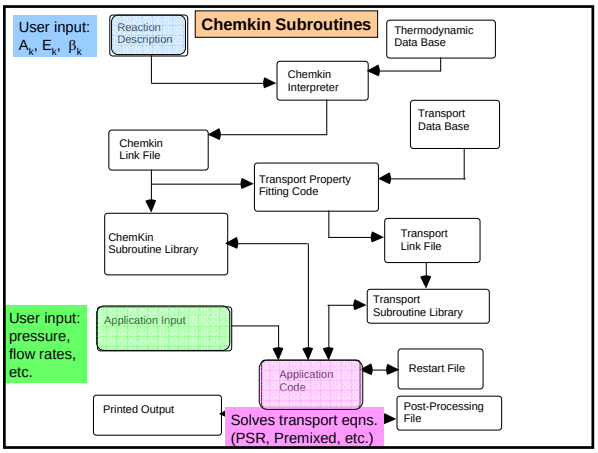
Intro to Chemkin



Examples of Chemkin Subroutines

What is the difference?

12. MEAN THERMODYNAMIC PROPERTIES (MOLAR UNITS)

SUBROUTINE CKABML (P, T, X, ICKWRK, RCKWRK, ABML)*
Returns the Helmholtz free energy of the mixture in molar units, given the pressure, temperature, and mole fractions; see Eq. (46).

SUBROUTINE CKCPBL (T, X, ICKWRK, RCKWRK, CPBML)
Returns the mean specific heat at constant pressure; see Eq. (33).

SUBROUTINE CKCVBL (T, X, ICKWRK, RCKWRK, CVBML)
Returns the mean specific heat at constant volume in molar units; see Eq. (35).

SUBROUTINE CKGBML (P, T, X, ICKWRK, RCKWRK, GBML)*
Returns the mean Gibbs free energy of the mixture in molar units, given the pressure, temperature and mole fractions; see Eq. (44).

SUBROUTINE CKHBML (T, X, ICKWRK, RCKWRK, HBML)
Returns the mean enthalpy of the mixture in molar units; see Eq. (37).

SUBROUTINE CKSBML (P, T, X, ICKWRK, RCKWRK, SBML)*
Returns the mean entropy of the mixture in molar units, given the pressure, temperature and mole fractions; see Eq. (42).

SUBROUTINE CKUBML (T, X, ICKWRK, RCKWRK, UBML)
Returns the mean internal energy of the mixture in molar units; see Eq. (39).

13. CHEMICAL PRODUCTION RATES

SUBROUTINE CKCDC (T, C, ICKWRK, RCKWRK, CDOT, DOOT)
Returns the molar creation and destruction rates of the species given the temperature and molar concentrations; see Eq. (73).

SUBROUTINE CKCDXP (P, T, X, ICKWRK, RCKWRK, CDOT, DDOT)
Returns the molar creation and destruction rates of the species given pressure, temperature and mole fractions; see Eq. (73).

SUBROUTINE CKCDXR (RHO, T, X, ICKWRK, RCKWRK, CDOT, DDOT)
Returns the molar creation and destruction rates of the species given the mass density, temperature and mole fractions; see Eq. (73).

SUBROUTINE CKCDYP (P, T, Y, ICKWRK, RCKWRK, CDOT, DDOT)
Returns the molar creation and destruction rates of the species given mass density, temperature and mass fractions; see Eq. (73).

More examples of Chemkin Subroutines

What is the difference?

SUBROUTINE CKCDYR (RHO, T, Y, ICKWRK, RCKWRK, CDOT, DDOT)
Returns the molar creation and destruction rates of the species given the mass density, temperature and mass fractions; see Eq. (73).

SUBROUTINE CKCCONT (K, Q, ICKWRK, RCKWRK, CIK)
Returns the contributions of the reactions to the molar production rate of a species; see Eqs. (49) and (51).

SUBROUTINE CKCTC (T, C, ICKWRK, RCKWRK, CDOT, TAU)
Returns the molar creation rates and characteristic destruction times of the species given temperature and molar concentrations; see Eqs. (76) and (78).

SUBROUTINE CKCTXP (P, T, X, ICKWRK, RCKWRK, CDOT, TAU)
Returns the molar creation rates and characteristic destruction times of the species given the pressure, temperature and mole fractions; see Eqs. (76) and (78).

SUBROUTINE CKCTXR (RHO, T, X, ICKWRK, RCKWRK, CDOT, TAU)
Returns the molar creation rates and characteristic destruction times of the species given the mass density, temperature and mole fractions; see Eqs. (76) and (78).

SUBROUTINE CKCTYP (P, T, Y, ICKWRK, RCKWRK, CDOT, TAU)
Returns the molar creation rates and characteristic destruction times of the species given the mass density, temperature and mass fractions; see Eqs. (76) and (78).

SUBROUTINE CKCTYR (RHO, T, Y, ICKWRK, RCKWRK, CDOT, TAU)
Returns the molar creation rates and characteristic destruction times of the species given the mass density, temperature and mass fractions; see Eqs. (76) and (78).

SUBROUTINE CKWC (T, C, ICKWRK, RCKWRK, WDOT)
Returns the molar production rates of the species given the temperature and molar concentrations; see Eq. (49).

SUBROUTINE CKWXP (P, T, X, ICKWRK, RCKWRK, WDOT)
Returns the molar production rates of the species given the pressure, temperature and mole fractions; see Eq. (49).

SUBROUTINE CKWXR (RHO, T, X, ICKWRK, RCKWRK, WDOT)
Returns the molar production rates of the species given the mass density, temperature and mole fractions; see Eq. (49).

SUBROUTINE CKWYP (P, T, Y, ICKWRK, RCKWRK, WDOT)
Returns the molar production rates of the species given the pressure, temperature and mass fractions; see Eq. (49).

SUBROUTINE CKWYR (RHO, T, Y, ICKWRK, RCKWRK, WDOT)
Returns the molar production rates of the species given the mass density, temperature and mass fractions; see Eq. (49).

$k = A T^{\beta} e^{-E/RT}$

```
ELEMENTS
O H N
END
SPECIES
  O   O2  H  H2  OH  HO2  H2O  H2O2
  N2
END
REACTIONS                                  A        β      E (cal/gmol)
  H+O2 = O+OH              (MILLER 81)     5.1E16  -0.82  16510
  H2+O = H+OH              (MILLER 77)     1.8E10   1.0    8830
  H2+OH = H2O+H            (DIXON-LEWIS 77) 1.2E09  1.3    3630
  OH+OH = H2O+O            (COHEN 79)      6.0E08   1.3     0.0
  H+OH+M = H2O+M           (MILLER 77)     7.5E23  -2.6     0.0
    H2O /20.0/
  O2+M = O+O+M             (MILLER 81)     1.9E11   0.5   95560
  H2+M = H+H+M             (MILLER 77)     2.2E12   0.5   92600
    H2O/6.0/  H/2.0/  H2/3.0/
  H2+O2 = OH+OH             (MILLER 77)    1.7E13   0.0   47780
  H+O2+M = HO2+M            (SLACK 77)     2.1E18  -1.0     0.0
    H2O/21.0/  H2/3.3/  O2/0.0/  N2/0.0/
  H+O2+O2 = HO2+O2         (SLACK 77)      6.7E19  -1.42    0.0
  H+O2+N2 = HO2+N2         (SLACK 77)      6.7E19  -1.42    0.0
  HO2+H = H2+O2            (LLOYD 74)      2.5E13   0.0    700
  HO2+H = OH+OH            (LLOYD 74)      2.5E14   0.0   1900
  HO2+O = OH+O2            (LLOYD 74)      4.8E13   0.0   1000
  HO2+OH = H2O+O2          (LLOYD 74)      5.0E13   0.0   1000
  HO2+HO2 = H2O2+O2        (TROE 69)       2.0E12   0.0    0.0
  H2O2+M = OH+OH+M         (BAULCH 72)     1.2E17   0.0  45500
  H2O2+H = HO2 + H2        (BAULCH 72)     1.7E12   0.0   3750
  H2O2+OH = H2O+HO2        (BAULCH 72)     1.0E13   0.0   1800
END
```

Figure 3. Example input file for the Chemkin Interpreter.

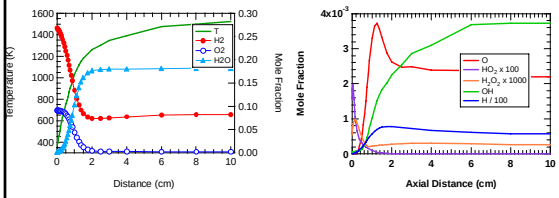
Example Subroutine

```
      SUBROUTINE FUN( NEQ, TIME, Y, F)
      DIMENSION Y(NEQ), F(NEQ)
C
C INPUT -
C   NEQ   - the number of dependent variables.
C   TIME  - the independent variable, time.
C   Y     - the dependent variable vector (length NEQ), structured as:
C           y(1)   = T, the temperature in Kelvins,
C           y(k+1) = Yk, the mass fraction of the k:th species.
C OUTPUT -
C   F     - The right-hand sides of the governing equations.
C-----------------------------------------------------------------------
      DIMENSION WT(10), H(10), WDOT(10)
C
C        These arrays are required to store output of some Chemkin
C     Subroutine calls.  They allow for up to 10 species.
C        WT(*)  - The molecular weights of the species (g/mole).
C        H(*)   - The species enthalpies (erg/mole*K)
C        WDOT(*)- The species molar production rates (moles/cc*sec).
C-----------------------------------------------------------------------
C
      COMMON /CHEMDIM/ KK, P, IWORK(200), WORK(200)
C
C        This common block contains parameters and data that are needed,
C     but not available through the FUN call list.
C        KK    - the number of species.
C        P     - the pressure in dynes/cm**2
C        IWORK - the Chemkin integer work space.
C        WORK  - the Chemkin real work space.
C
      CALL CKRHOY( P, T(1), T(2), IWORK, WORK, RHO)
      CALL CKCPBS( T(1), T(2), IWORK, WORK, CPB)
      CALL CKHMS (   T(1),       IWORK, WORK, H)
      CALL CKWYP ( P, T(1), T(2), IWORK, WORK, WDOT)
      CALL CKXTY (                IWORK, WORK, WT)
C
C        form the summation in eq. (6)
C
      SUM=0.
      DO 100 K=1,KK
         SUM = SUM + H(K)*WDOT(K)*WT(K)
  100 CONTINUE
C
C        form the right-hand sides of eqs. (6) and (7)
C
      F(1) = - SUM / (RHO*CPB)
      DO 200 K=1,KK
         F(K+1) = WDOT(K) * WT(K) / RHO
  200 CONTINUE
C
      RETURN
      END
```

ρ c_p h_i ω_i W_k (MW's) $= \sum_k h_k \omega_k W_k$ $= \frac{\sum_k h_k \omega_k W_k}{\rho c_p}$ $= \frac{\omega_k W_k}{\rho}$

Figure 4. Subroutine for defining governing equations for solution by LSODE.

Sample Chemkin Output



Example Premixed 1-D H_2 and O_2 in Ar