



Physics-Informed Neural Networks for Reacting Flow with Stiffness and Multicomponent Transport Process

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The numerical simulation of combustion presents a significant challenge due to the complex interactions of finite-rate chemistry and flowing transport phenomena, especially when addressing chemical mechanisms with multiple species and strong stiffness. While traditional numerical iterative methods have established a solid theoretical foundation and yield remarkable achievements in reacting flow problems, these methods suffer from the inherent numerical instability arising from discretization, which can further result in increased computation cost or convergence failures. Physical information neural networks (PINN), characterized by meshless nature and zero discretization error, offer a promising approach to this challenge. Leveraging the optimization approach, PINNs are capable of obtaining solutions of partial differential equation (PDE) systems on the continuous domain, and avoid the disadvantages of chemical stiffness and fluid-chemical coupling. Thus, these inherent challenges in solving PDE systems of reacting flow are transformed into the challenges of optimization algorithms.

However, the foundational framework of PINN tends to fail to converge during the training process or obtain the trivial solution, such as a non-reactive solution, due to the complexities of reacting flow. To address these challenges, a novel loss scheme developed from the Newton-iterative method is proposed to enhance the training convergence of PINN when solving complex PDE systems. This novel methodology, referred to as NewtonPINN, effectively modifies the optimization trajectory of PINNs and theoretically ensures convergence by incorporating the Newton-iterative scheme. The methane-hydrogen reacting system with a 3-step global mechanism and the ammonia-hydrogen reacting system are studied and validated for forward problems in one-dimensional reactors of freely-propagating premixed (FPP) flames and counterflow premixed (CFP) flames. To our knowledge, this is the first application of PINNs to reacting flows based on stiff and multi-step finite-rate chemistry models in the zero-shot learning task. Furthermore, some proposed strategies, such as importance sampling and input-output scaling transformations, have been demonstrated to be essential for the robust learning of PINN in reacting flow.

The results demonstrate that NewtonPINN can accurately reconstruct the fields with stiff, multi-step chemical models and infer unknown parameters across a series of equivalent ratios. Additionally, the reaction source terms of reactions are predicted with acceptable errors. This indicates the critical small-scale species, which play dominant roles in controlling the progress of reactions, are accurately captured by the NewtonPINN.