**Model used in the manuscript “Influence of Relative Humidity on the Heterogeneous Oxidation of Secondary Organic Aerosol”**

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The SOAHTChemistry.ipf file contains the code of the multilayer heterogeneous oxidation model presented in the manuscript “Influence of Relative Humidity on the Heterogeneous Oxidation of Secondary Organic Aerosol” by Li et al. that has been submitted to Atmospheric Chemistry and Physics. Igor Pro v.6.37 (<https://www.wavemetrics.com/>) is used to run the code.

1. Major functions:
   1. CreatekkWave\_3G\_basic() and CreatekkWave\_3G\_basicH2O(): Create a wave, named kkwave, containing all the parameters necessary for simulation, including rate constants, particle size, uptake coefficient, etc. The latter serves for high RH conditions where growth factor is taken into consideration
   2. OHexposure38s\_3G\_dry() and OHexposure38s\_3G\_H2O(): Simulate evolution of particles at a fixed OH concentration for certain amount of time.
      * A kkwave must be created before using these functions
      * Two functions are designed for low and high RH, respectively. The difference lies in the particle growth due to water uptake
      * Total simulation time is 38 s by default, but can be set differently in kkwave
      * RO radicals are treated implicitly in these functions (see manuscript for details)
   3. FullOHRange\_lowRH() and FullOHRange\_highRH(): Simulate evolution of particles after exposed to various OH concentrations at a fixed time
      * Number of OH concentrations and the largest OH concentration to be considered can be set in the functions
      * Simulation time for each OH concentration is set to 38 seconds by default, but can be changed in kkwave
      * These functions use OHexposure38s\_3G\_dry() and OHexposure38s\_3G\_H2O() respectively for each OH concentration
2. Example instruction:
   1. Example: simulation of particle evolution at a fixed OH concentration for a certain amount of time at low RH
   2. Compile the procedure and an “HT Oxidation” tab will appear on the menu bar
   3. Select “Create Rate Constants Wave -> Low RH-Simple”, enter the values in the pop-up window
      * Some values can’t be set in the pop-up window and need to be set in the function instead, such as particle initial diameter and total flow time. In this case, go to function “CreatekkWave\_3G\_basic()” in the procedure window, find the variable(s) and change the values by reentering the number right to the equal sign
   4. Select “Profiles at one OH conc - > Low RH”
   5. Multiple waves will be generated after the function is done running, including VFR\_38s, C\_RH, SL\_RO2, etc. Click on the wave in Data Browser to see the note for the wave for explanation on the meaning of the wave.
3. Advanced simulations:
   1. Functions CreatekkWave\_3G\_adv() and CreatekkWave\_3G\_advH2O() allow for input of different rate constant/fragmentation probability for different generation of the products. Major functions introduced in 1.b and 1.c can then be applied to explore the influence of generation-specific properties.
   2. Function OHexposure38s\_3G\_dry\_RO() is similar to 1.b but RO radicals are treated explicitly so that reactions such as RO+RH and RO decomposition are considered explicitly. Functions 3.a have pop-up menu where these two rate constants can be set. However, this function is not designed to simulation particle growth due to water uptake at high RH.
4. Miscellaneous functions:
   1. GraphFraction(ymatrix,xwave): Plot a stacked graph of the concentrations/fraction of all the species in the particle bulk. ymatrix should be wave “finalconc” generated by 1.b or wave “ConcAllspecies” or “FractionAllspecies” generated by 1.c. xwave should refer to wave “OHexposure\_38s” or “OHexposure”. y-axis: accumulated concentration/fraction; x-axis: OH exposure
   2. R2foroxidizedvsnon(finalconc): Calculate the R2 between oxidized particles and non-oxidized particles from linear fitting of the scatter plot. finalconc should refer to wave “finalconc” generated by 1.b or wave “ConcAllspecies” or “FractionAllspecies” generated by 1.c.