General CMAQ Changes

- Global Changes
  - USE RXNS_DATA replaces include statements for RXCM.EXT and RXDT.EXT files
- Chemistry Solvers
  - Routines in RXNS_FUNC MODULE replace *calcks and *calc_special routines in ROS3, EBI and SMVGEAR
- Aerosol Module
  - hetchem.f file removed from aero_subs.F
  - USE AEROSOL_CHEMISTRY statement enable access to data for aerosol diagnostic file such as GAMMA_N2O5
  - Other diagnostics variables are added such as the CLNO2 reaction, to be used in CMAQ version 5.1

Revisions to previous reaction data and types

- Changes to homogeneous chemistry
  - Duplicate products are combined into one product with net coefficient
    - *"→ a*OH + HCHO + b*OH"* becomes *"→ (a+b)*OH + HCHO"*
  - Type 9 Fall Reaction is modified to include rate constant such as for NO + HO2 -> HNO3
    - In mech.def : %3 # A^B@C & D^E@F & G@H;
    - Calculated : A*(T/300)**B*exp(-C/T)+ D*(T/300)**E*exp(-F/T)*N+G*exp(-H/T) where T = temperature and N = number density
    - Changes are backwardly compatible to old Type 9 expression
  - New Reaction Type for rate constants that depend sunlight, pressure and open ocean coverage
    - In mech.def: %H # A@-B & C@-D;
    - Equals A*exp(B*PRESSURE)+C*exp(D*PRESSURE) if sunlight is true and open/ice free water and 0.0 if not
      - Pressure in atmospheres
    - Implements ozone loss from non-chlorinated marine halogens

Source Code Files and New Reaction Type

- Two New F90 files (see build directory for example)
  - RXNS_DATA_MODULE.F90 contains same information in RXCM.EXT and RXDT.EXT files
  - RXNS_FUNC_MODULE.F90 contains subroutine and function to explicitly calculate standard rate constants
  - Latter file intends to make calculated rate constants more transparent and easier to change
- Reactions now possible between GC, AE and NR species, i.e., heterogeneous reactions
- New Reaction Type accomplishes heterogeneous reactions whose rate is calculated by a separate module called AEROSOL_CHEMISTRY (see build directory for example)
  - In mech.def fils, Reaction type denoted by the "~" symbol as below
    - <HET_N2O5> N2O5 = 2.0*HNO3 # 1.0~<HETERO_N2O5>;
    - <HET_N02> NO2 = 0.5*HONO + 0.5*HNO3 # 1.0~<HETERO_NO2>;

AEROSOL CHEMISTRY Module

- Calculate rate constants denoted by "~" in mechanism definition file.
- Module contains data and subroutines that set needed rate constants
  - Similar to how the phot routine returns photolysis rates
  - Unlike phot, available heterogeneous rate constants are hardwired into code
    - Model stops if requested rate constant not available
  - Several rates are available and will be used in CMAQ version 5.1
  - Only two rates used in the sent build directory's mechanism.
    - HETERO_N2O5 : N2O5 -> 2*HNO3
    - HETERO_NO2 : NO2 -> 0.5*HONO + 0.5*HNO3