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A data-driven complementary multi-level simulation framework for ammonia–syngas combustion optimisation

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Ammonia is regarded as an important energy carrier in power generation and maritime transport, but low flammability limits its combustion performance. Co-firing ammonia with syngas is considered an effective method to overcome this issue. Ammonia-syngas combustion has been widely explored through both experimental and computational methods. However, these traditional methods are limited by their intrinsic assumptions and modelling deficiencies. As a result, optimising combustion systems through these approaches can be time-consuming. Moreover, one level of simulation is often not sufficient enough to fully reveal the interactions involved in complex combustion processes. To address these challenges, we establish a machine learning based complementary multi-level simulation framework. The specific steps are illustrated in Fig.1 and described as follows:

(1) Construct the training dataset using one-dimensional laminar premixed flame simulations.

(2) Evaluate various ML models to identify the most suitable one for accurate prediction.

(3) Integrate the selected ML model into the Non-dominated Sorting Genetic Algorithm-III (NSGA-III) to find the optimal operating conditions.

(4) Perform Reynolds-Averaged Navier-Stokes (RANS) simulations to evaluate the spatial distribution of the optimal fuel composition.

(5)Apply reactive molecular dynamics (RMD) simulations to reveal the reaction mechanism.

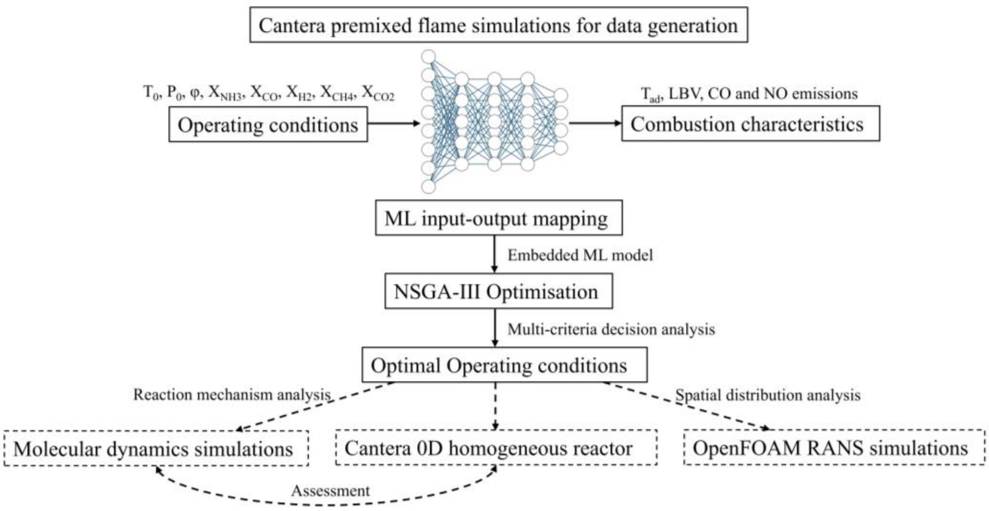

Fig.1. Overview of modeling framework for ammonia-syngas combustion optimisation.

Based on this simulation framework, we achieved laminar burning velocity (LBV) of ammonia-syngas combustion comparable to methane combustion, while maintaining low NO and CO emissions under adiabatic flame temperatures (T_{ad}) below 2000 °C. The optimal conditions obtained from modelling on one level were assessed using modelling from another level. This framework offers a new perspective for the efficient optimisation of combustion systems.