous molecules such as CO, CO₂, and light hydrocarbons. The isothermal simulations at different temperatures provided critical insight into the temperature-dependent reaction mechanism. The onset of significant bond cleavage was observed at approximately 2400 K, corresponding to the initiation of primary pyrolysis. As the temperature increased from 2600 K to 3000 K, the decomposition rate accelerated dramatically, and the product distribution shifted. At lower temperatures (e.g., 2600 K), the products were dominated by phenolic compounds and heavier hydrocarbons originating from the initial cleavage of ether (C-O) and C-N bonds. At higher temperatures (2800-3000 K), these primary products were rapidly consumed through secondary reactions, leading to a marked increase in the ultimate yields of syngas (CO, H₂) and small hydrocarbon gases (CH₄, C₂H₄). This atomic-scale observation correlates with the macroscopic TGA data, explaining the increased gas production at higher experimental temperatures. The results underscore that temperature primarily controls the reaction kinetics and product spectrum, while the heating rate governs the progression towards equilibrium products by affecting the time available for secondary reactions.

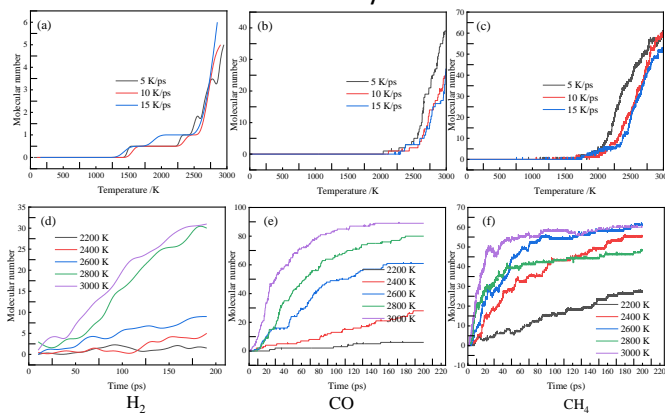


Fig. 5 Temporal evolution of the total number of H₂, CO, and CH₄ molecules at different temperatures

3.2.3. Initial Pyrolysis Pathways and Identification of Weak Linkages

The atomic-level trajectory analysis provides critical insights into the initial pyrolysis mechanisms. The

simulations reveal that the thermal degradation is initiated predominantly by the homolytic cleavage of two types of bonds: Ether linkages (C-O bonds) in the chain segments. C-N bonds adjacent to the aromatic rings, characteristic of the amine-based hardener. These scissions generate initial radical sites, which serve as precursors for a cascade of subsequent radical-driven reactions, including hydrogen abstraction, β -scission, and ring-opening events. The identified low bond dissociation energies (BDEs) for these linkages confirm them as the intrinsic weak points in the epoxy network structure.

3.2.4. Formation Pathways of Key Products

The simulations allow for the tracking of the detailed chemical routes leading to the formation of the observed major products: CO and CO₂: CO formation is primarily linked to the direct decomposition of carbonyl-containing intermediates or the rearrangement of radical fragments involving oxygen atoms. CO₂ is mainly generated from the decarboxylation of carboxyl groups (-COOH) formed through oxidative reactions. H₂O: The generation of water molecules is a result of dehydration reactions, often involving neighboring hydroxyl groups. Phenol: Phenol and its derivatives are produced through the fragmentation of the aromatic diamine hardener segments or the bisphenol-A units in the epoxy monomer, where C-Ar bond breakage is followed by hydrogen abstraction. Hydrocarbons: Small aliphatic hydrocarbons (CH₄, C₂H₄, C₂H₆) are formed from the cracking and hydrogenation of alkyl bridge segments (e.g., isopropylarene groups) connecting the aromatic rings.

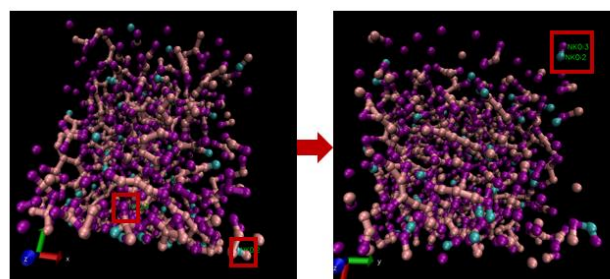


Fig. 6 Mechanism of CO generation in the pyrolysis reaction of epoxy resin

4. CONCLUSIONS

Through a combined experimental and ReaxFF MD simulation approach, this study reveals that the pyrolysis of epoxy resin from decommissioned wind turbine blades proceeds via a two-stage mechanism, initiated by the cleavage of weak C-O and C-N bonds. Major gaseous products include CO, CO₂, H₂O, phenols, and light

hydrocarbons, with an average activation energy of XXX kJ/mol. The simulations confirm the initial reaction pathways and product formation mechanisms, providing atomic-level insight essential for optimizing pyrolysis conditions toward efficient and high-value recycling of blade materials.

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