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Kinetic Parameter Estimation and Optimization of Bio-Oil and Phenol Production from Mahogany Wood Via Pyrolysis and Fluid Catalytic Cracking Using gPROMS

Samuel Ekamba, Uwem Inyang, Innocent Oboh, Kingsley Egemba

Abstract: ***The thermochemical conversion of wood waste into high-value biofuels and chemicals for energy use represents a promising approach to clean, sustainable energy. This research investigates the modeling, simulation, and optimization of bio-oil and phenol production from mahogany wood waste (Swietenia macrophylla) using an integrated process approach of fast pyrolysis and fluid catalytic cracking (FCC). Kinetic parameters were estimated, and process conditions were optimised using the gPROMS ModelBuilder 4.0 software. The application of a Franz kinetic model during the pyrolysis stage identified an activation energy of 106.7 kJ/mol and a maximum bio-oil yield of 41.98% under optimal conditions of 558.7°C, a residence time of 1.92 s, and a heat capacity of 2.50 kJ/kg·K. The ensuing fluid catalytic cracking stage, developed with a novel nine-lump kinetic model, realised a maximum phenol yield of 37.086% at 595.28°C, a residence time of 2.48 s, a weight hourly space velocity (WSHV) of 16.58 h^{-1}, and a catalyst-to-oil (C/O) ratio of 7.2. A statistical tool, analysis of variance (ANOVA), confirmed the models' statistical significance, with R^2 values of 0.9984 for pyrolysis and 0.8926 for fluid catalytic cracking (FCC), respectively. Model predictions showed 70.6% accuracy when computed against actual experimental data. These outcomes highlight the efficacy of gPROMS for kinetic modeling and simulation of complex biomass conversion processes.***

Keywords: Modelling, Methodology, Bio-Oil, gPROMS, Kinetic

Nomenclature:
FCC: Fluid Catalytic Cracking
PFD: Process Flow Diagram
gEST: gPROMS Parameter Estimation Tool
SSE: Sum of Squared Errors
SQP: Sequential Quadratic Programming

I. INTRODUCTION

The global energy crisis, health and environmental concerns associated with fossil fuel extraction, production, and consumption have intensified the search for renewable and carbon-neutral energy sources. Biomass, particularly lignocellulosic waste, presents a viable feedstock for producing biofuels and biochemicals [1]. Nigeria, as a major agricultural and wood-processing nation, generates significant quantities of wood waste, such as mahogany, which is often underutilized, leading to environmental issues [2].

Thermochemical conversion methods, notably pyrolysis, fluid catalytic cracking, and liquefaction, are effective and advanced pathways for transforming biomass and other types of waste into bio-oil, a liquid fuel that can be upgraded and converted into transportation fuels and valuable chemicals [3]. Flash pyrolysis, characterized by high heating rates, high temperature and short vapour residence times, maximises liquid bio-oil yield [4]. However, crude bio-oil is unstable, corrosive, and rich in oxygen content, necessitating further refining. Fluid Catalytic Cracking (FCC), a fireball in petroleum refining, has emerged as a promising technology for bio-oil upgrading, deoxygenating it into hydrocarbons and phenolics [5].

Pyrolysis and FCC are vital thermochemical processes extensively employed in the chemical industry [6]. The complexity of these processes, involving numerous reactions and sensitive operational parameters (temperature, residence time, catalyst type), makes experimental optimization costly and time-consuming. Although the financial implications of pyrolysis and FCC setup, operational cost, and revenue generation through bio-oil and other chemical sales make pyrolysis and FCC processes an economically competitive option [7]. Computer-aided modelling and simulation offer an efficient alternative [8]. While previous studies have modelled pyrolysis, few have focused on the integrated simulation of pyrolysis and FCC for specific feedstocks like mahogany wood, and even fewer have utilized the equation-oriented capabilities of gPROMS for detailed kinetic parameter estimation and optimization of this system [9, 10].

This research fills this gap by employing gPROMS to:

i. Develop and optimize a model for the rapid pyrolysis of mahogany wood to maximize bio-oil yield.
ii. Model the FCC upgrading of the produced bio-oil using a nine-lump kinetic model to maximize phenol yield.
iii. Estimate the kinetic parameters for both processes.
iv. Validate the model predictions against literature data and conduct an economic feasibility analysis.

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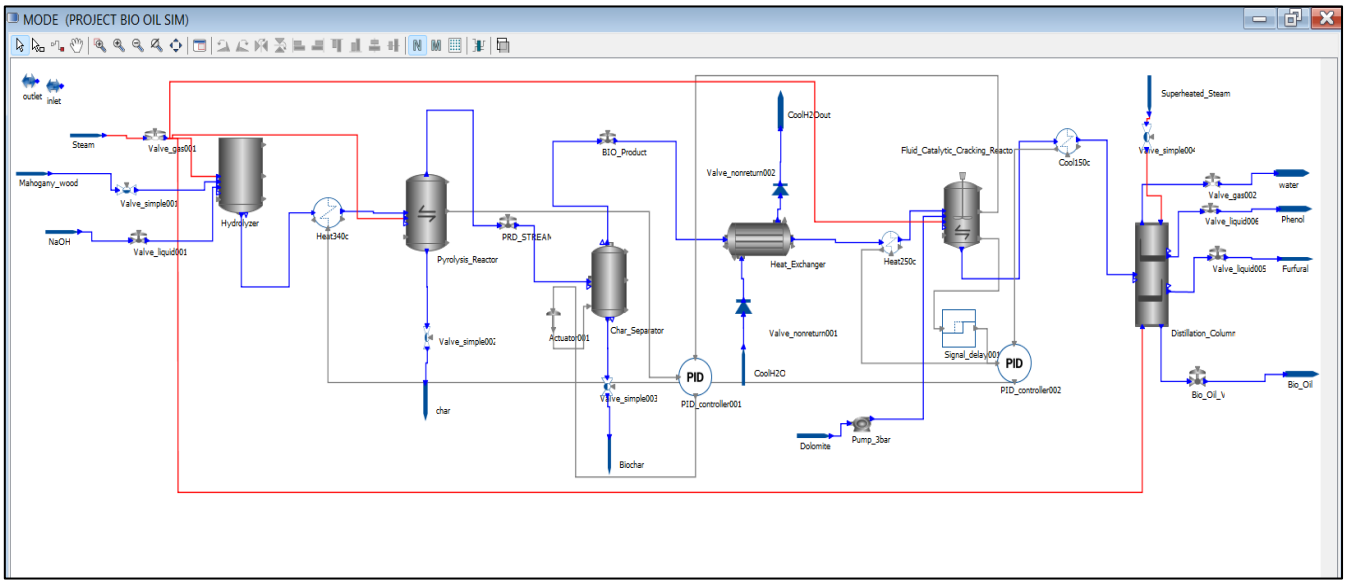
II. MATERIALS AND METHODS

A. Process Description and Feedstock

The study simulated an integrated plant comprising feedstock pretreatment (hydrolysis), pyrolysis, char separation, and FCC upgrading. The feedstock was mahogany wood waste, with properties detailed in Table 1. The process flow diagram (PFD) was developed and simulated in gPROMS (Figure 1).



[Fig.1: gPROMS PFD for the Production of Bio-Oil from Mahogany Wood Waste]

Table I: Proximate and Ultimate Analysis of Mahogany Wood Waste [11]

Ultimate Analysis (wt.%)	Value	Proximate Analysis (wt.%)	Value
Carbon	55.30	Moisture Content (wt.%)	9.80
Sulphur	<0.60	Volatile matter	79.11
Hydrogen	4.56	Fixed Carbon	13.85
Oxygen	39.26	Ash	1.24
Nitrogen	<0.34	HHV (MJ/kg)	21.26
		Cellulose	28.08
		Hemicellulose	29.52
		Lignin	21.9
		Particle size	0.8 mm

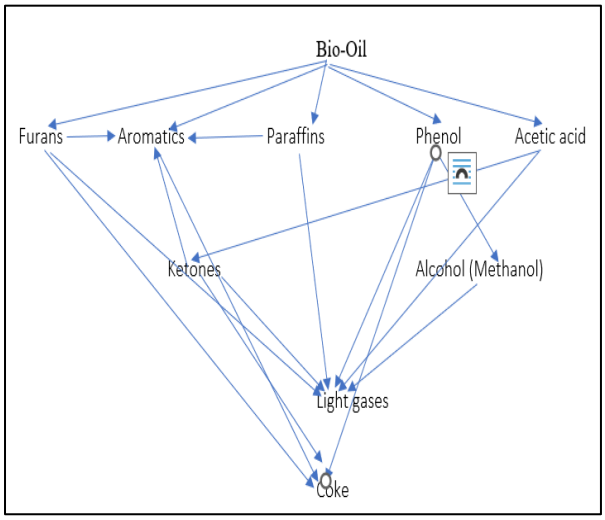
B. Modeling Framework In Gproms

gPROMS Model Builder 4.0 was used for all simulations, which were conducted at steady state. The key unit operations modelled were:

i. *Hydrolyzer:* Pretreatment with NaOH was modelled using Seaman's kinetic model for lignocellulose breakdown [12].

ii. *Pyrolysis Reactor:* A fluidized bed reactor was modeled. The kinetics of mahogany wood decomposition were described using the Franz model, a first-order competing reaction model for the production of gas, tar (bio-oil), and char [13].

iii. *Fluid Catalytic Cracking (FCC) Reactor:* The bio-oil vapour from pyrolysis was fed to an FCC unit. A nine-lump kinetic model was developed, categorizing the bio-oil into lumps: Aromatics (C_1), Paraffins (C_2), Phenols (C_3), Carboxylic Acids (C_4), Furans (C_5), Alcohols (C_6), Ketones (C_7), Light Gases (C_8), and Coke (C_9). The model comprised 20 reaction pathways (Figure 2).



[Fig.2: Bio-oil Reaction Pathways]

C. Kinetic Parameter Estimation

The gPROMS parameter estimation tool (gEST) was used to determine unknown kinetic parameters (pre-exponential factor *A* and activation energy *Ea*) by minimizing the sum of squared errors (SSE) between model predictions and data sourced from literature [14]. The Arrhenius equation was used for all rate constants.

D. Optimization and Statistical Analysis

The Sequential Quadratic Programming (SQP) algorithm in gPROMS was used to optimise the yields of bio-oil and phenol. The influence of process variables (temperature, residence time, heat capacity, WSHV, C/O ratio) was analyzed using Analysis of Variance (ANOVA) and 3D response surface plots.

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III. RESULTS AND DISCUSSION

A. Pyrolysis Process Optimization

Table 2 shows the simulated yields of bio-oil, char, and syngas at different temperatures. Bio-oil yield increased with temperature, peaking at 550°C (41.3%) before declining at 600°C due to secondary cracking, while char yield consistently decreased.

Table II: Simulated Product Yields from Pyrolysis

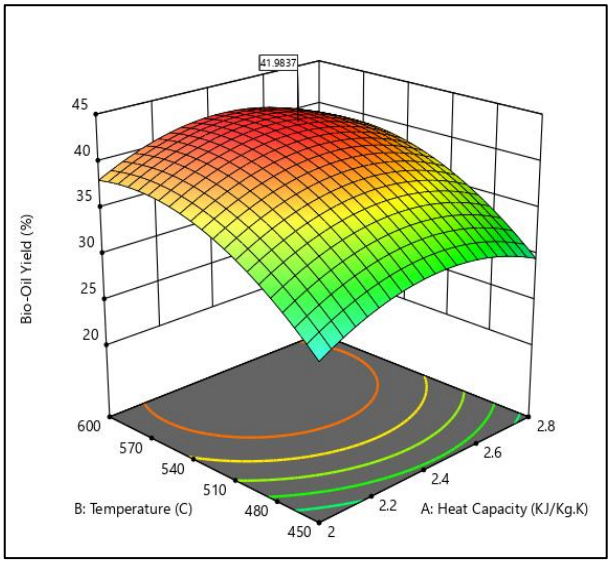
Temperature (°C)	Bio-Oil Yield (%)	Char Yield (%)	Syngas Yield (%)
450	27.5	29.5	38.7
500	33.5	23.0	43.0
550	41.3	20.6	38.0
600	37.8	16.9	44.2

ANOVA (Table 3) confirmed that temperature ($p < 0.0001$) and residence time ($p = 0.0002$) were the most significant factors affecting bio-oil yield. The model was highly important with an excellent R^2 of 0.9984.

Table III: ANOVA for Pyrolysis Bio-oil Yield (Response 1)

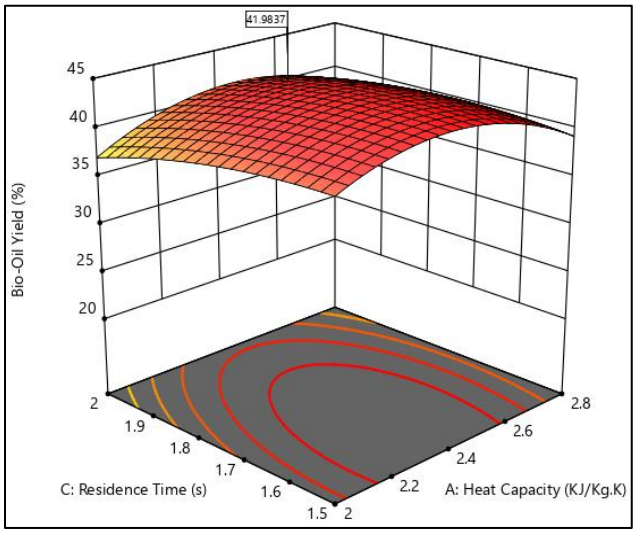
Source	Sum of Squares	F-value	p-value
Model	476.28	337.41	< 0.0001
A-Heat Capacity	0.0023	0.0146	0.9087
B-Temperature	329.30	2099.52	< 0.0001
C-Residence Time	15.70	100.08	0.0002
Residual	0.7842		

The 3D response surface plots in Figures 3, 4, and 5 illustrate the interactive effects among the variables. The optimization process found a maximum bio-oil yield of 41.98% at 558.7°C and a residence time of 1.92 s.



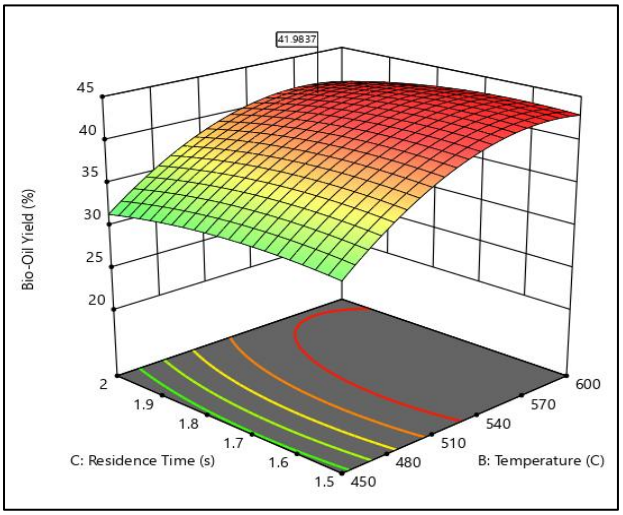
[Fig.3: 3D Plot of Temperature and Heat Capacity on Response 1]

The three-dimensional surface plot in Figure 3 shows the combined effect of heat capacity (A) and temperature (B) on bio-oil yield (%). The plot reveals that bio-oil yield increases with both parameters up to a specific optimal region, beyond which it begins to decline. The maximum yield of 41.98% is achieved at approximately 2.4–2.5 kJ/kg·K for heat capacity and 540–550 °C for temperature. This indicates that moderate thermal parameters and biomass properties favour the formation of bio-oil. However, excessive temperature or heat capacity can lead to secondary cracking or gasification, lowering the bio-oil yield and increasing the biochar yield. The contour map below further supports this trend, showing a distinct peak region surrounded by decreasing-yield zones, which helps identify optimal operating conditions for maximum efficiency.



[Fig.4: 3D Plot of Residence Time and Heat Capacity on Response 1]

The three-dimensional surface plot in Figure 4 shows the influence of heat capacity (A) and residence time (C) on bio-oil yield (%). The yield increases with both variables up to an optimal point, peaking at 41.98%. The maximum yield occurs at around 2.4–2.5 kJ/kg·K for heat capacity and 1.7 seconds for residence time. The contour plot shows a curved region of high values, displaying a defined optimal zone. This relationship suggests that controlling the thermal parameters and retention time maximises and minimises bio-oil yield.



[Fig.5: 3D Plot of Residence Time and Temperature on Response 1]

The three-dimensional surface plot in Figure 5 illustrates how temperature (450 °C – 600 °C) and residence time (1.5 s –2.0 s) affect bio-oil yield (%) from wood waste pyrolysis. The yield increases with both factors, reaching about 42% at higher temperatures and longer residence times. The smooth and convex response surface suggests a strong combined effect of these variables. The contour plot at the base highlights this gradient, with the red region indicating the optimal conditions, as also shown in Figure 6.

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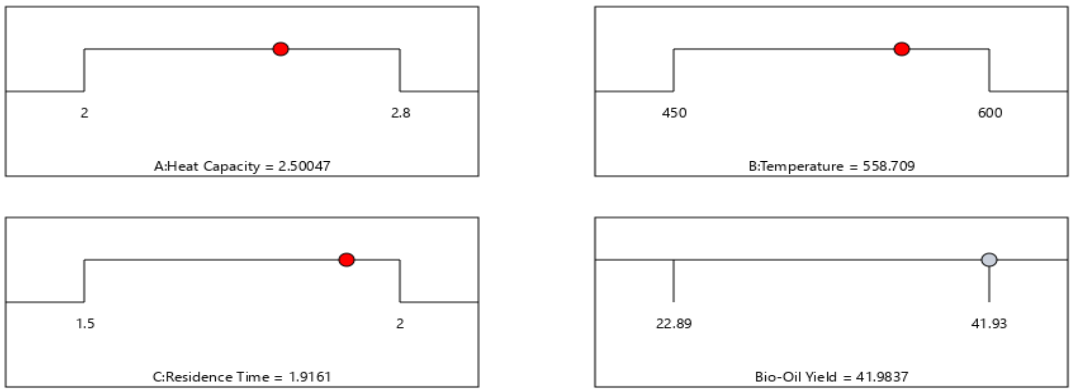


[Fig.6: Optimized Solution]

B. Fluid Catalytic Cracking (FCC) Optimization

The FCC simulation results (Table 4) showed that product distribution was susceptible to temperature. Phenol yield was targeted for optimization.

Table IV: FCC Product Yields (wt.%) at Varying Temperatures

Temp (°C)	Aro	Phe	Ket	Lg	Cok
450	6.51	14.7	18.0	12.0	8.56
500	7.33	15.5	18.7	12.4	9.80
550	8.20	15.6	18.2	12.8	10.2
600	7.10	13.1	17.6	13.0	11.9

For the FCC stage, ANOVA (Table 5) showed that residence time (p = 0.0012) and C/O ratio (p = 0.0003) were the most critical linear factors for phenol yield. The model R^2 was 0.8926.

Table V: ANOVA for FCC Phenol Yield (Response 3)

Source	Sum of Squares	F-value	p-value
Model	159.95	8.90	< 0.0001
A-Temperature	1.50	1.17	0.2967
B-Residence Time	20.17	15.17	0.0012
D-C/O Ratio	28.17	21.95	0.0003
Residual	19.25		

Optimization of the FCC process yielded a maximum phenol yield of 37.086% at 595.28°C, a residence time of 2.48 s, a WSHV of 16.58 h^{-1}, and a C/O ratio of 7.2.

C. Kinetic Parameter Estimation

The Franz model for pyrolysis provided a good fit to the data (R^2 = 0.7875), yielding a rate constant *k* of 0.4808 s^{-1} and an activation energy *Ea* of 106.7 kJ/mol as shown in Table 6. For the FCC process, the 20 kinetic parameters for the nine-lump model were successfully estimated [15]. The pre-exponential factors and activation energies (e.g., k_1: A=1.0×10⁶ s^{-1}, Ea=180 kJ/mol) were consistent with the highly reactive and complex nature of bio-oil cracking, as demonstrated in Table 7

Table VI: Franz model

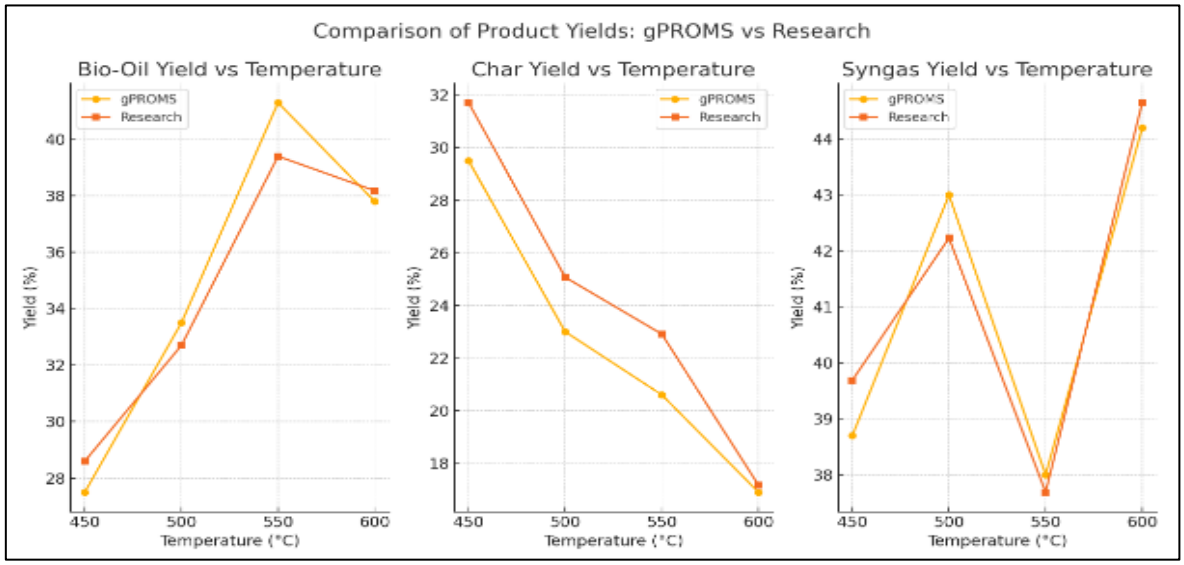
Parameters	Outcome
General model:	t) $= B[1 - \exp(-kt)]$
Coefficients (with 95% confidence bounds):	B = 16.71 (16.89, 17.54) k = 0.4808 E_a = 106.7 KJ/mol
Goodness of fit:	SSE: 23.67 R-square: 0.7875 Adjusted R-square: 0.7774 RMSE: 12.47

Table VII: Kinetic Parameter Estimation of FCC

K_n	Pathway	A (s^{-1})	Ea (kJ/mol)	Calculated K @ 450 °C	500 °C	550 °C	600 °C
k_1	$C_1 \rightarrow C_2$	1.0×10^6	180	9.95E-08	6.90E-07	3.78E-06	1.70E-05
k_2	$C_1 \rightarrow C_3$	1.0×10^5	200	3.57E-10	3.07E-09	2.03E-08	1.08E-07
k_3	$C_1 \rightarrow C_8$	1.0×10^7	220	1.28E-09	1.37E-08	1.09E-07	6.89E-07
k_4	$C_2 \rightarrow C_3$	5.0×10^5	170	2.62E-07	1.63E-06	8.14E-06	3.38E-05
k_5	$C_2 \rightarrow C_8$	5.0×10^6	190	9.43E-08	7.28E-07	4.38E-06	2.15E-05
k_6	$C_3 \rightarrow C_1$	1.0×10^5	200	3.57E-10	3.07E-09	2.03E-08	1.08E-07
k_7	$C_3 \rightarrow C_9$	2.0×10^5	230	4.86E-12	5.77E-11	5.07E-10	3.48E-09
k_8	$C_4 \rightarrow C_2$	2.0×10^6	190	3.77E-08	2.91E-07	1.75E-06	8.59E-06
k_9	$C_4 \rightarrow C_8$	2.0×10^7	210	1.35E-08	1.30E-07	9.43E-07	5.47E-06
k_{10}	$C_4 \rightarrow C_9$	5.0×10^5	240	2.30E-12	3.05E-11	2.94E-10	2.19E09
k_{11}	$C_5 \rightarrow C_3$	1.0×10^5	200	3.57E-10	3.07E-09	2.03E-O8	1.08E-07
k_{12}	$C_5 \rightarrow C_8$	1.0×10^6	220	1.28E-10	1.37E-09	1.09E-08	6.89E-08
k_{13}	$C_5 \rightarrow C_9$	2.0×10^5	240	9.22E-13	1.22E-11	1.18E-10	8.77E-10
k_{14}	$C_6 \rightarrow C_1$	5.0×10^5	200	1.79E-09	1.54E-08	1.02E-07	5.42E-07
k_{15}	$C_6 \rightarrow C_8$	5.0×10^6	220	6.42E-10	6.84E-09	5.47E-08	3.45E-07
k_{16}	$C_6 \rightarrow C_9$	1.0×10^6	250	8.74E-13	1.29E-11	1.37E-10	1.11E-09
k_{17}	$C_7 \rightarrow C_1$	5.0×10^5	200	1.79E-09	1.54E-08	1.02E-07	5.42E-07
k_{18}	$C_7 \rightarrow C_2$	5.0×10^5	210	3.39E-10	3.24E-09	2.36E-08	1.37E-07
k_{19}	$C_7 \rightarrow C_8$	5.0×10^6	230	1.22E-10	1.44E-09	1.27E-08	8.69E-08
k_{20}	$C_7 \rightarrow C_9$	1.0×10^6	260	1.66E-13	2.71E-12	3.17E-11	2.97E-10

D. Model Validation

A comparison between the gPROMS simulation and experimental data from literature [14] showed a strong correlation (Figure 7), with a prediction accuracy of 70.6% [16].



[Fig.7: Experimental Vs Simulated Comparison Plots]

IV. CONCLUSION

This study demonstrates the successful use of gPROMS for kinetic modelling and optimisation of an integrated pyrolysis-FCC process to convert mahogany wood waste into bio-oil and phenol. Key findings include the optimal conditions for maximising bio-oil yield (41.98%) from fast pyrolysis: 558.7°C and a residence time of 1.92 s. The optimal conditions for maximising phenol yield (37.086%) from FCC upgrading are 595.28°C, a residence time of 2.48 s, a WSHV of 16.58 h^{-1}, and a C/O ratio of 7.2. The Franz model and the novel nine-lump FCC model effectively describe the reaction kinetics, with estimated parameters providing a strong basis for reactor design. The high statistical significance of the models and the positive economic assessment highlight the potential for industrial application.

The use of gPROMS proved highly effective, conserving time and resources that would otherwise have been spent on extensive experimental work. This work provides a robust framework for simulating and optimising advanced biomass conversion processes.

DECLARATION STATEMENT

As the article's author, I must verify the accuracy of the following information after aggregating input from all authors.

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