How to use the Henry's Law Constant table with the MOZART options

The MOZART chemistry options (chem_opt = 111, 112, 201, 203) now use a table of Henry's Law constants for calculations in wet deposition (module_mozcart_wetscav.F), dry deposition (module_dep_simple.F), and convective wet deposition (module_ctrans_grell.F). The input file HLC.TBL is in the distribution run directory and must be copied into the simulation directory before execution. There are no changes required in the namelist.input file to run with the new Henry's Law constants.

The HLC.TBL file is an ascii, comma separated values (csv) table wherein each line has the following form:

Species, type, MW, KH_298, dH/R, K1_298, dE1/R, K2_298, dE2/R

Where:

- Species is a character variable (max length = 64)
- type is for future use, presently defaults to 0
- MW is a real defining the species molecular weight in amu
- KH_298, dH/R, … are real variables defining the Henry's Law constants

For all species, except ammonia(NH3), the effective coefficient is:

$$Heff = KH(T) * (1. + K1(T)/[H+] * (1. + K2(T))/[H+]))$$

And for ammonia (NH3) the effective coefficient is:

$$Heff = KH(T) * (1. + K1(T)*[H+]/K2(T))$$

With KH, K1, and K2 defined as:

$$KH(T) = KH\_298*\exp(dH/R*(1/T - 1/298))$$
$$K1(T) = K1\_298*\exp(dE1/R*(1/T - 1/298))$$
$$K2(T) = K2\_298*\exp(dE2/R*(1/T - 1/298))$$

To add a species or change the values in HLC.TBL, the following procedure is recommended.

1) Rename the file, HLC.TBL, to save the file: mv HLC.TBL HLC.TBL_org
2) Copy the original file to a new name for editing: cp HLC.TBL_orig HLC.TBL_new
3) Edit the new file, HLC.TBL_new
4) Link the new file to HLC.TBL: ln –sf HLC.TBL_new HLC.TBL

This method perserves both the original and new.