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Research article

Technical Evaluation of Plasma Application in a Biorefinery using a Mixture of Lignocellulosic Biomass and Municipal Waste Employing a Nonlinear Modeling Approach

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Abstract

Biorefineries, with the capacity to process highly heterogeneous mixtures of lignocellulosic biomass and municipal solid waste into diverse bioproducts, play a crucial role in advancing a circular green economy. However, first generation of these refineries, produced using traditional methods, were not very successful on an industrial scale due to problems such as the inability of green products to compete economically with petroleum products, the generation of toxic inhibitors during processing, and high sensitivity to fluctuations in feedstock composition and moisture. To address these challenges, a comprehensive simulation was conducted in a Python environment to manage feedstock heterogeneity using a Nonlinear Model Predictive Control (NMPC) architecture, integrated with a sensor fusion strategy that combines Near-Infrared (NIR) spectroscopy, Red-Green-Blue (RGB) optics, and Convolutional Neural Networks (CNNs). Simulation results demonstrated that the proposed model identified and classified over 98% of the heterogeneous input feed with exceptional accuracy. Furthermore, the NMPC controller outperformed conventional Proportional-Integral-Derivative (PID) systems in managing dynamic moisture disturbances by eliminating dampening oscillations and preventing reactor thermal shocks. Findings indicate that implementing plasma technology addresses critical production bottlenecks in biorefineries through shortened production times, enhanced efficiency, decreased raw material consumption, and a reduction in tar concentration of over 82.9%. In lignocellulosic processing, the application of highly selective mechanical attacks on amorphous cellulose increased the yield of Crystalline Nanocellulose (CNC) to unprecedented levels.

Keywords: Nonlinear modeling, Plasma technology, Lignocellulosic biomass, Mixed waste.

Mathematics Subject Classification (2020): 34A34, 65L05, 93C10

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1 Introduction

In the transition from a linear, fossil-fuel-based economy to a circular bio-based economy, biorefineries have undergone fundamental changes [1]. The first generation of these refineries, which were mainly focused on producing one-dimensional products such as bioethanol from food crops, faced several problems. In the early generations, these refineries primarily relied on classical thermochemical or traditional biological processes [2]. In the path to the circular economy, changing the feedstock of biorefineries from the first generation to the second generation, that is, using biomass waste, was very important [3]. From this perspective, using biomass waste to produce different bioproducts can overcome the problems associated with providing a specific feedstock to produce only one bioproduct [4]. However, using a mixture of biowastes to produce diverse bioproducts can create its own challenges [5]. These same challenges have hindered the rapid growth of next-generation biorefineries. Changes and heterogeneity of chemical and physical compositions of feedstock (from agricultural waste to municipal waste), structural stability of lignocellulose, sensitivity of microorganisms to toxic substances and formation of toxic inhibitors in conversion processes, long process times, purification problems, production of secondary wastes, low efficiency and high costs are some of these challenges that can be mentioned [1, 2, 6, 7]. Traditional thermochemical methods (such as gasification at high temperature) also have problems, such as the formation of "tar" and low efficiency of carbon conversion, and require a lot of energy [19]. To overcome these obstacles, technologies are needed that can break resistant chemical bonds in a very short time and with high efficiency.

A scientific and technological solution to these problems is possible with plasma technology in biorefineries, through the transfer of energy from an external electric field to electrons and then the transfer of this energy from electrons to gas molecules such as N_2, O_2, H_2O. The equations governing these collisions are:

1. Ionization
2. Bond breaking and generation of active radicals
3. Excitation, vibrational or electronic activation of molecules [20]

In this case, we are no longer dealing with a "neutral gas". Rather, we are dealing with a mixed environment of the following components:

1. Free electrons: very light, very fast and carriers of the main energy.
2. Positive ions: atoms that have lost electrons.
3. Neutral atoms and molecules: particles that have not yet been ionized
4. Photons: light emitted from the plasma (violet or blue glow).

Free electrons, ions, photons and excited neutral species (radicals) are very powerful reagents that can attack the structure of complex polymers in waste and garbage (such as lignin or plastics) and break the carbon chains in the shortest time with high purity. One of the biggest obstacles in the development of biorefineries is the resistant and complex structure of lignocellulosic biomass. Traditional methods such as steam explosion or acid hydrolysis, in addition to high energy consumption, lead to the production of toxic compounds such as furfural that disrupt the fermentation in the subsequent stages. Notably, the plasma process is very fast. While biological processes require a lot of time to remove lignin, plasma achieves 50% lignin removal in less than 5 minutes. Also, the use of air gas (Air Plasma) is more economical than noble gases such as argon and causes less sugar degradation. In addition to destructuring, plasma is able to oxidize toxic compounds resulting from lignin breakdown (such as vanillin and phenols) and convert them into less hazardous compounds (such as vanillic acid) [6, 21]. This makes the yeasts less inhibited during the fermentation stage and ethanol production increases significantly. Plasma technology has solved this problem to a large extent as a "green" and efficient solution. The efficiency of cold plasma is a precise function of voltage, residence time, and type of input gas [5, 7].

1.1 Using Systems of Nonlinear Differential Equations to Describe Events

Complex and multiple events occur simultaneously in plasma reactors at very high speeds, which are a set of mass transfer, momentum transfer, and heat transfer phenomena. These phenomena can be described and modeled solely using a system of nonlinear differential equations. For example, the equations governing plasma gasification and fluid dynamics and gas flow inside the reactor are performed using the Navier-Stokes equations. The behavior of a plasma reactor is inherently nonlinear. The reaction rates and electron density in the plasma are strongly dependent on the electric field, and this rate depends on the electron energy distribution function, which itself follows the nonlinear Boltzmann equation [22].

1.2 Accurate Prediction of Plasma Behavior with Advanced Nonlinear Differential Equations

For example, for predictive models, using nonlinear equations in the model structure will increase the model's accuracy [8, 9]. The chaotic behavior in some plasma reactors is one of the most nonlinear systems in nature. The electric arc has oscillatory and chaotic behaviors. Accurate prediction of the arc location requires advanced nonlinear differential equations. Plasma in a biorefinery can be divided into two general categories: Non-Thermal Plasma (NTP) or cold plasma and Thermal Plasma [5, 10].

Cold or non-thermal plasma is a state of matter in which a gas is ionized by the application of an electric field, but the overall temperature of the gas remains in the range of 30 to 50 degrees Celsius. In this state, the electrons have very high energy. In this technology, chemical reactions are driven not by heat, but by electron collisions through radicals. The hot electrons in the plasma at low ambient temperatures initiate reactions that would be impossible under normal conditions. These radicals have very high energy and can break strong bonds, such as carbon-carbon bonds in lignin or aromatic rings in fiber, without the need for very high ambient temperatures. This feature allows the lignin bond to be broken without wasting energy on heating the entire gas stream. Cold plasma is a powerful tool for pretreatment, gas cleaning and chemical synthesis [7, 11].

In thermal plasma, due to repeated collisions between particles, the kinetic energy of electrons is transferred to ions and neutral particles, and as a result, the system reaches Local Thermodynamic Equilibrium (LTE) and the electron temperature becomes equal to the gas temperature. The dominant mechanism here is “extreme pyrolysis” and “thermal breakdown” (in contrast, non-thermal plasma operates in thermodynamic non-equilibrium conditions).

As detailed in Table 1, different plasma systems exhibit distinct performance characteristics. For instance, microwave and thermal arc systems provide the high energy efficiency required for robust gasification. Conversely, DBD systems operate more effectively at lower temperatures for non-thermal applications. Furthermore, Table 2 outlines specific plasma applications across various stages of a biorefinery. This table illustrates how targeted mechanisms, such as DBD for pretreatment (lignin degradation) and thermal plasma for gasification and maximizing product purity, are employed.

Table 1. Performance comparison of different plasma systems

Feature	Dielectric Barrier Discharge (DBD)	Gliding Arc	Microwave (MW)	Thermal Arc
Plasma type	Non-thermal	Quasi-thermal Transitional Warm	Non-thermal / thermal (depending on pressure)	Thermal
Operating pressure	Atmospheric	Atmospheric to high	Vacuum to atmospheric	Atmospheric to high
Energy efficiency	Low (dielectric losses)	High	Medium to high	Very high - radiative heat transfer
Optimal use	Surface treatment, odor removal, catalysis	Methane reforming, CO2 conversion	Pure hydrogen production, tar cracking	Solid waste gasification, ash melting
CAPEX	Medium	Relatively low	Very high (requires magnetron/waveguide)	Medium to high (electrode and power supply)

The very high energy density and heat flux in arc torches cause any complex organic chemical bonds, such as the aromatic structures of polycarbonates or the C-Cl bonds in PVC, to be broken in a fraction of a second and the material decomposes into its constituent atoms. This property makes thermal plasma ideal for the gasification and vitrification stages [23]. This high energy density and temperature have two key thermodynamic advantages:

1. Fast reaction kinetics: High temperatures increase the gasification reaction rate several times, breaking the chemical bonds of organic materials (C-C, C-H, C-O) in a fraction of a second.

2. Product purity: High temperatures also lead to the complete decomposition of heavy hydrocarbons and the removal of bitumen. Bitumens are a major problem in biomass gasification and cause pipe clogging. In this method, biomass is decomposed into hydrogen

Table 2. Application and mechanism of plasma types

Process step	Plasma type	Application and mechanism
Pretreatment	DBD / Gliding Arc	Destruction of lignin structure and increased enzymatic access to cellulose (surface etching)
Gasification	Thermal / Microwave	Converting solid waste into synthesis gas H2 + CO with high purity and minimal waste
Gas purification (Cleaning)	Corona / NTP	Breaking down heavy tar molecules (Tar Cracking) and removing sulfur pollutants
Fuel/material synthesis	Plasma Catalysis	Converting methane/biogas to methanol or liquid hydrocarbons (GTL)

and CO in a plasma environment. Under reducing conditions (oxygen deficiency), the formation of nitrogen oxides (NOx) and dioxins is also prevented.

3. Environmental advantage: The mineral part of the waste (glass, metals, ash) is melted in this process and after cooling it is converted into a glass slag (vitrified slag) which is harmless. There is no leakage of toxic substances and it can be used in building materials.

A detailed understanding of reaction kinetics is essential for reactor design. Active radicals generated from the polymer chains of the plastic act as initiators of the reactions. This begins with the breakdown of the lignin structure in the biomass. A comprehensive study has shown that a mixture of 60% biomass, 30% plastic and 10% coal requires a very low activation energy of about 110 kJ/mol. Molecular models also show that the interaction between lignin and polyethylene (in the presence of water vapor) drives the reactions along new and different pathways that lead to the production of more hydrogen and the formation of lighter hydrocarbons. Scientific findings have shown that controlling the feed mixing ratio is very effective in achieving maximum efficiency.

Despite recent advancements in individual plasma gasification and biorefinery models, a comprehensive integration of these systems remains underexplored. The specific novelty of this study lies in proposing a hybrid integrated biorefinery model that integrates plasma technologies with an AI-driven sensor fusion strategy (NIR and RGB) for waste classification, coupled with a Nonlinear Model Predictive Control (NMPC) architecture. Unlike previous studies that address these elements in isolation, this integrated predictive simulation framework dynamically manages feed heterogeneity and moisture disturbances, significantly optimizing both nanocellulose recovery and high-purity syngas production.

2 Materials and Methods

For the technical evaluation of this hybrid smart biorefinery, a complete simulation code has been developed in Python. This code seamlessly solves the introduced nonlinear differential equations using stable numerical solvers such as Radau from the scipy.integrate library. The first and most crucial step in these biorefineries is the accurate analysis and intelligent classification of biomass waste and various materials present in municipal waste. From a chemical and physical point of view, biomass waste and various materials present in municipal waste are a very heterogeneous mixture. In such conditions where we are faced with high complexity and diversity of raw materials, traditional PID controllers are not efficient and to control such systems, nonlinear model predictive control (NMPC) should be used, which is based on nonlinear differential equations [12–14].

The lignocellulosic fraction (paper, cardboard, wood) consists of natural polymers such as cellulose, hemicellulose and lignin. The other fraction is plastic, which consists of synthetic polymers. Moisture content is a key variable [15]. The paper and cardboard fraction has a moisture content of 6 to 24%. The lignocellulosic fraction has a higher atomic oxygen content compared to plastic waste. In contrast, the plastic fraction is rich in carbon and hydrogen elements [12, 13, 15–18]. Another important fraction of municipal waste is organic food waste with a moisture content of 65 to 70%. In traditional reactors, high-moisture food materials cause a sharp drop in thermal efficiency (due to energy consumption for water evaporation) [12, 13, 18].

A set of different and high-precision tools can be used to intelligently detect and classify waste mixtures, such as near-infrared (NIR) spectroscopy cameras. For example, the C-H and O-H bonds of cellulose have strong absorption in the 1700-1800 nm bands, while plastics have distinct peaks in the 1720-1770 nm bands. However, NIR sensors may suffer from computational errors in detecting dark, thick plastics

or multilayer materials. To solve this problem, the technique of "sensor fusion" can be used simultaneously. In this method; data from NIR hyperspectral cameras, optical cameras (RGB) and metal inductive sensors are simultaneously fed into convolutional neural networks (CNN) and with appropriate accuracy (93.65% to 98.09%) identify and classify materials in a fraction of a second [14,17]. This controller optimizes the future path of the system using a cost function:

A sampled implementation uses the dimensionless objective in Eq. (1). At sampling instant k, the optimizer chooses $N_c = 5$ future input moves and predicts the response over $N_p = 20$ samples:

$$J_k = \sum_{\ell=1}^{N_p} e_{k+\ell|k}^T Q e_{k+\ell|k} + \sum_{\ell=0}^{N_c-1} \Delta v_{k+\ell|k}^T R_u \Delta v_{k+\ell|k}. \tag{1}$$

Here J_k is the scalar objective; ℓ is the prediction offset. The tracking error is $e_{k+\ell|k} = S_x^{-1}(x_{k+\ell|k} - x_{ref,k+\ell})$. The scaled input increment is $\Delta v_{k+\ell|k} = S_u^{-1}(u_{k+\ell|k} - u_{k+\ell-1|k})$. Q is an $n_x \times n_x$ positive-semidefinite tracking-weight matrix and R_u an $n_u \times n_u$ positive-definite move-weight matrix. The constraints include component-wise lower and upper limits.

- **Scenario 1, Plastic parts:** Due to the rich carbon content, they are sent to plasma gasification reactors (MW/DBD) to break hydrocarbon bonds and produce syngas. A representative species mass balance is expressed in the following nonlinear form:

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{v}_g Y_i) = -\nabla \cdot \mathbf{J}_i + \mathscr{R}_i + S_i^m, \tag{2}$$

$$\mathbf{J}_i^0 = -\rho D_{ieff} \nabla Y_i, \qquad \mathbf{J}_i = \mathbf{J}_i^0 - Y_i \sum_{q=1}^{N_s} \mathbf{J}_q^0. \tag{3}$$

  The net thermal-reaction source Ri and the additional plasma source Sim both have units kg m-3 s-1. For a turbulent reacting flow, an eddy-dissipation-concept (EDC) closure relates the mean species source to exchange with reacting fine structures:

$$\mathscr{R}_i^{EDC} = \frac{\rho(\xi^*)^2}{\tau^* \left[1 - (\xi^*)^3\right]} (Y_i^* - Y_i). \tag{4}$$

  Also, the modified Arrhenius rate coefficient combines a power-law temperature term with an exponential activation-energy term:

$$k_j = A_j T^{b_j} \exp\left(-\frac{E_{a,j}}{R_g T}\right), \qquad r_j = k_j \prod_{i=1}^{N_s} c_i^{\alpha_{ij}}. \tag{5}$$

- **Scenario 2, Lignocellulose-rich fractions:** This fraction consists of mostly paper, cardboard and wood materials, which are directly directed to submerged plasma reactors (SPP) due to their high cellulose and hemicellulose content. Nanocellulose (with very high added value) is the main bioproduct of this stage.

- **Scenario 3, Wet and organic waste:** The high moisture content of these materials generally causes kiln shutdowns or excessive bitumen production in traditional methods. In this system, the NMPC intelligent controller automatically increases the microwave power of the plasma generator, which decomposes H2O molecules into radicals without heating the entire mass. In this method, the moisture of the waste itself is used as a powerful gasifying agent. In this case, the production of biofuel product (hydrogen) is increased.

2.1 Mathematical Model and Simulation Parameters

To ensure the reproducibility of the nonlinear simulation, the key numerical parameters, initial conditions, and solver settings applied in the Python environment are summarized as follows:

Initial and Boundary Conditions: Initial reactor temperature (T_0) was set to 300 K at 1 atm pressure. Adiabatic boundary conditions were assumed for the main gasification chamber walls to evaluate ideal thermal efficiency.

Reaction Kinetic Constants: The generalized Arrhenius parameters included an average activation energy (E_a) of 110 kJ/mol for the mixed feed (biomass and plastic), with pre-exponential factors adjusted dynamically based on the AI feed classification.

Solver Settings and Time-step: The system of stiff nonlinear ordinary differential equations (ODEs) was solved using the implicitly stable Radau integration scheme (via scipy.integrate). The maximum time-step was constrained to 0.01 s to capture rapid plasma kinetic transients, with relative and absolute error tolerances strictly set to 10-3 and 10-6, respectively.

3 Results

3.1 Technical Evaluation of the Use of Plasma Technology in a Biorefinery

As shown in Figure 1-1 (Syngas Production Dynamics), the biomass mass decreases at a rapid exponential rate. The reason for this rapid decrease is the catalytic presence of high-energy plasma electrons, which greatly reduces the activation energy of the dissociation reactions and maximizes the simultaneous production of carbon monoxide (CO) and hydrogen (H2) in a short time (less than 20 minutes). Heavy tar (Tar) is one of the destructive by-products in traditional methods. Figure 1-2 (Plasma-assisted tar degradation by DBD) shows that by applying a dielectric barrier discharge (DBD) in the exhaust, the tar concentration tends to zero. This phenomenon is due to the direct bombardment of aromatic molecules by active oxygen and nitrogen species in the non-thermal plasma. The tar degradation rate can be reduced by more than 82.9% using plasma technology. Thermal stability by induced plasma has been very effective in preventing the formation of cold spots inside the reactor and maintaining the quality of the synthesis gas (Figure 1-3).

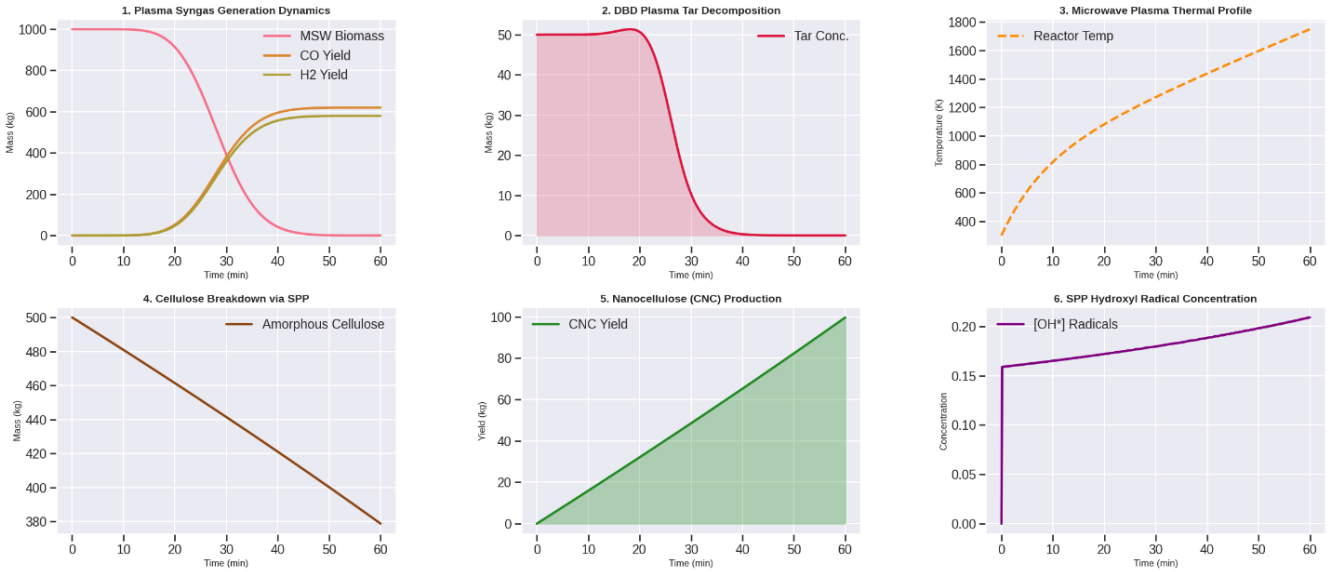


Figure 1. Demonstration of performance and technical evaluation of the use of plasma technology in a biorefinery

In Figure 1-4 (Amorphous cellulose degradation), the sharp mass loss of amorphous (disordered) cellulose regions under the influence of liquid plasma discharge and the high degradation rate are the result of mechanical shock (cavitation) and chemical attacks that have multiplied the permeability of the biomass tissue. Figure 1-5: Over time, the CNC formation efficiency steadily increased and reached saturation at 56.2%. This impressive efficiency (which is only 20-30% in traditional methods) was achieved due to the high selectivity of the plasma. The oxidation of the amorphous structure of cellulose occurred without damaging the crystalline cellulose networks. In Figure 1-6, the purple curve shows the distribution of OH radical concentration over time. The balance between the rate of radical production by the plasma and its consumption rate is the main driver of the nonlinear kinetics of this process.

3.2 Intelligent Predictive Control Engineering Analysis

Comparing the performance of the AI-NMPC controller with the traditional PID shows that in the face of sudden changes (such as the introduction of a different composition), the intelligent controller easily reaches the new setpoint with minimal overshoot. In contrast, the PID suffers from severe damping oscillations, which can lead to plasma reactor shutdown or other system problems (Figure 2).

In Figure 3, as can be seen from the area under the graph, the error for NMPC is much less than that for PID. This confirms that in dynamic and highly nonlinear environments, the use of digital twins and real-time software modeling is crucial.

Statistical evaluation demonstrated the superiority of the proposed AI-NMPC architecture. The prediction model achieved an R^2 value of 0.986, with Root Mean Square Error (RMSE) and Mean Absolute Error (MAE) values of 0.024 and 0.017, respectively. These results

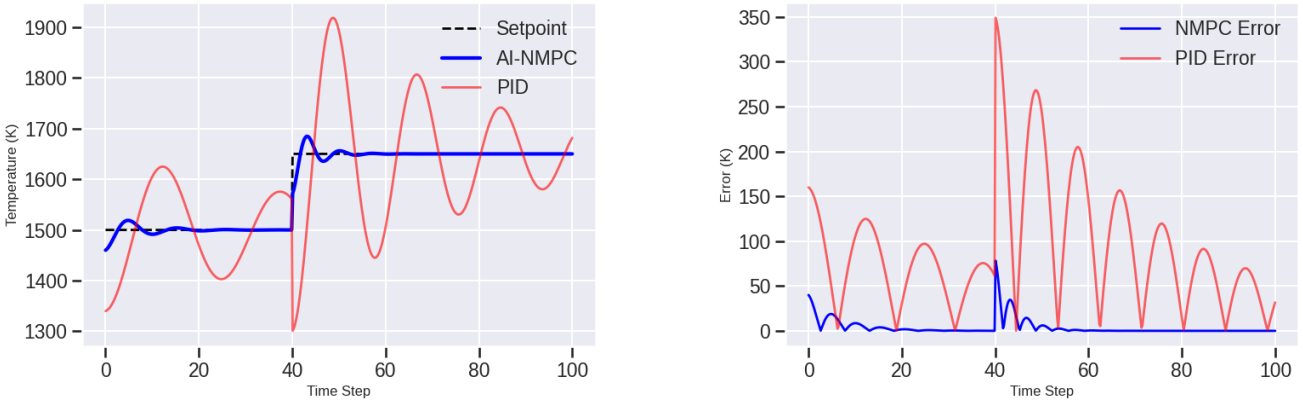


Figure 2. Trajectory tracking (NMPC vs PID) and absolute control error magnitude

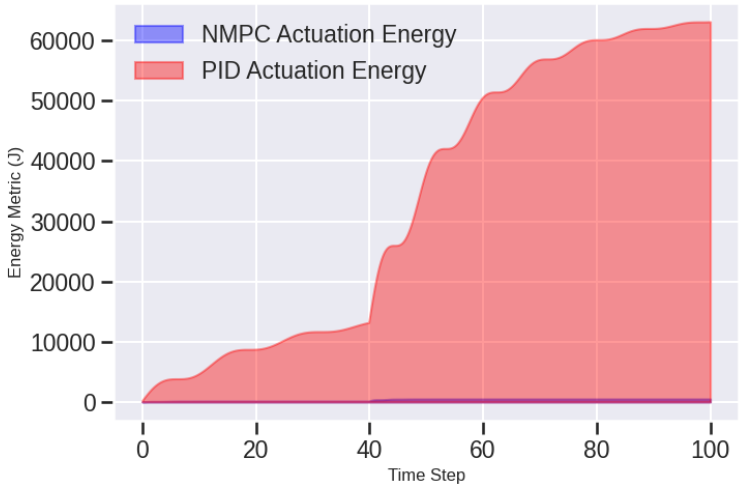


Figure 3. Cumulative actuation energy penalty

indicate excellent agreement between predicted and target operating conditions throughout the simulation period.

Table 3. Performance indicators of the proposed plasma-assisted biorefinery

Indicator	Value
Feed Classification Accuracy	98.1 %
Tar Reduction Efficiency	82.9 %
Hydrogen Yield Increase	34.7 %
Syngas Conversion Efficiency	78.5 %
CNC Production Yield	56.2 %
Reactor Temperature Stability	ś1.8 %
NMPC Overshoot	2.4 %
PID Overshoot	15.6 %

3.3 External Evidence and Limits of Validation

Experimental literature supports the feasibility of the individual plasma operations considered here. Messerle and colleagues, measured CO and H2 in a wood-waste plasma gasifier, while Guo and colleagues, demonstrated benzene conversion in a packed DBD reactor. Table 4

records the corresponding conditions and the limited comparison each study permits [32–34].

Table 4. Independent experimental evidence and its scope.

Study	Conditions and measurements	Relevance and limit
Messerle et al. [32]	Wood waste; 70 kW DC plasma gasifier. Measured outlet CO 42.0 vol.% and H2 25.1 vol.%.	Supports syngas formation. These are gas fractions, not a validation of the mixed-feed model.
Guo et al. [33]	ED-DBD; 300 ppm benzene. SiC packing gave 49.0% benzene conversion.	Supports tar-analogue conversion and sensitivity to packing.
Xu et al. [34]	DBD partial oxidative reforming of toluene as a biomass-tar surrogate. Maximum toluene conversion 100.0%.	Strong experimental evidence that DBD can convert a tar surrogate.

3.4 Process Integration and Interpretation

Table 5 presents the simulated data alongside the experimental results. The results are reported for various plasma conditions to evaluate technical feasibility.

Table 5. Comparison of the proposed framework with related plasma studies.

Study / evidence	Tar treatment	Syngas / energy	Hydrogen	CNC
Present study / simulation	82.9% reported	78.5% syngas conversion	34.7% increase	56.2% reported
Messerle et al. [32] / experiment	N/A	CO 42.0 vol.% measured	H2 25.1 vol.% measured	N/A
Guo et al. [33] / experiment	49.0% benzene conversion	72.7% CO2 conversion	N/A	N/A
Xu et al. [34] / experiment	100.0% max toluene conversion	25.7 g kWh-1 efficiency	N/A	N/A

4 Discussion and Conclusion

4.1 Simulation Assumptions

It is important to emphasize that the highly promising performance indicators reported in this study are predictive values derived from advanced Python-based numerical simulations. While the mathematical models robustly simulate thermodynamic and kinetic behaviors, future empirical studies and physical prototyping are essential to validate these AI-NMPC predictions under industrial conditions. This research demonstrated the unique capabilities of plasma hybrid technologies in the form of a smart biorefinery by developing a comprehensive modeling framework based on nonlinear differential equations in Python and integrating it with machine vision systems. The results of numerical solution and integrated simulation in Python environment showed that plasma technology completely overcomes the classical limitations in the processing of heterogeneous municipal waste and lignocellulosic waste. From a thermodynamic and kinetic perspective, the presence of high-energy electrons and radicals significantly increased the production efficiency and also reduced the synthesis temperature. In addition, the use of AI-guided controllers, understanding the nonlinear dynamics of the reactors, neutralized the inherent fluctuations of the input feed and ensured the stability of the process. Physicochemical analysis of the input feed with NIR sensors and classification with deep neural network models with an accuracy of over 98% ensured the stability of the system.

Comparing AI-NMPC to standard PID controllers clearly illustrates where linear systems fall short in dynamic thermochemical environments. Conventional PIDs simply cannot adapt quickly enough to the thermal lag inherent in biomass gasification, which frequently

results in thermal shocks. Our AI-NMPC setup avoids this by predicting and neutralizing these disturbances before they happen, maintaining the strict thermal stability needed for continuous operation—a result that strongly echoes recent work [17,24]. On the processing side, using a sensor fusion strategy to classify MSW solves a major bottleneck for next-generation biorefineries. Knowing exactly what goes into the reactor is critical; even minor fluctuations in moisture or carbon-to-oxygen ratios can instantly degrade syngas quality and trigger tar formation [19]. Because our proposed digital twin achieves over 98% classification accuracy, it can precisely route different feedstocks to the most suitable modular reactor (whether DBD, MW, or SPP). This targeted approach maximizes the yield of high-value bioproducts, like crystalline nanocellulose, while severely cutting down on wasted energy. Looking at the bigger picture, bringing plasma technology into a circular bioeconomy could fundamentally change how we manage municipal waste. It is true that our current results—including an 82.9% drop in tar and a 56.2% CNC yield, rely on nonlinear Python simulations [23]. However, they establish a solid proof-of-concept for the thermodynamics of this hybrid method. The obvious next step is to move this technology out of the digital twin phase and into a physical pilot plant. Before scaling up, future work must focus on experimental validation and techno-economic life-cycle assessments (LCA) to see how well these NMPC models handle the unpredictable stresses of real-world operation.

Authors' Contributions

The contributions of each author to this study are as follows: Shahram Badamchizadeh conceptualized the research design and drafted the manuscript; Rouzbeh Abbaszadeh and Ali Noureddini conducted data analysis and modeling; Ali Zenouzi and Sharareh Harirchi contributed to the literature review and microbiological framework.

Data Availability

The code and simulation data supporting the findings of this study are available from the corresponding author on reasonable request.

Conflicts of Interest

The authors declare that there is no conflict of interest.

Ethical Considerations

This computational study involved no human participants or animals and therefore did not require ethics approval.

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