TOWARDS REVOLUTIONIZING PROCESS- AND REACTION ENGINEERING WITH ARTIFICIAL INTELLIGENCE-BASED MODELS

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Abstract

Chemical reactor, -reaction and -process engineering can greatly benefit from recent developments in artificial intelligence and machine learning. With the vast amounts of process data available to industrial players, AI models can be constructed which are faster, more accurate and more memory efficient than current models. The use of deep learning artificial neural networks at three different scales of the steam cracking process is discussed. For reconstructing steam cracker feedstocks and predicting effluent compositions, it is proven that highly accurate, predictive machine learning models can be constructed. A deep learning artificial neural network can predict the product yields of 31 important compounds. With other potential applications such as increasing the efficiency of reactor (profile) simulations and more accurate property estimation at a molecular scale coming within reach, the sky promises to be the limit for the application of artificial neural networks.

Keywords

Artificial Intelligence, Deep Neural Networks, Steam Cracking, Multi-Scale Modelling

Introduction

Despite the continued search for alternative production methods for light olefins, steam cracking is the predominant route and is expected to remain so in the foreseeable future (Amghizar et al. 2017). In recent years, artificial intelligence (AI) and specifically artificial neural networks (ANNs) have proven to be revolutionary in many applications, from gaming (Gibney 2016) over autonomous cars (Li and Gao 2018) to industrial manufacturing (Day 2018). The impact of AI in industry can barely be underestimated and has been named “Industry 4.0” (Lasi et al. 2014).

The traditionally conservative (petro-)chemical has been slow to adopt AI methods. However, their capacity to tackle highly complex problems poses great potential to develop more efficient and more accurate models at several scales within the process. This has been proven by the work of several researchers. Pyl et al. used artificial neural networks to reconstruct detailed naphtha compositions from commercial indices (Pyl et al. 2010). Other researchers have modeled stream cracker yields using ANNs (Ghadrdan et al. 2009; Niaei et al. 2007; Sedighi et al. 2011).

The drawback of traditional ANNs is that they still require manual engineering of the relevant features. The deep learning approach that is presented here circumvents this issue by including this step in the learning process. The model itself will determine and select the relevant features. In what follows, the application of deep learning at three different scales in steam cracking will be discussed: process, reactor and molecular scale.

AI-Based Multi-Scale Modelling of Steam Cracking

Process Modeling

Currently companies are unable to fully exploit the potential of real time optimization, as detailed process stream analyses are time-consuming. To avoid this, an AI-based model has been constructed that is capable of predicting steam cracker effluent compositions using no more than a limited number of commercial indices of the feedstock: boiling points, vapor pressure, density and basic PIONA composition. Figure 1 shows the parity plot for the most important target in steam cracking – ethene. Using just the abovementioned feedstock characteristics, process temperature, pressure and the product ratios ethene/ethane, methane/propene and ethene/propene, the model predicts the effluent ethene fraction within 5%, along with 30 other (pseudo-)components.

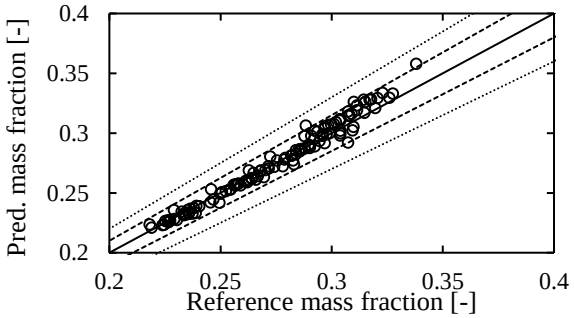

Figure 1: Parity plot for the predicted ethylene mass fraction.

Reactor Modeling

A second scale at which artificial intelligence can be of use, is the detailed modeling of reactors. At the moment, this requires the solution of several differential equations: momentum, energy and species balances. For detailed, large kinetic networks, this may become prohibitively expensive, especially in applications such as computational fluid dynamics. While tabulation techniques, such as in situ adaptive tabulation (Pope 1997), address this issue, ANNs can potentially provide the same acceleration, but with more efficient memory usage.

Molecular Properties

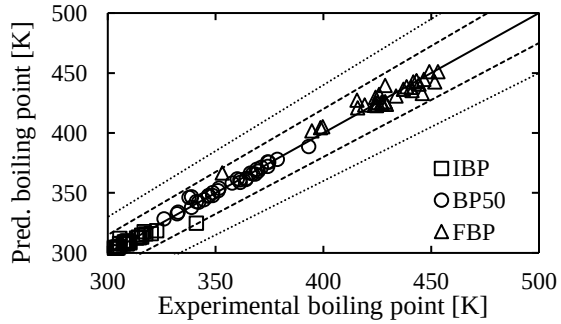

Figure 2: Parity plot for the predicted boiling points.

A final scale which is considered for the application of deep learning methods is the molecular scale. For naphthas typically used as steam cracking feedstocks, the density, vapor pressure, initial-, mid- and final boiling points are estimated with high accuracy using a deep learning ANN. This is illustrated by Figure 2, which shows that the boiling points are predicted with less than 5% error.

Conclusions

Artificial intelligence is having a major impact in several applications, though in chemical process and reaction engineering, the true breakthrough has not yet been made. Regardless, AI has the potential to become an indispensable tool in the chemical industry. We have shown that ANNs can be successfully applied in process modeling. Product yields are predicted within 5% of the reference yields. On the reactor scale, initial steps have been taken towards further optimizing detailed simulations. On a molecular scale, ANNs have been used with success to predict boiling points, again with less than 5% error. Based on these findings, it can be concluded that (deep) ANNs are on the verge of taking over many aspects of chemical engineering.

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