Numerical Analysis for Real-time NMPC of Ethanol Steam Reformers

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1 Introduction

The growth in population has resulted in a considerable increase in global energy consumption. This is due to the fact that energy is required for practically all activities like transportation, heating etc. Nowadays, hydrogen has emerged as an attractive energy vector that may be utilized to store energy from renewable sources. The time has come to capitalize on hydrogen's potential to play a significant role in addressing critical energy challenges. Recent breakthroughs in renewable energy technology have proved that technical innovation has the potential to build worldwide clean energy firms that do not rely on hydrocarbon-based fuels, therefore helping to reduce pollution levels [3].

Because it possesses one of the highest *energy* densities per unit mass, hydrogen is appealing as a fuel. According to [5], energy density is defined as the quantity of energy stored per unit volume in a specific system or region of space. According to this statistic, hydrogen has an energy density of 35,000 watts per kilogram (W/kg), but lithium-ion batteries have an energy density of just 200 watts per kilogram (W/kg) and because hydrogen has a tenfold higher energy-to-weight ratio than lithium-ion batteries, it can deliver a greater range while being substantially lighter. The usage of fuel cells when *pure hydrogen* is used can be turned into electricity at high efficiency, durability, and efficiency as needed.

Because of the physical features of hydrogen, it is difficult to *transport* and *store*, prompting us to study safe ways for effectively producing hydrogen locally. One conceivable method for safe hydrogen transportation that appears to be the most efficient is to store the fuel as a low-pressure liquid and then use an on-board ethanol steam reformer (ESR) to produce hydrogen as needed [1]. This is owing to its mobility, renewable nature, and low toxicity.

The development of real-time efficient and trustworthy control systems to assure device efficiency while reducing the impact of interruptions such as significant variations in interior and external temperatures during transportation, as mentioned in [1] are crucial for the design of ethanol steam reformers. There have been few mathematically modelled studies on the best design of control techniques for ethanol steam reformers. Previous research has examined the steady-state behaviour of ethanol steam reformers in order to build proportional-integral-derivative (PID)-based decoupled control loops while disregarding physical and operational restrictions and needs [6] and [7]. Another study [4] presented the use of a model which manages a mass flow control of ethanol/water and a temperature regulation of 1 kWe thermal plasma reformer. Although these work they have certain limitations such as neglecting physical and operational constraints and do not take maximum use of the system's accessible information. Some of the research rely on linear process models, which might be inaccurate in general as in [4]. Given the complexity of nonlinear models for ethanol steam reformers, research has been done to employ nonlinear process models, which have a relatively high computational cost for computing the control rule.

The authors [2] conducted the first research to conduct a rigorous examination of the extent of nonlinear model predictive control, in which they analyze a mechanistic model that is a single distributed parameter system which in fact makes this physics-based distributed parameter system for ethanol steam reformer a *unique* system. In addition, the same paper presented a method for constructing an approximation reduced-order nonlinear dynamics model with lower computing cost while preserving the same structure of the original equations and physical model parameters.

Further extending the study [1] the authors now introduced a *zero error* approach in the model reformulation. When putting the model into a nonlinear model predictive control algorithm, this new formulation preserves the same advantages of being dependent on physical model parameters and considerably lowering the real-time computations required. Figure 1 shows the ESR which is a nonlinear dynamical system comprised of a catalytic ethanol steam reactor in series with a separation stage that includes a selective membrane for hydrogen removal as described in [1]. The mechanistic model described are a function of time and axial direction only (only one spatial dimension) for the system of partial differential equations.

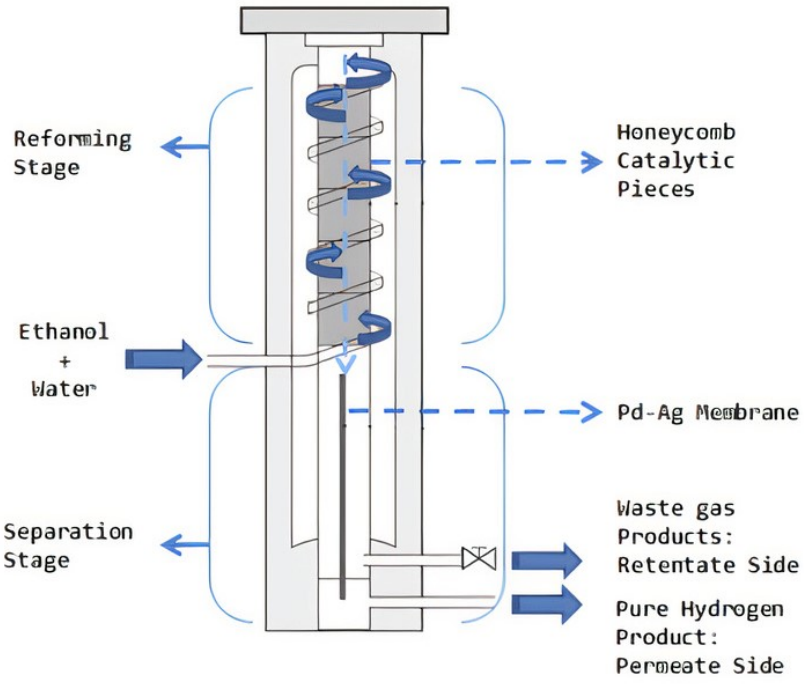

Figure 1: Staged membrane reactor scheme

This will be the first in-depth examination of the aforementioned reformed system, with the goal of attempting to turn it into some type of conservation law or similar standard method (examples include convection form, diffusion form etc.). We will rigorously prove the uniqueness and existence of our system's solutions by understanding their characteristic system which is usually done by the *Riemann* method. Expanding on this, we look at any potential singularities, such as hypothetical shock developments and how the system might behave under time limitations. This is particularly crucial since any numerical approach we wish to utilize requires us to discretize the domain (i.e. discretize both the *spatial* and *temporal* parts of the domain and consider a bounded domain). This is significant because it allows us to avoid using numerical approaches that might cause the system to blow up and instead utilize more efficient numerical methods created expressly for 1D conservation rules (examples include The finite volume method, Approximate Riemann Solvers etc).

Our main contribution to this paper is to perform a numerical comparison based on dependability and efficiency, as defined by computation time and the number of analyses required to achieve a specific level of accuracy, as well as to precisely guarantee that the algorithm is stable, converges and is consistent [3]. This would be accomplished by converting the systems of partial differential equations to a system of ordinary differential equations, for which there are already various techniques for solving this system of ODEs (examples include Euler Methods, Adaptive methods etc). This may also be compared to a direct approach to solving PDE problems utilizing numerical techniques like as finite difference methods, finite element methods, finite volume methods, spectral methods etc. Finally, we take this to the further by determining the best system formulation and refining the accompanying numerical approach even more to reduce computing costs.

The end goals of this study, as stated in [3], are to enable a mechanistic model to be employed in real-time control calculations while explicitly accounting for input, state and output constraints with minimal computation cost. This would open up a new field of research into nonlinear distributed parameter systems with additional features such as mass, particle number all of which are common in other areas of research (examples include thermodynamics, fluid dynamics etc). This research may be extended to other reactor systems that are frequently encountered in chemical process control applications etc. Lastly this would bring us closer to our goal of manufacturing hydrogen safely which in turn could be used as green energy.

References

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