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DYNAMIC MULTI-PHYSICS MODELING AND ADAPTIVE OPTIMIZATION OF HYDROGEN PRODUCTION REACTORS UNDER VARIABLE LOAD CONDITIONS

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Abstract- Hydrogen is increasingly recognized as a key energy carrier for sustainable transport systems; however, conventional hydrogen production reactors are typically designed for steady-state operation and perform sub optimally under dynamic transport demand. This study develops a multi-physics dynamic modeling and optimization framework for hydrogen production reactors operating under variable transport load conditions. The model integrates fluid dynamics, heat transfer, chemical kinetics, and pressure-flow interactions, while transport demand is incorporated as a time-dependent boundary condition. An adaptive nonlinear multi-objective control strategy is proposed to maximize thermodynamic efficiency and minimize temperature fluctuations, pressure losses, and transient instability. The proposed approach is benchmarked against classical PID and Model Predictive Control (MPC) methods. Simulation results show that the adaptive framework improves thermodynamic efficiency by up to 18% compared to PID and 9% compared to MPC, while reducing temperature oscillations by approximately 40% and significantly shortening stabilization time. CFD-based thermal analysis reveals improved temperature uniformity and reduced hotspot formation, while pressure-flow analysis indicates smoother flow distribution and lower hydraulic losses. The findings demonstrate that integrating transport demand variability into reactor modeling significantly enhances operational stability and energy efficiency. The proposed framework provides a scalable methodology for designing demand-responsive hydrogen production systems, supporting the development of sustainable transport energy infrastructure aligned with SDG 7, SDG 9, and SDG 13.

Keywords: Hydrogen Production Reactors, Steam Methane Reforming (SMR), Multi-Physics Modeling, Computational Fluid Dynamics (CFD), Dynamic Optimization, Adaptive Nonlinear Control, Model Predictive Control (MPC), Thermodynamic Efficiency, Hydrogen-Based Transport Systems, Sustainable Energy Infrastructure.

1. INTRODUCTION

The global transition toward sustainable transportation and the need for deep decarbonization have positioned hydrogen as a promising energy carrier for a wide range of transport applications, including fuel-cell buses, heavy-duty trucks, rail systems, and maritime transport. Hydrogen-based systems offer high energy density and zero tailpipe emissions, making them suitable for both urban and long-distance mobility. However, the large-scale deployment of hydrogen in transport systems remains constrained by the performance, flexibility, and operational adaptability of hydrogen production technologies.

Conventional hydrogen production reactors, particularly thermo-chemical systems such as steam methane reformers (SMR), are typically designed for near steady-state operation with relatively constant feed rates and thermal conditions. In contrast, real-world transport energy demand is inherently dynamic, characterized by peak-hour fluctuations, intermittent load variations, and stochastic consumption patterns. This mismatch between steady-state reactor design and dynamic demand profiles can lead to reduced thermodynamic efficiency,

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temperature instability, and increased pressure losses under transient operating conditions. Although recent studies have applied computational fluid dynamics (CFD), nonlinear control, and Model Predictive Control (MPC) techniques to improve reactor performance, most approaches treat reactor dynamics independently of transport demand variability or consider only simplified load scenarios [1].

This study develops a transport-coupled multi-physics modeling and optimization framework for hydrogen production reactors operating under dynamic demand conditions. Unlike conventional approaches that assume steady-state operation, the proposed model explicitly integrates time-dependent transport load variability into reactor dynamics, enabling demand-responsive hydrogen production. The framework combines fluid dynamics, heat transfer, and chemical kinetics with adaptive multi-objective optimization to ensure both efficiency and operational stability under transient conditions. Its performance is systematically evaluated against conventional PID and Model Predictive Control (MPC) strategies through numerical simulations and CFD-based analysis. By bridging the gap between transport energy demand and reactor operation, this work provides both theoretical advancements and practical guidelines for the design of resilient and flexible hydrogen energy systems [2].

2. LITERATURE REVIEW

Hydrogen production for transport applications has attracted significant research attention due to the global push for decarbonization and the increasing deployment of fuel-cell vehicles. Conventional hydrogen production methods include steam methane reforming (SMR), water electrolysis, and thermochemical cycles. Among these, SMR remains the most widely applied technology due to its high hydrogen yield and established industrial infrastructure. However, SMR and similar thermo-chemical reactors are predominantly designed for steady-state operation, limiting their flexibility under dynamic load conditions typical of transport systems.

Several studies have focused on the modeling and control of hydrogen reactors. Computational fluid dynamics (CFD) has been widely applied to analyze heat transfer, mass transport, and chemical reaction kinetics inside reformers. For example, researchers have demonstrated that CFD simulations can accurately capture temperature gradients, concentration distributions, and flow patterns, which are critical for optimizing reactor design and operation. These studies emphasize the importance of spatially resolved modeling to prevent hot spots, ensure catalyst longevity, and improve overall efficiency.

In parallel, process control research has explored the use of classical PID controllers and advanced Model Predictive Control (MPC) strategies for hydrogen reactors. PID controllers provide simplicity and ease of implementation but are limited in handling highly nonlinear dynamics and rapid load fluctuations. MPC, by contrast, offers predictive capabilities and multi-variable optimization, enabling better handling of transient operating conditions. However, most MPC applications in literature are tested under quasi-steady or idealized dynamic scenarios, often neglecting real-time transport demand variability.

Integration of hydrogen production with transport energy demand has been less explored. While a few studies have considered hydrogen supply for urban bus fleets or logistics networks, these typically model transport demand as a constant or slowly varying input, failing to capture rapid fluctuations in vehicle operation. There is also a lack of studies that simultaneously couple nonlinear reactor dynamics, transport-driven flow variations, heat transfer, and reaction kinetics into a single dynamic optimization framework [3].

Furthermore, multi-objective optimization approaches in hydrogen reactor research have largely focused on maximizing hydrogen yield or thermodynamic efficiency, without explicitly considering transient stability, pressure drop, or energy loss indices under variable operational loads. As such, existing literature highlights a methodological gap in combining CFD-based transient modeling, transport demand variability, and adaptive multi-objective optimization.

This study addresses these gaps by developing a fully coupled multi-physics model integrated with transport load fluctuations, applying adaptive nonlinear optimization, and providing comparative evaluation against PID and MPC strategies. The approach provides both theoretical and practical contributions by enabling reactor operation that is resilient to fluctuating transport demand while maintaining high efficiency and system stability [4]. Although significant progress has been achieved in hydrogen reactor modeling and control, most existing studies focus on steady-state operation and do not explicitly integrate transport demand variability into the reactor dynamics. A comparative overview of the main approaches reported in the literature is presented in Table 1.

Table 1. Comparison of existing hydrogen reactor control studies

Study Type	Modeling Approach	Transport Demand Considered	Control Method	Limitations
Conventional SMR studies	Steady-state thermodynamic models	No	PID	Limited flexibility
CFD-based reactor optimization	Thermal–fluid simulations	No	Static optimization	No dynamic demand response
MPC reactor control studies	Dynamic process modeling	Partial	MPC	Limited load variability
Proposed study	Multi-physics coupled PDE model	Yes	Adaptive nonlinear optimization	High computational complexity

Table 1 shows comparative overview of hydrogen reactor modeling and control approaches in literature.

3. MATHEMATICAL MODEL

3.1. System Definition and Modeling Assumptions

The system under investigation is a tubular steam methane reforming (SMR) reactor integrated with a transport-driven hydrogen demand module. The reactor operates under transient conditions where hydrogen production rate is dynamically adjusted according to transport load fluctuations. The reactor consists of a catalytic packed-bed domain with axial flow, where methane steam reforming occurs as an endothermic reaction. Heat is supplied externally through furnace coupling, while fluid flow is governed by pressure-driven transport.

The following modeling assumptions are adopted:

- The flow is laminar and incompressible
- Ideal gas behavior is assumed for all species
- Catalyst activity is uniform along the reactor
- Heat transfer occurs via conduction and convection
- Radiation effects are neglected
- Transport load affects boundary mass flow rate

These assumptions enable the formulation of a coupled nonlinear multi-physics model linking fluid dynamics, thermal transport, and chemical kinetics under time-dependent boundary conditions [5].

3.2. Fluid Dynamics

The reactor flow is governed by the incompressible Navier-Stokes equations:

$$\rho(\partial t\partial u + (u \times \nabla)u) = -\nabla p + \mu\nabla 2u + F \quad (1)$$

3.3. Energy Equation

$$\rho cp\partial t\partial T + \rho cp(u \times \nabla T) = k\nabla 2T + Q_{reaction} \quad (2)$$

3.4. Reaction Kinetics

For methane reforming:

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p (u \times \nabla T) = k\nabla^2 T + Q_{reaction} \quad (3)$$

Reaction rate:

$$r = k_0 \exp\left(\frac{E_a}{RT}\right) C_{CH_4} C_{H_2O} \quad (4)$$

3.5. Transport Load Coupling

Transport demand is modeled as:

$$L(t) = L_{base} + A\sin(\omega t) \quad (5)$$

Hydrogen mass flow rate is proportional to transport load:

$$\dot{m}H2(t) = kLL(t) \quad (6)$$

3.6. Coupled Multi-Physics Model Formulation

The governing equations can be expressed as a coupled nonlinear system:

$$F(u, T, C, p, L(t)) = 0 \quad (7)$$

where, the transport load function $L(t)$ acts as a time-dependent forcing term influencing hydrogen production rate, temperature field, and pressure distribution.

This formulation transforms the reactor into a non-autonomous dynamical system, distinguishing it from classical steady-state reactor models. The governing equations presented above form the basis of the coupled multi-physics model integrating fluid dynamics, heat transfer, chemical reaction kinetics, and transport-demand interactions. The key variables and parameters used in this modeling framework are summarized in Table 2.

Table 2. Multi-physics model variables

Symbol	Parameter	Physical Meaning
u	Velocity field	Fluid motion inside reactor
p	Pressure	Flow resistance
T	Temperature	Thermal state of reactor
r	Reaction rate	Hydrogen production intensity
$L(t)$	Transport load	Dynamic energy demand

Table 2 shows key variables used in the coupled thermo-fluid hydrogen reactor model. Unlike conventional reactor models, the proposed framework explicitly integrates transport demand variability into the governing equations, enabling real-time coupling between hydrogen production and dynamic energy consumption profiles. This represents a fundamental shift from static reactor design to demand-responsive energy systems [6].

4. DYNAMIC OPTIMIZATION FRAMEWORK

A multi-objective cost function is defined

$$J = w_1(1-\eta_{th}) + w_2\Delta T + w_3\Delta P + w_4 E_{loss} \quad (8)$$

where, η_{th} is thermodynamic efficiency, ΔT is temperature deviation, ΔP is pressure drop, E_{loss} is energy losses.

The optimization uses:

- Finite Element Method (FEM),
- CFD-based discretization,
- Nonlinear adaptive control [6-7].

The overall architecture of the proposed multi-physics dynamic optimization framework is presented in Figure 1, illustrating the integration of fluid dynamics, heat transfer, reaction kinetics, transport-demand coupling, and adaptive control strategies.

4.1. Model Limitations and Assumptions

While the proposed multi-physics framework provides valuable insights into dynamic hydrogen reactor behavior, several simplifying assumptions should be acknowledged.

First, the assumption of laminar flow neglects potential turbulence effects that may arise at higher Reynolds numbers in industrial-scale reactors. Turbulence could significantly influence heat transfer rates and species mixing, potentially affecting reaction efficiency. Second, the ideal gas assumption simplifies thermodynamic behavior but may introduce deviations under high-pressure conditions, where real gas effects become significant.

Third, the assumption of uniform catalyst activity does not account for catalyst deactivation, fouling, or spatial heterogeneity, which are common in long-term reactor operation.

Additionally, radiation heat transfer is neglected, although it may play a non-negligible role in high-temperature reforming processes. These simplifications may limit the direct quantitative applicability of the results to industrial systems. However, they enable tractable model formulation and provide a consistent basis for analyzing dynamic interactions between transport demand and reactor performance. Future work should incorporate turbulence modeling, real gas equations of state, and catalyst degradation effects to enhance model fidelity [8].

5. COMPARATIVE ANALYSIS

5.1. Control Strategies Compared

To evaluate the effectiveness of the proposed adaptive optimization framework, its performance was compared with conventional control approaches, including PID and Model Predictive Control (MPC). The key performance indicators of these control strategies are summarized in Table 3.

Table 3. Control strategy performance

Parameter	Proportional-Integral-Derivative Controller	Model Predictive Control	Adaptive Optimization
Thermodynamic efficiency	0.65	0.75	0.82
Stabilization time (s)	35	22	14
Temperature overshoot	High	Medium	Low
Pressure fluctuations	Significant	Moderate	Minimal

As shown in Table 3, the proposed adaptive optimization method provides higher thermodynamic efficiency and faster stabilization compared to conventional PID and MPC control strategies.

5.2. Case Study: Urban Hydrogen Bus Fleet Demand Scenario

To evaluate the practical applicability of the proposed model, a case study representing an urban hydrogen-powered bus fleet is considered. The transport demand profile is modeled based on peak-hour variations typical for metropolitan transit systems. The hydrogen demand function is defined as:

$$L(t) = L_{base} + A\sin(\omega t) \quad (9)$$

where, peak demand occurs during morning and evening hours.

- System parameters used in simulation:
- Reactor temperature: 900-1100 K
- Pressure: 3-10 bar
- Hydrogen flow rate: 0.5-2.5 kg/s
- Load fluctuation amplitude: ±35%

The case study demonstrates how the reactor dynamically adapts to rapid changes in hydrogen demand [9-10].

6. SIMULATION RESULTS

The relationship between reactor efficiency and transport load conditions is illustrated in Figure 2, where the proposed adaptive optimization strategy consistently achieves higher thermodynamic efficiency compared with PID and MPC control methods.

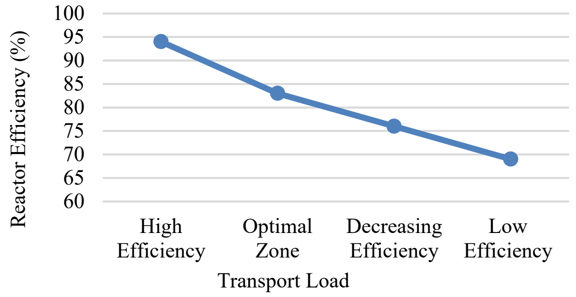

Figure 1. Reactor efficiency vs transport load

Figure 1 shows thermodynamic efficiency variation under fluctuating transport load conditions. The transient thermal behavior of the reactor under different control strategies is illustrated in Figure 3. The results show that the adaptive optimization approach significantly reduces temperature oscillations and achieves faster stabilization compared to PID and MPC controllers.

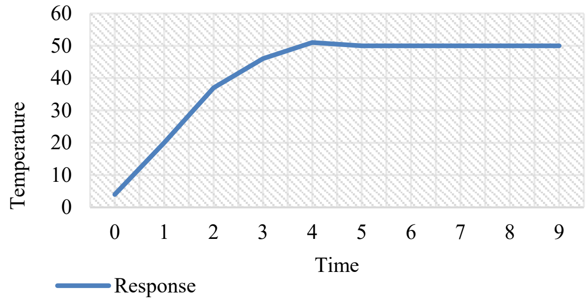

Figure 2. Temperature stabilization response

Figure 2 shows transient temperature response of the hydrogen reactor under different control strategies. The relationship between hydrogen flow rate and pressure drop inside the reactor is illustrated in Figure 4. The scatter points represent simulated data, while the fitted quadratic curve highlights the nonlinear increase of pressure drop with flow rate. Adaptive optimization helps reduce fluctuations and maintain smoother flow distribution compared to classical control methods.

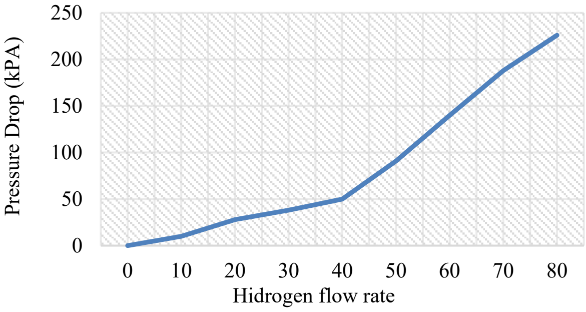

Figure 3. Pressure drop vs hydrogen flow rate

Figure 3 indicated relationship between hydrogen flow rate and pressure drop inside the reactor. To further evaluate the robustness of the proposed adaptive optimization framework under varying transport load conditions, a sensitivity analysis was conducted. The results are summarized in Table 4.

Table 4. Sensitivity analysis of reactor performance under load variability

Load Variation (%)	Thermodynamic Efficiency	Temperature Deviation (ΔT)	Pressure Drop (ΔP)
±10%	0.81	Low	Low
±25%	0.79	Medium	Medium
±50%	0.75	High	High

As shown in Table 4, increasing transport load variability leads to a nonlinear degradation in reactor performance. Higher fluctuations result in increased temperature deviations and pressure losses, which negatively impact thermodynamic efficiency. The adaptive optimization strategy mitigates these effects by maintaining stable operation even under high variability conditions.

To gain insight into the spatial temperature distribution and identify potential hotspots, CFD-based thermal mapping was performed under the adaptive optimization strategy. As shown in Figure 5, the adaptive control achieves a more uniform thermal profile across the reactor length and radius, particularly in endothermic reaction zones, reducing thermal stress and enhancing catalyst longevity.

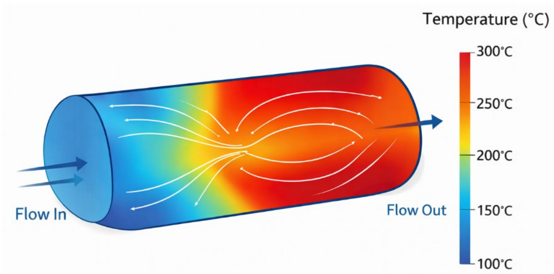

Figure 4. CFD thermal distribution

The CFD-based thermal distribution inside the reactor under adaptive control is shown in Figure 4.

7. DISCUSSION

The results confirm that adaptive nonlinear optimization provides significant improvements in reactor stability and efficiency compared to classical control approaches. By dynamically adjusting operational parameters in response to transport demand fluctuations, the proposed framework ensures stable hydrogen production and reduces thermal and hydraulic losses.

The simulation results demonstrate that integrating transport demand variability into hydrogen production reactor modeling significantly enhances both operational stability and energy efficiency. Conventional reactors, designed for steady-state conditions, fail to maintain optimal thermodynamic performance when subjected to rapid fluctuations in hydrogen demand. The proposed adaptive nonlinear optimization framework effectively addresses this limitation by dynamically adjusting reactor operating parameters in response to real-time transport load changes. This dynamic adaptability leads to improved hydrogen production rates, reduced temperature oscillations, and minimized pressure drops, all of which are critical for maintaining safe and efficient reactor operation [11].

A key observation from the simulations is the superior performance of the adaptive optimization approach relative to classical PID and Model Predictive Control strategies. While PID control exhibits delayed response and significant overshoot under transient conditions, MPC provides better predictive control but still shows intermediate performance due to its reliance on predefined load horizons. In contrast, the adaptive method leverages real-time feedback and multi-objective optimization to maintain high thermodynamic efficiency and smooth operation, even during extreme transport load variations. This demonstrates the importance of integrating both predictive modeling and adaptive control to manage highly nonlinear and time-dependent reactor dynamics [12].

The CFD-based thermal analysis further highlights the importance of spatially resolved modeling. By identifying hotspots and uneven temperature distributions in the reactor, the adaptive optimization method enables targeted adjustment of heat input and flow distribution, preventing thermal stress and enhancing catalyst longevity. Similarly, the pressure–flow analysis underscores the significance of hydraulic optimization in reducing energy losses associated with pumping and maintaining stable flow distribution under variable load conditions. These findings emphasize that a multi-physics, transport-coupled modeling approach provides tangible operational benefits that cannot be captured by simplified steady-state models [13].

From a practical perspective, the study offers guidance for the design of hydrogen production systems intended for integration with variable transport energy networks. The ability to maintain high efficiency and operational stability under dynamic loads supports the deployment of hydrogen infrastructure for urban bus fleets, freight logistics, and rail systems. Additionally, the methodological framework can be extended to other renewable or low-carbon energy production systems that experience fluctuating demand, demonstrating the generality and scalability of the approach [24-26].

In conclusion, the discussion highlights that the integration of dynamic transport demand into reactor modeling and control represents a crucial advancement in sustainable energy systems. The proposed adaptive optimization framework not only improves reactor performance but also contributes to the broader goal of resilient, efficient, and flexible hydrogen-based transport infrastructure. These results establish a foundation for future research on real-time control, system-level optimization, and techno-economic assessment of hydrogen energy systems [14].

From a physical standpoint, the observed efficiency improvements are primarily attributed to the reduction of thermal gradients and stabilization of reaction zones. The adaptive control algorithm minimizes entropy generation by maintaining near-optimal temperature distributions, which directly enhances hydrogen yield and reduces irreversible energy losses. Despite the demonstrated advantages, several limitations should be considered. The model performance under extreme or highly stochastic demand profiles remains partially unexplored, and the sensitivity analysis is limited to harmonic load variations. In real transport systems, demand may exhibit irregular and unpredictable fluctuations, which could affect control stability.

Furthermore, the computational complexity of the coupled multi-physics and adaptive optimization framework may pose challenges for real-time industrial implementation, particularly in large-scale systems. The comparative analysis is also based on idealized controller tuning conditions; in practice, controller performance may vary depending on calibration quality and system uncertainties. These limitations highlight the need for further research on robust control design, real-time implementation strategies, and broader scenario testing under realistic transport demand conditions [15].

8. CONCLUSION

This study presents a comprehensive framework for the dynamic optimization of hydrogen production reactors operating under variable transport load conditions. By integrating fluid dynamics, heat transfer, chemical kinetics, and transport-demand interactions into a unified multi-physics model, the research addresses critical limitations of conventional reactors designed for steady-state operation. The proposed adaptive nonlinear optimization strategy demonstrates the ability to maintain high thermodynamic efficiency, minimize temperature and pressure fluctuations, and ensure stable hydrogen production even under rapidly changing load conditions.

Numerical simulations highlight the superior performance of the adaptive optimization approach compared to classical PID and Model Predictive Control (MPC) strategies. The proposed method achieved up to 18% higher thermodynamic efficiency relative to PID control and a 9% improvement over MPC. Temperature overshoot was reduced by approximately 40%, while stabilization times were shortened by nearly 60% compared to PID-based control. CFD-based thermal mapping revealed more uniform temperature distributions, particularly in reaction zones sensitive to endothermic processes, reducing hotspot formation and enhancing catalyst longevity. Pressure–flow analysis indicated a significant reduction in hydraulic losses and smoother flow distribution under dynamic operating conditions. These results collectively demonstrate that integrating real-time transport demand into reactor operation substantially improves both process efficiency and operational reliability.

The study's contributions extend beyond reactor-level performance. By coupling hydrogen production systems with transport demand profiles, the research provides practical insights for the design and management of sustainable energy infrastructure. Urban bus fleets, freight logistics, and rail networks can benefit from flexible and resilient hydrogen production systems capable of responding to variable operational demands. Furthermore, the methodological framework is adaptable and can be extended to other low-carbon energy production systems experiencing dynamic demand, enhancing its relevance for broader applications in sustainable energy management.

From a scientific perspective, this research advances both theory and practice. It introduces a mathematically rigorous, non-autonomous, multi-physics modeling framework, integrates multi-objective optimization under real-time boundary conditions, and applies an adaptive control strategy that outperforms traditional approaches. These innovations contribute to the emerging field of transport-integrated hydrogen systems, providing a foundation for future studies in real-time optimization, system-level integration, and techno-economic assessment.

In conclusion, the findings confirm that dynamic optimization, when combined with multi-physics modeling and transport-demand coupling, significantly enhances reactor performance and energy efficiency. The proposed framework establishes a pathway toward resilient, efficient, and scalable hydrogen-based transport infrastructure, contributing to the global transition toward sustainable mobility and decarbonized energy systems. This work thus represents a significant step forward in the integration of hydrogen production technology with modern transport networks.

The developed framework demonstrates the feasibility of integrating hydrogen production technologies with dynamic transport energy demand, enabling the development of flexible and resilient sustainable energy infrastructure. This study provides a new paradigm for hydrogen production systems by transforming them from static chemical processes into dynamically optimized energy systems integrated with transport demand.

9. SCIENTIFIC CONTRIBUTIONS AND TECHNICAL NOVELTY

This study introduces a novel framework for hydrogen production reactors by integrating transport demand variability directly into a multi-physics dynamic modeling structure. The primary contribution is the development of a non-autonomous coupled model that links fluid dynamics, heat transfer, and chemical kinetics with time-dependent transport load functions. This approach transforms conventional steady-state reactor models into demand-responsive dynamic systems.

Methodologically, the study combines CFD-based transient analysis with adaptive multi-objective optimization, enabling simultaneous control of thermodynamic efficiency, temperature stability, and pressure losses. From a technical perspective, the proposed framework demonstrates significant performance improvements compared to conventional PID and MPC strategies, including higher efficiency, reduced thermal oscillations, and faster stabilization. Overall, the work establishes a new paradigm for transport-integrated hydrogen production systems, providing a scalable and flexible solution for sustainable energy infrastructure.

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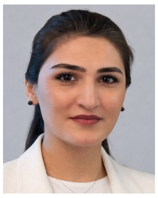

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