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**Explanatory Document:**

There are two folders enclosed. Their contents are explained below:

**Folder 1\_CO Oxidation Simple Kinetics**

*Contains*:

1. Code file: **CO Oxidation Simple Kinetics.ipynb**
2. Code pdf: **CO Oxidation Simple Kinetics - Jupyter Notebook.pdf**

This folder contains a hardcoded simple microkinetic model for (4 step) CO Oxidation written using python 3.7 on jupyter notebook. It simply solves resulting 4 differential equations for the coverages.

**Folder 2\_Matrix CO Oxidation Microkinetic model (with Fitting)**

Contains:

1. Code file: **Curve\_fit | L-BFGS-B\_Diff\_eval | Spline-Feature Scaling.ipynb**
2. Code pdf: **Curve\_fit | L-BFGS-B\_Diff\_eval | Spline-Feature Scaling - Jupyter Notebook.pdf**
3. Atomic Matrix: **Atom\_Input.csv**
4. Stoichiometric Matrix: **Stoic\_Input.csv**
5. Known rate constants: **Param\_Input.csv**
6. Guess rate constants: **Param\_Input\_Guess.csv**

This folder contains a generic code to solve for the coverages from a user defined microkinetic model in the form of matrices (therefore allowing for any reaction mechanism(s) to be implemented in making the model). Similarly, the code was written using python 3.7 on jupyter notebook. The same 4 step CO Oxidation model was still used. An attempt is then made to fit data using the microkinetic model defined.

A sample set was obtained from the outputted coverages and used to perform fitting to re-obtain the kinetic rate constants. It was used as the input of which a microkinetic model is being fitted into. This sample set was normalized to allow for ease in fitting. The goal behind the fitting of coverages is to create the possibility of externally obtained coverage profiles (obtained through KMC, TAP, etc.) to be fitted based on a speculated reaction mechanism defined in the matrices (i.e., the reaction mechanism) and have the corresponding rate constants predicted. *Note: Numerical solvers were used to perform fitting therefore needing guess rate constants to be provided. These are crucial to generating good predictions which is why multiple fitting techniques were explored and their dependency on initial conditions was qualitatively analyzed.*