Uncertainty Reduction Software

# Simulations Module

## class model\_data

### This object is used for the storage of data from simulations of various types (JSR, shock tube, burner, etc). It is meant to act as a single storage container type for all different simulation types. Simulation results such as speciation profiles are stored as Pandas DataFrame objects, and sensitivities are arrays accessible via indexing.

#### model\_data.k\_sens

##### Three dimensional array containing kinetic sensitivities of the model. First axis is the independent variable (time,position, temperature), second axis is the sensitivity parameter (k1, k2,…), and the third axis is the observable against which the sensitivity is calculated (i.e. NO, OH, CO2)

#### model\_data.p\_sens

##### Three dimensional array containing physical sensitivities of the model. First axis is the independent variable (time,position, temperature), second axis is the sensitivity parameter (i.e. T,P), and the third axis is the observable against which the sensitivity is calculated (i.e. NO, OH, CO2)

#### model\_data.sensitivities

##### Three dimensional array containing physical sensitivities of the model. First axis is the independent variable (time,position, temperature), second axis is the sensitivity parameter (i.e. T,P, k1, k2,…), and the third axis is the observable against which the sensitivity is calculated (i.e. NO, OH, CO2)

#### model\_data.solution

##### The results of the simulation. Stored as a Pandas DataFrame. Column titles depend on type of simulation but generally may include information such as speciation profiles for species contained in mechanism used for simulation.

#### model\_data.Index

##### A list of lists used for indexing of the kinetic sensitivity array. First list contains independent variables (times, positions, temperatures), 2nd list contains the reaction equation, 3rd list contains a list of observables. Order of list corresponds to the order of axes in the sensitivity array

#### model\_data.pIndex

##### Serves the same purpose as model\_data.Index but for physical sensitivities. 2nd list is instead a list of the physical parameter varied such as ‘T’ or ‘P’.

#### model\_data.overall\_index

##### Same purpose as the above two functions but is a combined version where the second list contains first a list of physical parameters and then contains the reaction equation in the same axis. To be used if it is desired to use all sensitivities.

#### model\_data.simtype

##### Variable holds a string indicating what type of simulation was run. For example, a jet-stirred-reactor would be given the string ‘jsr’.

#### model\_data.\_\_init\_\_(self, simtype, kinetic\_sens=np.array(()), physical\_sens=np.array(()), Solution=pandas.DataFrame, Index=[], pIndex[])

##### Function to initialize model\_data instance. Each option is written to one of the class variables described previously.

#### model\_data.\_\_add\_\_(self, data)

##### Overloading of the addition operator returns the sum of two model data objects, where the sum is defined as joining of data along axis=0 such that the length of axis=0 is increased. The two model\_data objects must have equivalent values of model\_data.simtype.