Surrogate Modeling of Biomass Gasification in Fluidized Beds Using GRU-RNN

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Abstract

A machine learning surrogate model was developed to predict syngas and tar species along the reactor length in biomass gasification. Using a GRU-based Recurrent Neural Network (RNN), the model reduced computation time from 3696 CPU hours to just a few seconds, achieving a 10 orders of magnitude improvement in efficiency compared to traditional CFD simulations, while maintaining high accuracy. This approach enables faster and more cost-effective predictions for high temperature biomass pyrolysis process.

1 Introduction

Thermochemical processes like pyrolysis and gasification hold great potential for converting biomass into valuable chemicals and fuels. Gasification transforms lignocellulosic materials into syngas (mainly CO and H_2) and tar under controlled oxidizing conditions, with syngas serving as a precursor for producing liquid fuels via the Fischer-Tropsch process. A significant challenge in gasification is controlling the yield and composition of tar, a complex mixture of aromatic hydrocarbons that disrupts the process and demands extensive cleanup. Experimental investigations are often limited by harsh reactor conditions and the intricate coupling of hydrodynamics with reaction chemistry. Traditionally, Computational Fluid Dynamics (CFD) simulations have been used to study these reactors, but their high computational cost restricts the use of detailed chemical kinetic models crucial for predicting tar composition. This work proposes a surrogate model based on a Recurrent Neural Network (RNN) to replicate CFD predictions, utilizing detailed chemistry for secondary gas-phase reactions responsible for syngas and tar formation, while significantly reducing computational demand.

2 Methods

CFD-DEM simulations are performed to model biomass gasification in a lab-scale fluidized bed reactor Xue et al. [2012]. Devolatilization of biomass particles is modeled using a spatially- resolved 1D intraparticle model Goyal and Pepiot [2018] incorporating a lumped devolatilization chemistry model Corbetta et al. [2014]. Biomass feedstock and reactor conditions are varied to generate an extensive database of biomass devolatilization products. A compact kinetic model for the secondary gas phase reaction Goyal and Pepiot [2017] is used with ideal reactor models - Continuous Stirred Tank Reactor (CSTR) for the multiphase region and Plug Flow Reactor (PFR) for the freeboard

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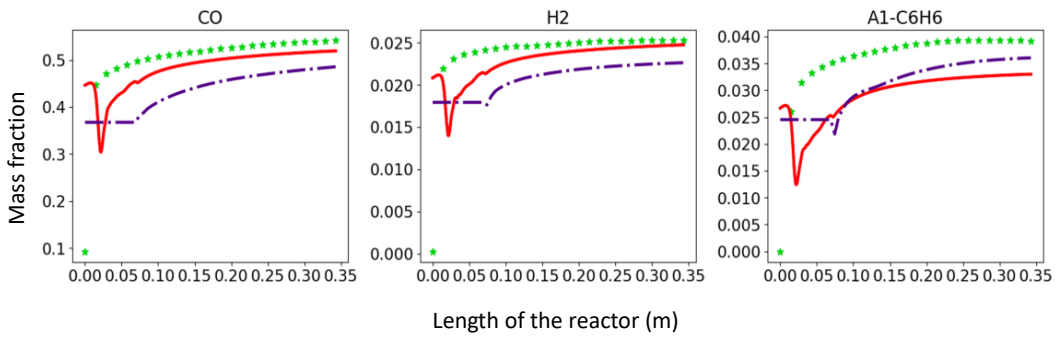

Figure 1: Comparison between the selected product species mass fractions obtained from the CFD-DEM simulations (solid red lines), ML-CSTR and ML-PFR in series (dash-dotted purple lines), and ML-PFR (green symbols).

region. The data sets for both models include mass fractions of 27 product species spanning different residence times. The resulting data set comprises approximately 165 million data points. Gated recurrent units based Recurrent Neural Network models (GRU-RNN) Sharma et al. [2022] are built for the ideal reactor models. The input to the ML models consist of mass fractions of the primary product species obtained through the biomass devolatilization model. The two ML models are used in series and their predictions are compared CFD-DEM simulations.

3 Results and discussion

Figure 1 shows the cross-sectional and time-averaged CFD-DEM predictions (solid red line) of CO, H_2, and single-ring aromatics mass fractions along the reactor length at 800 C. A significant variation in the species mass fraction is observed in the multiphase region (0 to 0.06 m) with a sharp peak near the injection location of biomass. These results demonstrate improper mixing in the multiphase region and inadequacy of the CSTR assumption commonly used in the literature. The CFD-DEM results are compared with the developed ML models: 1) ML-CSTR and ML-PFR in series (dash-dotted purple lines) and 2) ML-PFR for the entire reactor (green symbols). Both the models can adequately capture the overall trend, including the outlet species mass fractions. However, the comparison within the multiphase region is semi-quantitative. Interestingly, Model 1 predictions are in better agreement with the CFD-DEM despite improper mixing in the bed region. The input of both the ML models is the composition of biomass devolatilization products, whereas in CFD simulations biomass particles release primary products within the multiphase region. Overall, the developed ML model enabled a significant reduction in computational cost compared to CFD, reducing computation time from 3696 CPU hours to just a few seconds, achieving a 10 orders of magnitude improvement. Similar observations were made at higher reactor temperatures of 900°C and 1000°C.

4 Conclusions

We perform CFD-DEM simulations of biomass gasification in a lab-scale fluidized bed reactor utilizing a 1D intraparticle biomass devolatilization model and a compact kinetics model for the secondary gas-phase reactions. To reduce the computational cost of these CFD simulations, Recurrent Neural Network based surrogate models are developed that are based on CSTR and PFR assumptions and uses the same particle-scale model and chemistry as used in the CFD simulations. The developed ML model adequately replicates the evolution of syngas and tar species along the reactor length as predicted by computationally expensive CFD simulations

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