Title: Application of machine learning to pyrolysis reaction networks: reducing model solution time to enable process optimization

Authors: Blake R. Hough, David A.C. Beck, Daniel T. Schwartz, Jim Pfaendtner

PII: S0098-1354(17)30171-0
DOI: http://dx.doi.org/doi:10.1016/j.compchemeng.2017.04.012
Reference: CACE 5786

To appear in: *Computers and Chemical Engineering*

Received date: 3-11-2016
Revised date: 1-4-2017
Accepted date: 8-4-2017

Please cite this article as: Hough, Blake R., Beck, David AC., Schwartz, Daniel T., & Pfaendtner, Jim., Application of machine learning to pyrolysis reaction networks: reducing model solution time to enable process optimization.*Computers and Chemical Engineering* http://dx.doi.org/10.1016/j.compchemeng.2017.04.012

Application of machine learning to pyrolysis reaction networks: reducing model solution time to enable process optimization

Blake R. Hough[1], David A.C. Beck[1,2], Daniel T. Schwartz[1], Jim Pfaendtner[1,*]

[1] Department of Chemical Engineering, University of Washington, Seattle, WA, USA
[2] eScience Institute, University of Washington, Seattle, WA, USA

* Jim Pfaendtner, Department of Chemical Engineering, University of Washington, Box 351750, Seattle, WA 98195. E-mail: jpfaendt@uw.edu

Highlights

- Neural networks are an appropriate modeling tool to represent high dimensional detailed kinetic models with high accuracy and reduced computational cost
- The increased speed of a kinetic model solved with a neural network could facilitate use of detailed kinetic models in reactor or process models that have complex spatiotemporal heterogeneity
- The information content contained within the neural network is tunable depending on the desired outputs

Abstract

Comprehensive models of biomass pyrolysis are needed to develop renewable fuels and chemicals from biomass. Unfortunately, the detailed kinetic schemes required to optimize industrial biomass pyrolysis processes are too computationally expensive to include in models that account for both kinetics and transport within reacting particles. Here we present a machine learning approach using artificial neural networks and decision trees to reduce the computational expense of detailed kinetic models by four orders of magnitude, enabling their use in comprehensive models. The trained neural networks generalize very well, predicting the outputs of the detailed kinetic model with over 99.9% accuracy on new data. The machine learning approach we outline is not specific to kinetic modeling and can be applied to any set of input and output data, even if the underlying relationship between inputs and outputs is unknown.

Keywords: neural network, kinetic modeling, pyrolysis, biomass

1. Introduction

Interest in developing comprehensive models that describe biomass pyrolysis is high due to growing scientific and industrial interest in lignocellulosic biomass as a feedstock for renewable fuels and chemicals.(Ragauskas et al., 2006) These models couple descriptions