Version 0.4.1 - 01/26/2015

**Change log:**

* Special rate coef importer improved.
* "MCM\_Constants.txt" file updated.
* Special forms TDBR1 - 4 tested and are calculating the rate coef correctly.

**Detailed/Technical Change log:**

* Special rate coef importer script improved. Many lines removed and if statements improved:
  + Script will now add to unknown rate arr if certain irregularities occur. This should stop the script writing over default Kintecus Arrhenius input and claiming all is right with the world.
  + "MCM\_constants.txt" now includes the required default Arrhenius input for Kintecus. This was changed to enable better coding and MCM2 functionality. Headers also updated.
* Tested TDBR1 - 4 against hand calculated values at 298 K and all rates were calculated correctly. TDBR3 and 4 were the opposite way to expected, but no big issue there.

**Current issues/improvements:**

* First runs of T2B model have shown that RO2 chemistry might not be being calculated correctly. This could be due to the special kinetic forms which need to be figured out!
  + Special kinetic forms checked out to be OK
  + Problem lies with the calculation of RO2 using the "OUTC[..]" command in the species spreadsheet.



* + Problem appears to be related to a model stiffness/integration issue. If integration step size is set to 1 second then get reasonable agreement with AtChem model:



* + However, set integration time to 10 seconds and not such a good fit:



* + Possible model stiffness or integration error?
  + Constraining the model to the profile of the RO2 predicted by AtChem almost matches (discrepancy here in the HO2 + CH3O2 reaction, which is not being calculated the same for some reason).



* + So kinetic equations are being calculated correctly. Something to do with the RO2 calculation making the model quite stiff in that case?
* Currently some minor debugging enabled to help code, but would be good to have a debugging option so that the various parts of the script are printed through the analysis process.
* Check that all rates are being calculated correctly.
* SP4 contains M but does not need it. Also, it is hard coded to multiply rate coefficient by 2, when this is currently done by the import script. One of them needs to change...
* Arrays need to be size-defined to avoid memory overflow issues with large models.
* Documentation is required. Not a full manual, but an improvement of the description below.
  + Example spreadsheet explaining the complex and special rate forms would be good. Can modify James' one perhaps?
* reactions that need different signs:
  + Most equations you must enter the data in the inverse sign form for Kintecus to read the data. As Kintecus calculates "EXP(-B/Temp)" you don't want to put "-1000", but "1000". This is not always the case, and so:
  + TDBR1 and 2 require the Ea as it appears in the MCM code. They also appear to be the wrong way around!

**Error code these things:**

* Um....

**Longer term goals:**

* Potentially written in Fortran/C/C# to make this compatible with other ways of running kintecus (Text based)
* Integration of temperature and photolysis profiles
* Testing alongside a Facsimile run (Lisa's data maybe?)
* Get HIRAC data comparison with AtChem. Talk to Iusti.
* HO2 import script is not very clever. Could improve perhaps?
* Script currently only imports MCM special forms and complex forms. No support for photolysis rates yet.
* Ask user if they are OK with the model and species sheets being destroyed, or if they would prefer to append.
* Decode complex rate forms instead of using a case structure with hard-coded values. This would allow greater flexibility for any future updates or any other reactions that followed the same general rule. *This is mainly for the SP4 case...*

**Previous Versions:**

Version 0.4 - 01/21/2015

**Change log:**

* Transfered code to a Kintecus blank model workbook.
* Added button on control panel to activate macro (Don't know if James will want this, but is useful to test if the whole thing works.
* Updated code to be independent of which sheet is active at the start.
* Importer will complain if there is no "MCM", "model" or "species" sheets. These are the 3 that are used.
* Importer now reads complex reaction constants from the tab delimited text file "MCM\_Constants.txt" located in the Kintecus directory.

**Detailed/Technical Change log:**

* Added some extra functions to check for sheet existence and check for headers based on comment character "#".
* Variables have been tidied up and moved to top. Code now runs in "Option explicit" mode to avoid undeclared variables.

Version 0.3.2 - 01/14/2015

**Change log:**

* Tidied up variables. Now defined and initialised at the beginning.
* Improved search functions.
* RO2 now counted as species and not enhancers.
* Code now recognizes double exponential rate coefficients and interprets them as TDBR3.

**Detailed/Technical Change log:**

* Improved search functions.
  + String searches were basic and not looking for exact matches. Caused mismatching errors and some rates that were let through, even though not identified!

Version 0.3.1 - 01/14/2015

**Change log:**

* Fixed the complex rate importer.
* Now imports "M" correctly.

**Detailed/Technical Change log:**

* Removed "ignore M" feature, as it wasn't necessary. You can specify "+M" as a reactant (I just hadn't read the manual correctly).
* Now imports remaining complex rates from the MCM. Will throw an error if not recognised and dump the unknowns at the end of the model spreadsheet, commented out.
  + This is done through a case structure function and the expressions are matched explicitly.
  + Hence, values and expressions are hard coded into the script.

Version 0.2 - 29/12/2014

**Change log:**

* Now copes with multiple "M" species in Rate Expression.
* Code should now be able to handle some minor unknown rate expressions and prompt user if so.
* HO2 self reaction now imports correctly

**Detailed/Technical Change log:**

* Multiple "M" Species:
  + Code rewritten to build a string of unique 'M' species instead of assuming all left over terms are 'M's.
  + Checks for 'M' in the list of species compiled earlier in code - if 'M' then puts in O2 and N2 as specified enhancers.
* Added function to find end character termination. Speeds up code.
* Reshuffled code so not all in one big loop. Nested if statements were looking for 'VARIABLE' and 'RO2' at every line. There was no point! These are now separated and terminate their loops when something is found.
* Added boolean variables to deal with certain changes during the main loop (PreExpSet for example).
* Altered the way Special Reactions and Complex reactions are handled
  + Better adaptation to multiple enhancers and Spec Rates.
  + Code does not now assume that something not found in the nested if statements is a 3rd body enhancer (which was silly).
* If part of rate expression is not recognised, then error dialog displayed and reactions can be entered "AS IS" or appended to model sheet but commented out (whichever the user prefers).
* HO2 self reaction
  + Importer works, but have had to include some very specific code to deal with this one case.
  + What if there are others? - Unlikely.
  + Think of a better way?
* Added "IgnoreM" boolean - could be useful later on?