STEP 1:

Create the top of the Cantera YAML file. The simplest thing to do is to take an existing file and copy it.

The beginning of the file will be the model name (here , the model name will be “Example5”).

The phases here include one named *gas* phase and one named *surf* . Later, these will be “linked” by a Cantera interface object where the gas phase species can thereby impinge upon the surface.

In this example, we are going to two possible surface species, Acetaldehyde1-Ce(S), Acetaldehyde2-Ce(S), in addition to empty sites. We are only going to use one of the surface species.

We **cannot** have a pressure of 0, so we use 1E-20.

STEP 2:

Add actual thermodynamics quantities for the gas phase acetaldehyde and surface species

Some NASA polynomials came from. <https://doi.org/10.1016/j.combustflame.2014.12.010>

Acetaldehyde 3D Sackur-Tetrode 156.06 J/molK

**TODO:** Provide explanation for how to make the surface species thermodynamics using Sackur-Tetrode, adsorption enthalpy calculations, and info from following link: https://myengineeringworld.net/2013/10/Excel-thermochemical-NASA-polynomials-Burcat.html

STEP 3:

Create a set of reactions and rate constants. In this case, we will be using Example5\_input\_reactions\_parameters.csv which is based on some previous model.

canteraReactionType should be “reaction” (or ‘surface\_reaction’). The fact that it is as surface reaction is actually gleaned from the (S) inside reactionEquation.

We have made a few reactions, but we are only going to use the ones related to Acetaldehyde species 11. The way we will do that is simply by having the surface covered with only species 1 during the initial coverages. There are already some coverages inside Example5\_yaml\_top\_info.yaml, but we are going to overwrite those later.

STEP 4:

Inside model\_functions\_example5.py we will need to create the simulation function that PEUQSE will call. First, we will put all of the settings at the top of the file for the “Example5\_input\_simulation\_settings”, these are for the cantera simulation model (not for PEUQSE).

In these lines of code we have set the surface coverage to have only the Acetaldehyde1 surface species, and nothing of anything else.

Then we have some piecewise intervals and parameters. These are the cantera parameters – we are only going to modify some subset of these using PEUQSE.

In order to help the parameter estimation find a solution, we are going to make the samplings like “*offsets*” from each other that then get converted into modifiers: this way we can confine ourselves to monotonically decreasing activation energies.

STEP 5:

It is a best practice to create an example simulation prior to running the parameter estimation. We will do so inside a function called “test\_run”

The output from “test\_run” looks strange, but that is fine because it is not intended to be a “good” output.

STEP 6:

Now create a simulation function that will serve as a simulation wrapper.

Then test that also from the man function. Make 2 cases to make sure we can see a difference.

STEP 7:

Now create a PEUQSE runfile to change the PEUQSE inputs.

runfile\_example5 has a short mcmc run

runfile\_example5b has a doOptimizeLogP using the MAP from one of the short mcmc runs.

This example was not run to the point of reaching a good fit: just long enough to provide some examples. It looks like there should be some coefficient of scaling on the data.