Lumped Model for Fluid Catalytic Cracking

Objective: Kinetic Parameter Estimation for FCC using a Lumped model
In this example, we build a lumped model for catalytic cracking of heavy feedstock. Lumping strategies, where species of similar carbon numbers are grouped together, allow us to build simplified models that can be practical for operational use. Here, we use a six-lump model and data from [1] to estimate the kinetic parameters. You may download the zipped rex file for this project.

Features Illustrated
- Building a lumped model for FCC
- Direct use of compound mass in a project, instead of moles
- Using REX for non-standard reaction engineering applications
- Pie Chart Reports of weighted and unweighted Least Square Errors (LSQ)
- Parity Charts for Sets that have several Experimental Data points

Reaction Model
We consider a six lump model described in [1]. The lump for feedstock contains compounds present in Vacuum Gas Oil (VGO) and Light Cycle Oil (LCO). The product lumps are Gasoline, Coke, C4 species, C3 species and Dry Gases (C1, C2 and H2). This lumped cracking model as represented in [1] is shown below:
Along with the above pathways, there is usually a catalyst deactivation pathway that is considered. However, the experiments from [1] consider constant catalyst activity, so deactivation is not modeled here. In addition, they eliminate the cracking reactions of gasoline, C3 and C4, which results in a simplified network:

All reactions are assumed with order of two with respect VGO+LCO. The mass balance for product lump $i$ can be expressed by the following equation:

$$\frac{dM_i}{dt} = k_i \phi m_c C_{VGO+LCO}^2$$

where $m_c$ is the catalyst mass, $\Phi$ represents the catalyst activity, $C_{VGO+LCO}$ is the mass concentration (gr/l) of [VGO+LGO] and $M_i$ is the mass of product lump $i$.

The experimental data in [1] is collected in a batch reactor and measurements of mass fraction are provided with time. The conversion from mass fraction to mass is straightforward by multiplying the fractions with the total mass in the batch reactor.

Setting up the REX Project
We first enter the lumps and inert $N_2$ in the compounds node. Since we work with mass units in this example, we must enter the molecular weights for the species in the Compound→Formula node to allow the calculation of pressure.
In the Reactions node, the five reactions of the simplified reaction network above are entered. The following units are chosen in the Units Configuration node:

<table>
<thead>
<tr>
<th>Variable</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time</td>
<td>sec</td>
</tr>
<tr>
<td>Temperature</td>
<td>°C</td>
</tr>
<tr>
<td>Pressure</td>
<td>atm</td>
</tr>
<tr>
<td>Volume</td>
<td>L</td>
</tr>
<tr>
<td>Mass</td>
<td>g</td>
</tr>
<tr>
<td>Moles</td>
<td>mmol</td>
</tr>
<tr>
<td>Specific Energy</td>
<td>kJ/mol</td>
</tr>
<tr>
<td>Surface Area</td>
<td>m²</td>
</tr>
<tr>
<td>Rate Basis</td>
<td>Catalyst Mass</td>
</tr>
<tr>
<td>Concentrations</td>
<td>Mass Density</td>
</tr>
</tbody>
</table>

In particular, we chose to work with Mass Density as units of Concentrations. Kinetics rates will thus depend on the mass concentration of compounds.

In Kinetics node we include the forward direction only for each reaction.

In Kinetics→Parameters node, we set order two with respect to the reactant for all reactions and enter some initial values for other parameters:
In this model, we assumed that the catalyst activity $\Phi$ is constant which is merged into the preexponential value in the REX model.

In the Estimation node, we consider all reactions to be estimated. We have experimental data at two temperatures, thus we open bounds for both pre-exponentials and activation energies in the Estimation→Parameters node:

In the Reactor node, we select a single gas batch reactor; all other options are kept to default:

Then we enter the experimental data for the experiments. We have two sets of data at different temperature, the measurements of mass along time is shown below:
In the Weights node, hybrid weights are used and we select all lumps to be reconciled, considering that we have independent measurements for them. Finally, we enable the Estimate option in the Solution Options node.

Model Results

The Results node reports the weighted and unweighted prediction errors (LSQ) summed across all sets, showing the contribution of each reconciled compound:
Finally, pie charts show the distribution of the prediction errors, by experimental set or by variable (usually a compound). The example below shows the contribution of compounds to the total weighted LSQ:
In the Model-Data Comparison node, you may inspect the model fit:

An alternative way to visualize the model match is by enabling parity charts. When doing that, the profiles along time are not shown, all experimental data for the compound is plotted against the calculated values. The 45 degree line represents perfect fit. For every set, all data-points are shown except the first one that corresponds to the initial condition. The line that connect the points in the parity chart only means that the connected points belong to the same experimental set. For example,
the Gasoline parity chart is shown below:

![Gasoline parity chart](chart.png)

Further Studies
Due to the limited amount of temperature data, there may be uncertainty in the activation energy values. You may enable Confidence Calculations in Solutions Options node, and then rerun the model. The confidence interval of the estimated parameters is reported in Results→Parameters node.

References