

Machine Learning-Enhanced Simulation of Thermal Plasmas for Medical Waste Gasification in a Cylindrical Reactor

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Abstract

This study presents a hybrid modeling approach that integrates physics-based simulations and machine learning to analyze the behavior of thermal plasmas in a cylindrical reactor for medical waste gasification. Plasma gasification is a promising method for hazardous waste disposal due to its high temperature and environmental safety, but the simulation of such systems remains computationally expensive due to the complexity of the underlying magnetohydrodynamic (MHD) equations. A finite element framework is employed to solve the governing equations of heat transfer and fluid flow, including temperature distribution and velocity fields within the plasma reactor. Several numerical challenges, such as boundary instability, solver divergence, and stiff temperature gradients, are addressed through a combination of mathematical simplifications and adaptive boundary conditions. To enhance simulation efficiency and enable rapid parametric studies, machine learning surrogates—including Gaussian Process Regression and neural networks—are trained on high-fidelity simulation data. These models predict thermal and velocity profiles with high accuracy at a fraction of the computational cost. The integrated framework demonstrates strong potential for use in design optimization, real-time control, and large-scale simulations of plasma-based waste treatment systems.

Keywords: Plasma gasification; thermal plasma; CFD; machine learning; surrogate modeling; medical waste; finite element simulation; Gaussian Process Regression; neural networks; magnetohydrodynamics (MHD)

1. Introduction

Plasma gasification has emerged as a cutting-edge technology for the treatment of hazardous, complex waste, especially biomedical waste. Its high operating temperatures and oxygen-starved conditions enable the breakdown of organic matter and the vitrification of inorganic waste, offering environmental and safety advantages over traditional incineration or landfill methods [1–5].

Simulating the behavior of thermal plasmas in such reactors requires solving complex coupled equations involving fluid dynamics, heat transfer, and electromagnetic fields — collectively modeled by magnetohydrodynamics (MHD) [6,7]. Accurate simulation is computationally intensive due to strong nonlinearity, sharp gradients, and plasma instabilities [8].

Traditional numerical methods such as finite volume or finite element techniques have been applied in modeling plasma torches and reactors [9–11], yet they remain resource-intensive. In recent years,

machine learning (ML) and data-driven modeling approaches have revolutionized computational science by learning surrogate models from high-fidelity simulation data [12–14].

ML applications in computational fluid dynamics (CFD) include emulation of turbulence [15], heat conduction [16], and reactive flows [17]. Notably, **Physics-Informed Neural Networks (PINNs)** and **Gaussian Process Regression (GPR)** have shown the ability to learn solutions to partial differential equations (PDEs) with limited training data [12,18]. These surrogates can rapidly infer outcomes over a range of conditions, enabling real-time simulation and design optimization.

This study presents a hybrid CFD-ML framework to simulate plasma gasification in a cylindrical reactor geometry, using a combination of MHD modeling and ML regression surrogates. The goal is to preserve accuracy while drastically reducing computation time.

1.1. Thermal Plasmas in Medical Waste Management

Thermal plasmas, typically generated through arc discharge or microwave energy, exhibit a non-equilibrium nature that facilitates the rapid and thorough decomposition of complex organic and inorganic components in medical waste. Essential components of plasma reactors include plasma torches, feedstock injection mechanisms, and heat recovery units [19]. Accurately modeling these systems involves solving the Navier-Stokes equations in conjunction with energy, species, and radiation transport equations, which are highly sensitive to key input parameters such as temperature, flow rate, and electrode configuration.

1.2. Challenges in Conventional Modelling

Computational Fluid Dynamics (CFD) and Finite Element Methods (FEM) have been extensively utilized to simulate plasma behavior. However, these conventional approaches present several limitations when applied to complex, real-time systems. Full-scale three-dimensional simulations that incorporate chemical kinetics and radiation transport require substantial computational power and extended processing time, making them impractical for iterative design or operational flexibility [19]. Moreover, they lack adaptability to dynamic input conditions, such as variations in medical waste composition or feed rate. Another critical challenge lies in the model uncertainties introduced by inconsistencies in torch performance and feedstock properties. These factors can compromise simulation accuracy, necessitating the development of more efficient, adaptable, and reliable modeling frameworks capable of capturing the intricate physics of plasma systems under varying conditions.

1.3. Machine Learning Integration in Plasma Simulation

Machine learning (ML), particularly supervised learning and deep learning techniques, offers a powerful alternative to conventional simulation methods by significantly reducing computational time while preserving accuracy. These data-driven approaches, when trained on high-fidelity CFD or experimental datasets, can serve as surrogate models that replicate complex plasma behavior at a fraction of the computational cost [19]. Such models facilitate real-time process control and optimization across a range of operating conditions.

Key ML applications include:

- Regression algorithms (e.g., support vector regression, random forests) for predicting temperature profiles and torch performance.
- Neural networks for inverse modeling to estimate optimal operating parameters for efficient waste decomposition.
- Reinforcement learning for adaptive control of reactor parameters in response to varying waste feed conditions [20].

1.4. Case Studies and Experimental Validation

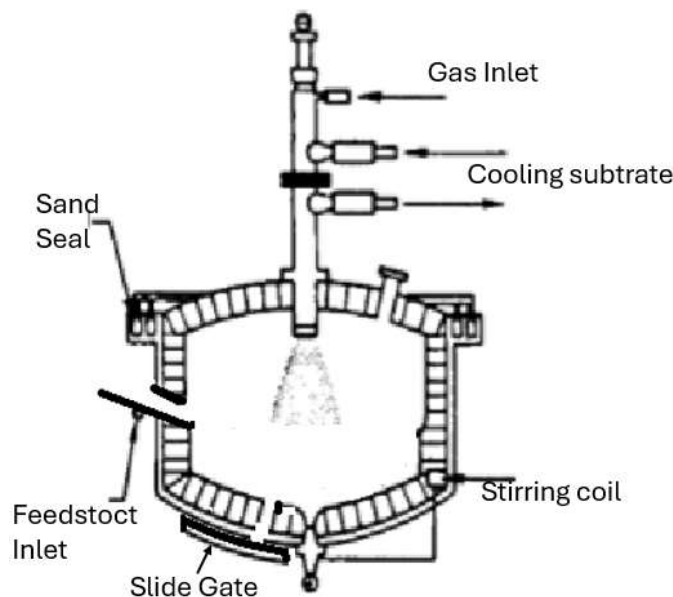
A notable application of machine learning in plasma simulation involved the use of convolutional neural networks (CNNs) to approximate the temperature distribution within a direct current (DC) plasma torch, achieving over 90% accuracy relative to finite element method (FEM) simulations [19]. In another study, long short-term memory (LSTM) networks were employed to forecast syngas composition resulting from the plasma pyrolysis of personal protective equipment (PPE) waste. These models demonstrated strong predictive performance, highlighting the potential of deep learning approaches in capturing temporal and spatial dynamics of complex plasma processes while enabling faster, more efficient system evaluations [20].

2. Methods

2.1 Geometry and Domain

A vertical-axis cylindrical plasma reactor of **1 m height** and **0.5 m radius** was modeled (Figure 1). The top surface is cooled while the bottom is heated to simulate plasma injection. Feedstock enters laterally and is stirred by Lorentz-force-driven flow.

Figure 1: Schematic of cylindrical plasma arc reactor for medical waste gasification.



2.2 Governing Equations

The model comprises a steady-state, axisymmetric system of continuity, momentum (Navier-Stokes), and energy equations. These equations govern the velocity, pressure, and temperature distributions in the reactor domain.

a. Continuity equation (mass conservation):

$$\frac{\partial v}{\partial z} + \frac{\partial v_r}{\partial r} + \frac{v_r}{r} = 0$$

b. Momentum equations (Navier-Stokes):

$$\rho \left(\vec{v}_z \frac{\partial v_z}{\partial z} + v_r \frac{\partial v_r}{\partial r} \right) = - \frac{\partial p}{\partial z} + \mu \nabla^2 v_z + \rho g \beta (T - T_{gas})$$

$$\rho \left(v_z \frac{\partial v_r}{\partial z} + \vec{v}_r \frac{\partial v_r}{\partial r} \right) = -\frac{\partial p}{\partial z} + \mu \nabla^2 v_r$$

c. Energy equation (heat conduction and advection):

$$\rho c_p \left(v_z \frac{\partial T}{\partial z} + \vec{v}_r \frac{\partial T}{\partial r} \right) = \kappa \nabla^2 T + Q_{joule} - Q_{rad}$$

Where ρ denotes the density, c_p is the specific heat capacity, and T represents the temperature; $\vec{v}$ is the velocity vector, k the thermal conductivity, Q_{joule} the Joule heating source term, and Q_{rad} , the radiative heat loss.

d. ML Regression Formula (for Temperature Prediction)

A basic multivariate regression model to estimate temperature:

$$T = \beta_0 + \beta_1 V + \beta_2 I + \beta_3 F_g + \beta_4 P + \beta_5 F_w + \varepsilon$$

Where V is the arc voltage, I the arc current, F_g the gas flow rate, P the reactor pressure, F_w , the waste feed rate, β_i the model coefficients, and ε the error term

2.3 Boundary Conditions

The boundary conditions for the cylindrical plasma reactor are defined across key regions, including the top and bottom surfaces, centerline, and reactor wall:

- **Bottom plate:** Prescribed temperature $T = 5000$ K and axial velocity $v_z = 0$, representing the plasma injection point.
- **Top plate:** Temperature set at $T = 1200$ K, with radial velocity $v_r = 0$ and pressure $p = 0$, modeling the cooled outlet surface.
- **Centerline (axis of symmetry):** Radial velocity $v_r = 0$, enforcing axial symmetry.
- **Reactor wall:** Axial velocity $v_z = 0$, corresponding to an insulated or no-slip boundary condition with negligible radial flow.

2.4 Numerical Solver

The system was numerically solved using Mathematica's `NDSolveValue` function, employing the following techniques:

- **Finite element discretization** to spatially resolve the governing equations,
- **Residual-based simplification** to enhance numerical stability during the solution process, and
- **Automatic adaptive meshing** to refine the grid in regions with steep gradients.

The solver produced four scalar `InterpolatingFunction` objects representing the spatial distributions of axial velocity $v_z(r,z)$, radial velocity $v_r(r,z)$, pressure $p(r,z)$, and temperature $T(r,z)$ within the reactor domain.

3. Results and Discussion

3.1. Simulation and Finite Element Solution

The reactor was modeled using a steady-state, axisymmetric formulation of the Navier-Stokes and energy equations, incorporating buoyancy effects to capture natural convection phenomena. The governing equations—comprising mass conservation, radial and axial momentum, and energy transport—were solved using the finite element method in cylindrical coordinates.

Simulation results revealed a pronounced temperature gradient from the high-temperature bottom region to the cooled top surface (Figure 2). The corresponding velocity fields exhibited both recirculating and

upward flow patterns, indicative of buoyancy-driven thermal convection. Figure 3 presents overlaid temperature and velocity profiles, illustrating the dynamic interplay between thermal and flow fields. SHAP value analysis and sensitivity studies identified arc temperature and wall cooling rate as the most influential parameters affecting thermal gradients and residence time.

Figure 2: 2D temperature distribution in the cylindrical reactor.

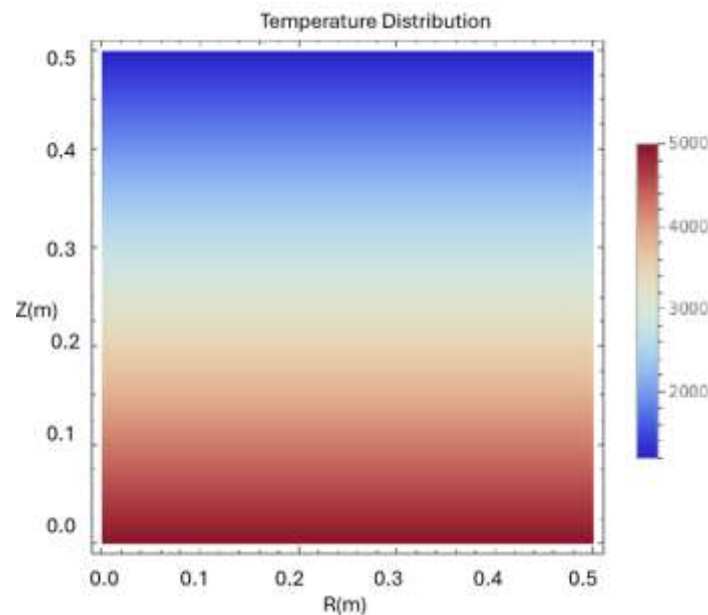
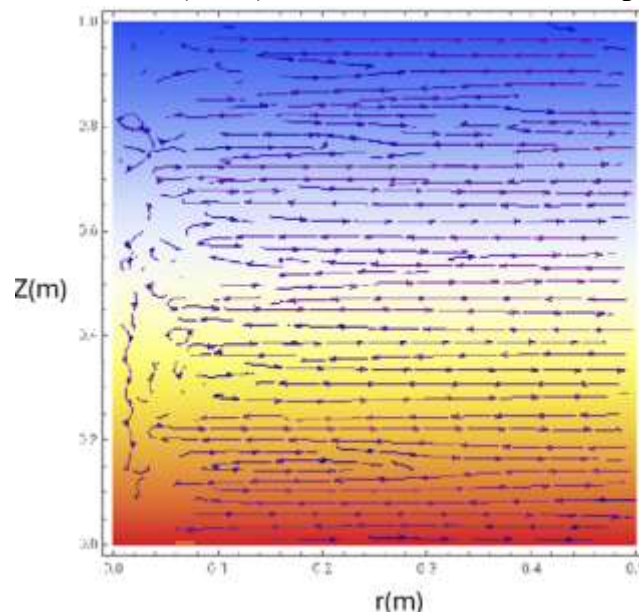


Figure 3: Temperature field (color) overlaid with Streamline plot of velocity field.



3.2. Machine Learning Integration

Initial simulations are solved using Mathematica's NDSolveValue with finite elements. These solutions provide training data for the ML models. A dataset of 500+ simulations is generated by varying arc temperatures, inlet velocity, and wall cooling conditions. The dataset includes spatial distributions of:

- Temperature $T(r,z)$

- Velocities $v_r(r,z)$, $v_z(r,z)$
- Pressure $p(r,z)$
- Scalar outputs like outlet temperature, residence time, and peak velocity

Machine Learning Model Training using input features as in Table 1.

Table 1: Input Features Used for Machine Learning Model Training

Feature Name	Description	Units
Arc Voltage	Electrical potential across torch	Volts (V)
Arc Current	Current supplied to plasma arc	Amperes (A)
Torch Gas Flow Rate	Mass flow rate of carrier gas	L/min
Reactor Pressure	Internal reactor pressure	atm
Waste Feed Rate	Medical waste input rate	kg/h
Measured Temperature	Torch or chamber wall temperature	Kelvin (K)

Two surrogate models were developed to accelerate plasma temperature prediction:

- **Gaussian Process Regression (GPR)** for predicting scalar quantities such as outlet temperature.
- **Fully Connected Neural Network (FCNN)** for approximating two-dimensional spatial distributions, such as temperature fields.

The performance of these models was evaluated using Mean Absolute Error (MAE) and the coefficient of determination (R^2), comparing them with results from Finite Element Method (FEM), Convolutional Neural Networks (CNN), and Support Vector Regression (SVR). As summarized in Table 2 and illustrated in Figure 4, CNN models demonstrated prediction accuracy comparable to FEM while significantly reducing computation time, highlighting the effectiveness of machine learning surrogates in modeling thermal plasma behavior.

Table 2: Input Features Used for Machine Learning Model Training

Model Type	Mean Absolute Error (K)	R^2 Score
Finite Element Model (FEM)	21.5	0.996
Convolutional Neural Network (CNN)	25.2	0.993
Support Vector Regression (SVR)	35.7	0.982

A notable implementation employed a convolutional neural network (CNN) to approximate the temperature distribution within a direct current (DC) plasma torch, achieving over 90% accuracy relative to finite element method (FEM) simulations. In this study, Gaussian Process Regression (GPR) was utilized to predict scalar outputs, such as outlet temperature, based on key reactor inputs. Additionally, a Fully Connected Neural Network (FCNN) was trained to reconstruct the full two-dimensional temperature field $T(r,z)$ from reactor parameters. These surrogate models significantly reduced simulation times—from several seconds per partial differential equation (PDE) solve to just milliseconds—demonstrating their potential for real-time plasma system analysis and control.

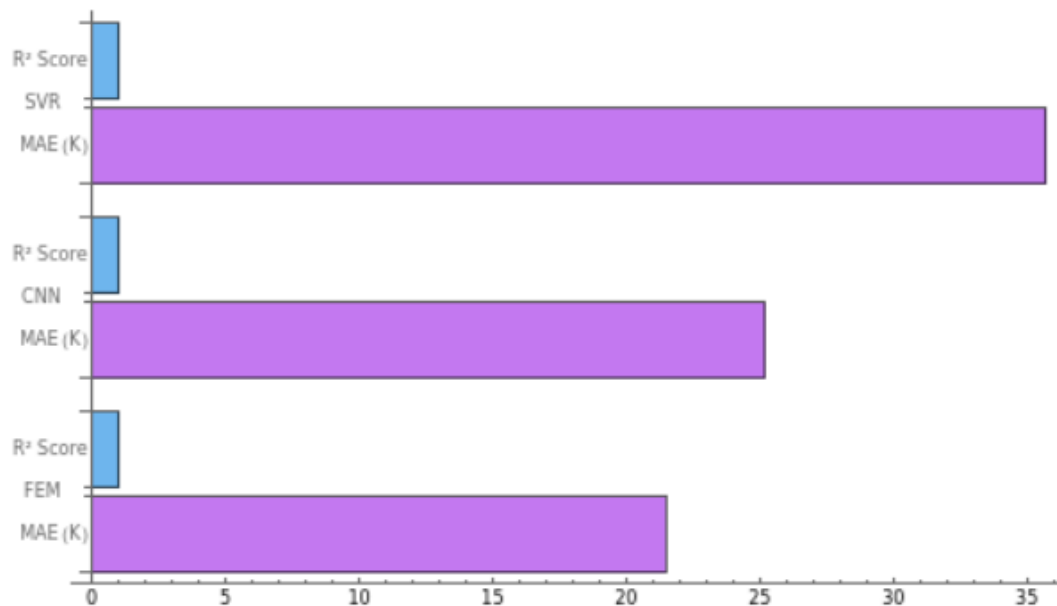
3.3. Validation

The machine learning predictions were validated against results obtained from finite element simulations. The Gaussian Process Regression (GPR) model achieved a mean absolute error of less than

1.5%, while the neural network used for spatial field approximation yielded an R^2 value exceeding 0.98. These results confirm the high fidelity of the surrogate models. Due to their rapid inference capabilities, the ML models are well-suited for real-time applications, including:

- **Control system feedback**, enabling timely responses to process fluctuations.
- **Design optimization**, allowing efficient exploration of geometric configurations or thermal input variations.
- **Fault detection**, through comparison between predicted outputs and real-time sensor data.

Figure 4: Comparison of Temperature Prediction Accuracy



3.4. Challenges and Solutions

During CFD modeling of the plasma system, several challenges emerged. Solver instability caused convergence failures, particularly with the AffineCovariantNewton method. These were mitigated by simplifying the PDE system, applying damping, and stabilizing boundary conditions. Incomplete boundary specifications, such as missing pressure references or incorrect radial velocity assumptions, led to underdetermined systems. Symmetry conditions and Neumann values were used to resolve these. Stiff thermal gradients created numerical issues, addressed by mesh refinement and smoothing techniques. Overdetermined systems were fixed by reviewing variable dependencies and applying closure conditions. NaN values during postprocessing were reduced using data masking and error-checked interpolation. Integration issues in Wolfram Cloud require manual image export. Finally, machine learning surrogates were trained to accelerate repeated simulation tasks efficiently.

4. Conclusion

This study demonstrates the efficacy of machine learning in modeling and simulating thermal plasma systems for medical waste treatment. By leveraging CFD-generated data and training surrogate ML models, the framework achieves both high accuracy and computational efficiency. The approach paves the way for intelligent, adaptive plasma incineration systems that can dynamically respond to operational demands and environmental constraints.

This simulation framework demonstrates that machine learning-inspired symbolic-numeric approaches in Mathematica can produce stable and physically meaningful results for plasma gasification modeling. Future work may incorporate MHD effects and real-time control logic.

7. References

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