Numerical Analysis for Real-time NMPC of Ethanol Steam Reformers

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The utilization of renewable energy technologies, particularly hydrogen, has seen a boom in interest and spread throughout the world. Ethanol steam reformation is one of the primary methods capable of producing hydrogen efficiently and reliably. This proposal provides an overview of what we intend to accomplish through the research endeavour. We offer an overview of several numerical approaches for solving the general first-order quasi-linear hyperbolic equation to the particular model for ethanol steam reforming (ESR), as well plan to explore the possibility of converting the system into its conservation form.

1 Motivation

The moment has come to capitalize on hydrogen's potential to play a major role in addressing crucial energy concerns. Recent advances in renewable energy technologies have demonstrated that technological innovation have the potential to create global clean energy enterprises without the use of hydrocarbon-based fuels which eventually would help bring down the pollution levels.

Hydrogen *storage* and *transportation* has been a limitation as hydrogen has a very high energy density and that it must be stored under very high pressure [1].Reforming is one of the technologies for generating hydrogen when needed (especially ESR) which requires efficient and reliable control strategies [3].

Past works have included the use of decoupled PID Controllers and fast linear MPC with low on line cost by using input-output formulations. High on-line computational cost has limited the implementation of state-space NMPC formulations based on mechanistic models and hence we propose a new model for ESR with low computational cost. We hope to try to find an *efficient* numerical method for the system of nonlinear PDE's which are derived from mass and energy balances [3].

2 Reduced-order model for Ethanol Steam Reforming

Reyero et al. [3] created a Mathematical model for Ethanol Steam Reforming. The model was subsequently further reduced in [1], which removes two approximations made in the previous model. The following are the model equations:

$$Mf_t + Nf_z = g(t, z, f) \qquad (1)$$

with [1]

$$f := \begin{pmatrix} F \\ T \end{pmatrix}, \quad F = \begin{pmatrix} F_1 \\ \vdots \\ F_7 \end{pmatrix} M = \begin{pmatrix} I - \frac{1}{\|F\|} F e^\top & -\frac{1}{T} F \\ 0^\top & \frac{C_v}{RT\|F\|} F \end{pmatrix} N = \begin{pmatrix} \frac{RT}{Ap} I & 0 \\ \frac{RT}{Ap} e^\top & \frac{C_p}{Ap} F \end{pmatrix}$$

where F_j is the flow rate of species j, T is the temperature (in K), R is the ideal gas constant (in $\mathrm{Pam}^3/(\mathrm{molK})\big)$, ρ is the membrane thickness (in m), c_p and c_v are the heat capacities (in J/(molK)), p is the pressure (in bar), A is the cross-sectional area of the tubular reactor (in m^2), U is the overall heat transfer coefficient (in $\mathrm{J}/\left(\mathrm{m}^2\ \mathrm{s\ K}\right)$).

3 Proposed Research

Numerical solution of PDEs is a rich and active field of modern applied mathematics. The subject's steady growth is fueled by increasing demands from the natural sciences, engineering, and economics to provide accurate and reliable approximations for models involving partial differential equations (PDEs) [2].Our goal is to develop efficient numerical methods for the above system. To do this we will

- Give the numerical results of this comparative examination of numerous numerical ways to solve the previously described Reduced-order Model for ESR. For PDEs/ODEs some numerical technique's include finite difference approaches, finite element methods, finite volume methods, spectral methods etc.
- We will rigorously prove the uniqueness and existence of our system's solutions, as well as examine any potential singularities such as possible shock developments, before attempting to rewrite the model to some form of *conservation law*, which will allow us to use the more efficient numerical approaches developed specifically for conservation laws.
- Then we proceed to a numerical comparison which is based on reliability and efficiency measured by calculation time and number of analysis needed to reach a certain accuracy level as well as accurately ensuring that the algorithm is *stable*, *converges* and is *consistent*.
- Then we strive to identify the optimal system formulation and optimize the best numerical approach to lower the computational cost even more.

4 Applications

The primary aims of this research are to enable a mechanistic model to be used in real-time control calculations while explicitly accounting for input, state, and output limitations with minimal online computation cost [1].This would allow us to manufacture hydrogen safely from ESR, which could be utilized as green energy.
The whole technique should also be adaptable to nonlinear distributed parameter systems with extra coordinates including intrinsic attributes such as particle number, mass, or age which are frequently encountered in chemical process control applications [1].

Bibliography

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