Accelerated Machine Learning Model for Biomass Gasification in Fluidized Beds

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Highlights

- Machine learning model to predict syngas and tar species along the reactor length
- Maximum mean relative error between the ML predictions and test data is 0.47%
- GRU-based RNN model reduced computation from 3696 CPU hours to few seconds

1. Introduction

Thermochemical processes like pyrolysis and gasification have the potential to convert biomass into valuable chemicals and fuels. Gasification transforms lignocellulose materials into syngas (mainly CO and H_2) and tar under controlled oxidizing conditions. Syngas serves as a precursor for producing liquid fuels through the Fischer-Tropsch process. A primary challenge in gasification is managing the composition and yield of tar, a complex mixture of aromatic hydrocarbons, that disrupts the process and requires extensive cleanup. Experimental insights are limited due to harsh reactor conditions and the complex coupling between hydrodynamics and reaction chemistry. Currently, Computational Fluid Dynamics (CFD) simulations are key for studying these reactors. However, their high computational demand limits the use of detailed chemical kinetic models necessary to predict tar composition. Machine learning provides an opportunity to develop surrogate models for biomass gasification at an affordable computational cost. This work demonstrates the use of Recurrent Neural Network model to replicate CFD simulation predictions utilizing detailed chemistry models for secondary gas-phase reactions responsible for syngas and tar formation.

2. Methods

CFD-DEM simulations are performed to model biomass gasification in a lab-scale fluidized bed reactor (Q. Xue et al., 2012). Devolatilization of biomass particles is modeled using a spatially-resolved 1D intraparticle model (Goyal et al., 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 et al., 2017) is used with ideal reactor models - Continuous Stirred Tank Reactor (CSTR) for the multiphase region and Plug Flow Reactor (PFR) for the freeboard 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 (K. G. 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.

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3. Results and discussion

Figure 1 shows the cross-sectional and time-averaged CFD-DEM predictions (solid red line) of CO, H2, 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 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 allowed significant reduction in the computational cost than CFD (3696 CPU hours to few seconds) . Similar observations are made at higher reactor temperatures: 900°C and 1000°C.

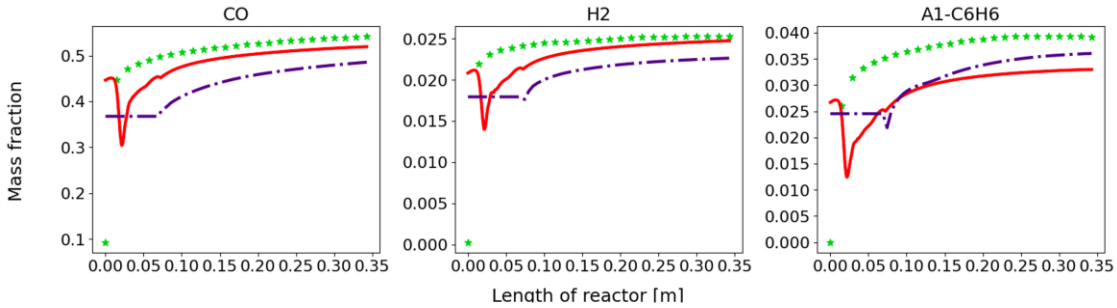

Figure 1. Comparison between the selected product species mass fractions obtained from the CFD-DEM simulations (solid red lines), ML-CSTR and ML-PFR in series (dash-dotted purple lines), and ML-PFR (green symbols).

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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Keywords: CFD, Machine Learning, RNN, Kinetic model, Biomass gasification