Units of Concentrations and Reaction Rates

In Chemked-II, the two sets of units are used, which are based on the unit volume and on the unit mass.

Units based on the unit volume

Among a great number of concentration units we have chosen mol/cm^3. These units are most frequently used in published reaction mechanisms and they are the default units in the CHEMKIN subroutines. Reaction rates have units mol/cm^3 sec.

Example ----------
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OH + M = O + H + M         9.88E+17 -0.74 102100
H2/2.5/ H2O/12./ AR/0.75/
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Concentrations [OH], [O], [H], [M] mol/cm^3
Forward reaction rate $q_{for} = k_{for}$ [OH][M]
Reverse reaction rate $q_{rev} = k_{rev}$ [O][H][M]
Net reaction rate $q_{net} = q_{for} - q_{rev}$
The all reaction rates have units mol/cm^3 sec.

The time functions of these values can be viewed with the post-processor tools (see the help topic **Analyzing Output Data**).

Note. To calculate the molar production w_{jn} of species n in reaction j, the net reaction rate should be multiplied by stoichiometric factor s_{jn} of this species. $w_{jn} = s_{jn} * q_{net}$, mol/cm^3 sec

Units based on the unit mass

These concentration units are mol/g. The units are natural for the constant pressure processes; conservation equations for species have a simple form.

$$\frac{dZ_n}{dt} = \sum_j b_{jn} \;;\; b_{jn} = \frac{w_{jn}}{\rho}$$

where Z_n is content of species n per 1 gram of gas mixture (mol/g); ρ is gas density (g/cm^3) and b_{jn} is production rate of species n in the jth reaction (mol/g

sec). Sum is over reactions that involve the *n*th species The integral production (mol/g) of species *n* on the time interval t_1-t_2 is

$$Z_n(t_2) - Z_n(t_1) = \sum_j B_{jn} \; ; \quad B_{jn} = \int_{t_1}^{t_2} b_{jn}\, dt$$

Time functions of the production rates b_{jn} and the total productions B_{jn} can be viewed with the post-processor tools (see the help topic **Analyzing Output Data**).