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Toward Generalizable and Adaptive Chemical Reactor Networks for Hydrogen Combustion

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Climate change poses significant challenges, prompting policies for carbon neutrality by 2050. Renewable energies, mainly hydrogen as a Smart Energy Carrier (SEC), offer high efficiency and zero direct CO_2 emissions. However, its combustion creates challenges, such as increased nitrogen oxide (NO_x) emissions, necessitating innovative combustion technologies for cleaner use. Chemical Reactor Networks (CRNs) provide an effective approach for simulating detailed kinetic mechanisms with reduced computational demands. Introduced by Bragg [2], this method divides the combustor into discrete compartments that represent homogeneous flow zones, modelled as Perfectly Stirred Reactors (PSRs) or Plug Flow Reactors (PFRs). The reactors, interconnected by mass and heat exchanges, form a network designed to preserve the main characteristics of the global flow field. Data for CRNs can come from semi-empirical relationships or CFD simulations. The combined CFD-CRN method effectively predicts pollutant emissions, while unsupervised clustering algorithms like Principal Component Analysis (PCA) help automatically select features and group observations [1]. The primary objective of this analysis is to explore how CRNs vary with changes in input database conditions, such as the composition of a methane-hydrogen mixture, and to evaluate how these variations impact predictive performance. Subsequently, the study aims to determine whether it is possible to identify an average network capable of adequately representing all the examined conditions. The integration of Graph Neural Networks (GNNs) is envisioned as a predictive approach to generalize CRNs for unseen scenarios, leveraging their ability to learn complex patterns and relationships within graph-structured data.

References

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