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Accelerating alkali metal chemistry simulations in solid fuel combustion via artificial neural networks

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Alkali metal reactions play a crucial role in solid fuel combustion, significantly influencing slag formation, ash deposition, and pollutant emissions. Understanding and accurately modeling these reactions are essential for optimizing combustion efficiency and reducing environmental impact. However, solving complex alkali metal reactions with detailed mechanisms in turbulent combustion simulations is computationally expensive. To address this issue, this study develops a neural network-based approach to reduce computational cost. The combustion characteristics of Loy Yang lignite are investigated. The chemical percolation devolatilization (CPD) model is employed to obtain hydrocarbon volatile compositions, with tar species approximated by C_2H_2. The initial sodium species in the volatile is set to be NaOH, while those of S and Cl are set to be SO_2 and HCl, respectively. The volatile combustion mechanism is constructed by integrating the DRM22 hydrocarbon mechanism [1] with Glarborg's detailed alkali mechanism [2].

To facilitate the generation of alkali metal reaction datasets, an approach is proposed to rapidly produce compatible datasets from existing combustion data. For each dataset point, the initial alkali-related species, i.e., NaOH, HCl, and SO_2, are supplemented based on the volatile mixture fraction. To maintain mass conservation, hydrocarbon species are proportionally reduced. Alkali metal reactions are simulated using the detailed mechanism with the CVODE solver, allowing the free evolution of alkali metal species while keeping hydrocarbon species and temperature constant. Initial and final species values are first averaged with a weighted random proportion and then subjected to random perturbations (±40%) to construct the dataset.

Five artificial neural networks (ANN) are trained to predict the source terms of five primary alkali metal species, i.e., Na, NaCl, Na_2SO_4, $NaHSO_4$, and SO_3. Each network comprises seven fully connected layers and four batch normalization layers, employing the ReLU activation function. The model input features include 24 chemical species and temperature, totaling 25 inputs, with one output corresponding to an alkali metal species source term. Network training and implementation are performed using the TensorFlow open-source framework. A-priori validation shows that ANN predictions closely align with CANTERA simulation results based on the detailed mechanism.

The ANN model is then integrated into three-dimensional direct numerical simulations (DNS) to predict alkali metal reactions in pulverized coal combustion as an a-posterior test. The predicted sodium species distributions show good agreement with both the detailed and reduced mechanisms, though the prediction of Na_2SO_4 shows a slight positive bias. The proposed ANN model effectively captures alkali metal chemistry in multiphase turbulent combustion of solid fuel while significantly enhancing computational efficiency.

References

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[2] Glarborg P, Marshall P. Mechanism and modeling of the formation of gaseous alkali sulfates. Combustion and Flame, 2005, 141 (1–2): 22-39.