Computational Modeling of the Combustion Reaction Kinetics of the Oil Palm's Empty Fruit Bunch and Mesocarp Fiber

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Abstract

Empty Fruit Bunch (EFB) and Palm Mesocarp Fiber (PMF) are abundant by-products of palm-oil milling whose energetic valorisation is limited by high moisture and corrosive ash constituents (K, Cl). Using a computational model developed in Python and solved with the Livermore Solver for Ordinary Differential Equations with Automatic method switching algorithm, this study presents a moisture-free, mass- and energy-balanced kinetic framework that predicts the time-resolved combustion behavior of both biomasses, thereby strengthening the reproducibility and transparency of the modeling framework. The kinetic model tracks the consumption of elemental species and formation of combustion products, calibrated with data from the NIST Chemical Kinetics Database. The model accurately reproduces the low-heating-value energy releases reported in the literature—147.11 MJ for EFB and 158.27 MJ for PMF—while additionally resolving transient species profiles, heat-release rates and combustion-power curves. Simulations reveal that EFB attains its maximum heat release at an Air to Fuel Ratio ≈ 13 % lower than PMF, yet still delivers greater boiler-usable enthalpy after accounting for moisture-free energy balance. Our results demonstrate that rigorous physicochemical characterisation combined with detailed chemical kinetics provides a reliable, transferable toolset for designing next-generation

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biomass boilers and unlocking the energy potential of agro-industrial residues such as EFB.

Keywords: Combustion, Empty Fruit Bunch (EFB), Palm Mesocarp Fiber (PMF), Reaction Kinetics, Combustion Modeling, Biomass Boilers

1. Introduction

Palm oil has become the world's most important vegetable oil, with global output exceeding ≈ 78 million tons in 2023, driven chiefly by Indonesia and Malaysia, which together supply more than four-fifths of the total [1, 2]. Rapid acreage expansion is also occurring in emerging producer regions such as Latin America and sub-Saharan Africa, motivated by biofuel mandates, export demand and rural-development policies.

The milling process simultaneously generates large quantities of lignocellulosic residues—chiefly Empty Fruit Bunch (EFB) and Palm Mesocarp Fiber (PMF)—whose energetic valorisation can improve both the economic and environmental performance of the industry worldwide. Among these, EFB account for approximately 20% of the FFB weight, followed by PMF at 13% and Palm Kernel Shells (PKS) at 4% [3], as depicted in Figure 1. These by-products represent a significant waste, yet less than 10% of EFB and PMF are currently used for energy or industrial purposes [4].

Despite its high carbon content and energy potential, EFB is often underutilized as a fertilizer after it is buried openly, leading to material loss and contributing to environmental pollution. This uncontrolled practice results in the emission of greenhouse gases such as methane, which has a global warming potential over 80 times greater than that of carbon dioxide over a 20 year horizon [5]. In response, the exploitation of EFB in energy demanding processes is proposed.

Recent studies have shown that partially replacing PMF (the primary biofuel currently used in industrial boilers for energy generation in oil palm industries) with EFB can lead to a 28,81% increase in energy potential and fulfill a cycle process of energy production [3]. Moreover, this substitution would enable the reallocation of PMF to value-added applications such as paper production and structural enhancement of recycled cardboard, due to

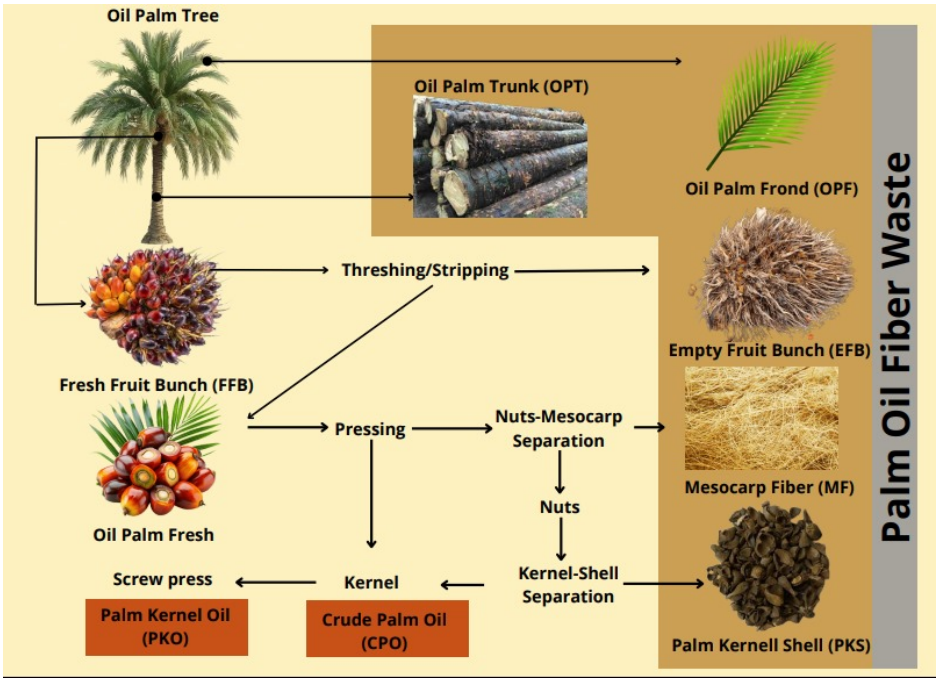

Figure 1: Main biomass residues generated in the palm oil industry.

its high cellulose content [6, 7].

To examine the viability of this substitution and assess the feasibility of using EFB as an alternative biofuel, understanding its chemical potential with the Low Heating Values (LHV) and kinetics (composition over time) is crucial, as these factors directly influence the energy yield and combustion behavior. A higher LHV indicates greater energy content per unit mass, while favorable kinetics ensure efficient and stable conversion during combustion. Using the LHV is the first possible model in early-stage boiler design or adaptation. Nonetheless, it is limited to quantify released thermal energy and no information about combustion gases composition can be obtained. On the other hand, combustion kinetics models of EFB is able to predict the deposition of alkali metals and chlorine, and the detailed chemical species distribution in the exhaust gases.

Previous studies on biomass combustion modeling have focused on Thermo Gravimetric Analysis (TGA) as the primary method for deriving kinetic pa-

rameters [8]. Some works have applied the Coats–Redfern method to TGA and Derivative Thermogravimetry (DTG) data from oil palm residues to fit multi-stage decomposition models and calculate activation energies for different stages [9, 10]. Others have combined TGA with Differential Scanning Calorimetry (DSC) to derive thermal degradation profiles and adjust parallel reaction schemes for palm oil by-products [11]. Although these methods offer detailed insights into thermal decomposition, they rely on fixed laboratory conditions, are not easily adaptable to iterative system-scale analysis, and require extensive recalibration for each scenario.

More complex kinetic approaches have also been developed, including detailed reaction networks of biomass pyrolysis or combustion [12, 13]. Those models can involve hundreds of elementary reactions and are often constructed for wood or municipal solid waste, as in [14, 15]. While accurate, such models require high computational effort and extensive chemical data, making them less feasible for practical, early-stage boiler design or adaptation to diverse fuels. Other works have employed empirical kinetics combined with CFD or simplified reactor models to simulate ignition and burnout phases [16, 17], but without resolving species evolution over time or applying the method to oil palm biomass. A recent example of empirical kinetic modeling that prioritizes simplicity and curve fitting over mechanistic detail is presented in [18], though it does not address time-resolved species profiles or specific applications for palm biomass.

By now, no previous study has developed a combustion model capable of simulating the temporal evolution of reactants and products for oil palm EFB and PMF. Most published works for these biomass either focus on fuel characterization, heating value, or static equilibrium outputs. Even existing models for EFB gasification [19, 20] do not resolve the dynamic behavior of species concentrations during the reaction process. As a result, there is a lack of tools capable of supporting time-dependent combustion diagnostics for this biomass in boiler systems.

In contrast, the model proposed in this study introduces an accessible method to simulate EFB and PMF combustion, for easier numerical resolution and visualization of the results (in Python). It uses a system of coupled ordinary differential equations derived from mass balance principles for each biomass. While the LHV of the biomass is used to validate the final energy

output, the model allows for the resolution of species evolution, combustion duration, and conversion completeness. Additionally, it supports a dynamic energy and power analysis based on the simulated temporal profiles and a defined combustion chamber volume, enabling thermochemical evaluation throughout the reaction. The model can also be extended to perform parametric Air-Fuel Ratio (AFR) analysis to identify the value that maximizes thermal energy release for each biomass, facilitating direct fuel comparisons under standardized conditions. This structure offers insight into reactant depletion, intermediate formation, and product stabilization (information not captured by static models) inside the combustion chamber. Moreover, it permits integration into future studies on flame control, biomass injection techniques, air injection optimization, and material selection within biomass boilers.

By filling this methodological gap, the present model contributes a new perspective to the combustion analysis of oil palm biomass, focused on simplicity, adaptability, and temporal resolution. Thus, the main objective of this study is to develop and validate a combustion model for EFB and PMF, two of the most representative residues from the oil palm industry, in order to assess their chemical potential as biofuels in industrial boiler applications.

Previous kinetic approaches for biomass combustion often rely on semi-empirical formulations derived from thermogravimetric analysis, such as model-free methods applied to forest residues [21], or on semi-global kinetic schemes where pyrolysis and combustion are represented through lumped pseudo-components fitted to experimental curves [22]. Although these approaches allow estimating global kinetic parameters, they do not resolve the time-dependent evolution of real chemical species. On the other hand, detailed kinetic mechanisms include hundreds of elementary reactions and demand substantial computational resources, which limits their applicability for iterative studies or early-stage design [16].

Within this landscape, the model proposed in the present work positions itself between these two extremes. It explicitly predicts the temporal evolution of key reactants and products for EFB and PMF while maintaining low computational cost and a mathematically simple structure. To our knowledge, this combination of multi-species tracking, time-resolved combustion behavior, and computational efficiency has not been previously reported for