Neural Networks for Fast Analysis of Complex Chemical Reaction Mechanisms

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Background and Challenges

Biomass as an new source of sustainable energy is composed of high content of lignin, a highly cross-linked amorphous copolymer of three randomly polymerized phenylpropane units that account for up to 35 wt% of dry biomass and carries the highest specific energy content of biomass. Such that, developing a comprehensive kinetic models for such energy extraction from lignin pyrolysis can be challenging. Empirical and global models of biomass or lignin pyrolysis have always been relying on apparent kinetic derived from TGA studies. The main limitation of these models are their inability to predict the composition and distribution of product over a wide range of heating rates and temperature parameters. Thus this severely limited its practical application.

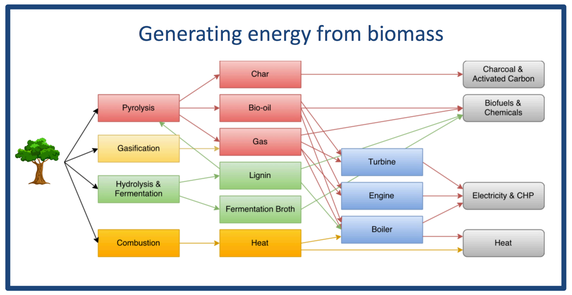

Figure 1. energy generation profile for lignin

In order to address the above limitations, and to continue Blake Hough's extensive studies on developing a open source predictive model with low computational cost. This capstone project aimed to replace the old ODE solver (DDASAC) with an open source ODE solver in SciPy. Additionally, team has also been investigating a third party simulation package called Cantera, is suite of object orientated software tools for problem involving chemical kinetics, thermodynamics, and/or transport processes.

The challenging parts are mainly come from the implementation of compatible ODE solver that would replace the DDASAC. Such that DDASAC had been offering an extremely low computational cost for the old model. Switching to open source SciPy solver can compromise the computational cost as well as accuracy. Cantera implementation has shed some promising lights on replacing the entire model, with further investigation will hopefully address the limitation from lignin pyrolysis models.

Objective and Methods

The objective of this project is to develop an open-source package in Python to solve chemical kinetic model, which focuses on lignin pyrolysis system (including 93 species and over 400 reactions). It compiles input data of reactions and constants list into both Cantera and Scipy package.

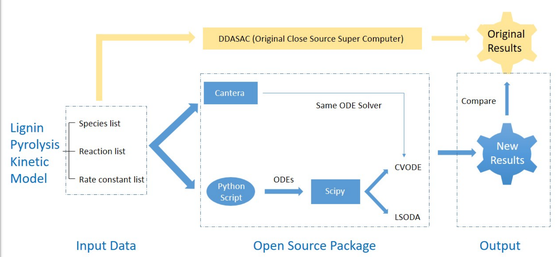

Figure 2. objective pipeline

SciPy is an open source Python library used for scientific and technical computing. In this project, the ordinary differential equations (ODEs) generated from input data can be solved by built-in ODE solvers in scipy.integrate. Here we choose two best-known ODE solvers -- LSODA and CVODE to solve ODEs. The methods used in LSODA and CVODE are variable-order, variable-step multistep methods. It provides automatic method switching between implicit Adams method for non-stiff problems, and a method based on backward differentiation formulas (BDF) for stiff problems. So LSODA and CVODE are widely used in industrial applications for its convenience and simplicity.

Cantera is an open source collection of object-oriented software tools for problems involving chemical kinetics, thermodynamics, and transport processes. It combines two steps: generating ODEs from reaction information and solve ODEs by built-in CVODE solver. The ODE solver method in Cantera is same as that in Scipy.integrate, so if the ODE equations are all the same, we can expect to get the same results from Cantera and Scipy.integrate. But it may take less time to compute in Cantera, because it is written in C++, which has higher operating efficiency than Python, the foundation of Scipy.

Workflow

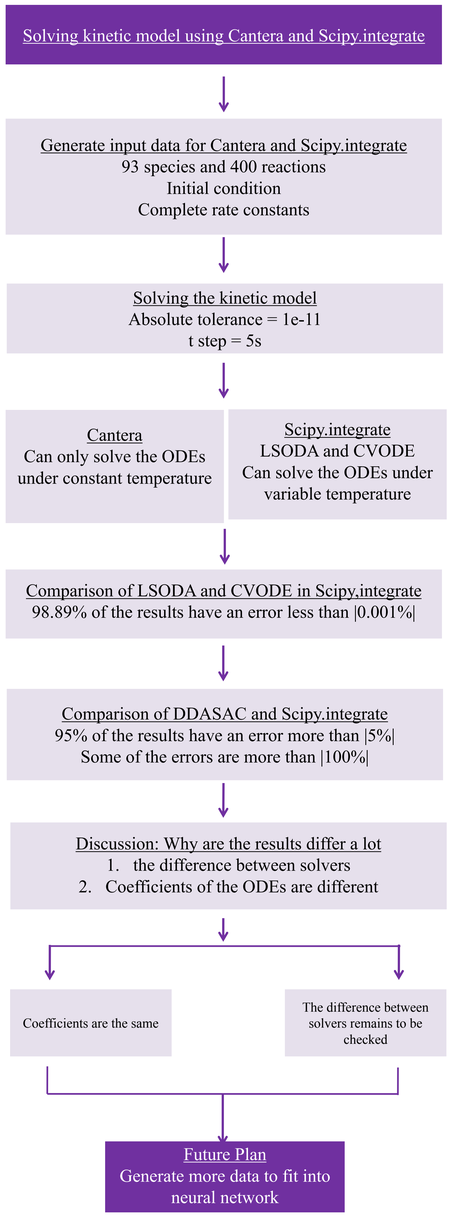

Figure 3. Workflow

Results and Discussion

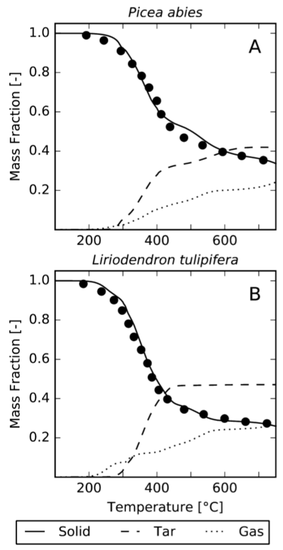

Figure 4. weight loss curve comparison

The typical strategy for validating kinetic models of biomass slow pyrolysis is comparing predicted weight loss curves with experimental results from TGA experiments. In Figure 4 model predictions for total solid yields is compared to the experiments of Jakab et al. This model shows excellent temporal agreement with solid yield for lignin from the two species shown, and the same level of agreement is observed with the other 14 species in the experimental study.

Open source licensing is popular because it helps produce reliable and high quality software quickly and inexpensively. In addition, it is innovative since open source programs are the product of collaboration among a large number of different programmers. Our goal is to make the neural network for Lignin pyrolysis open source. This kind of code renewal progress is common in the industry. Now we successfully script in Python to solve the kinetic model which containing 93 species and 400 ordinary differential equations, while previous work could only be executed on the high-performance computer called CMOL and the commercial tool called DDASAC. However, our result is still different from previous one due to numeric accuracy and ODE solvers. During the period, we put much effort on debugging and various ODE solving methods. Furthermore, the computational time has been successfully reduced to one minute for one initial condition. Our next step is to use this result to feed into machine learning model. 250 thousand different initial conditions will be generated and neural network method will be used for our Lignin model. We will build an open source package based on Python. Thus, ODEs will no longer need to solve again and results can get in seconds.

Capstone Project
UNIVERSITY of WASHINGTON

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