**Extended Fall-off reactions**

This is a first example in which only 1 bath species is specified:

H2O2 (+M) = 2OH (+M) 2.00E12 0.9 48749. ! High-pr kinf

LOWMX / 2.49E24 -2.3 48749. / ! Low-pr klow

TROEMX / 0.43 1.E-30 1.E+30 / ! Troe parameters

LOWSP / H2O 1.86E25 -2.3 48749. / ! klow for (+H2O)

TROESP / H2O 0.51 1.E-30 1.E+30 / ! Troe for (+H2O)

H2O/1.0/ CO2/ 1.60/ N2/ 1.50/ O2/ 1.20/ !Other 3rd body eff.

Here we explicitly specify H2O as a bath species, by providing the low-pressure kinetic parameters (LOWSP) and the Troe coefficients (TROESP). The LOWMX and LOWMX keywords are used to specified the low-pressure kinetic parameters and the Troe parameters for all the remaining species (MX stands for mixture). The overall reaction rate is calculates as the weighted sum of 2 reaction rates: one associated to the mixture parameters (MX) and one associated to the H2O species. The weights are represented by the mole fractions:

In the following example, we specify two bath species, in addition to the mixture (please consider that the numbers I put are random):

H2O2 (+M) = 2OH (+M) 2.00E12 0.9 48749. ! High-pr kinf

LOWMX / 2.49E24 -2.3 48749. / ! Low-pr klow

TROEMX / 0.43 1.E-30 1.E+30 / ! Troe parameters

LOWSP / H2O 1.86E25 -2.3 48749. / ! klow for (+H2O)

TROESP / H2O 0.51 1.E-30 1.E+30 / ! Troe for (+H2O)

LOWSP / CO2 1.86E21 -1.3 38649. / ! klow for (+CO2)

TROESP / CO2 0.71 1.E-20 1.E+29 / ! Troe for (+CO2)

H2O/1/ CO2/1/ N2/ 1.50/ O2/ 1.20/ !Other 3rd body eff.

In this case, the overall reaction rate would be:

More in general, if you specify N bath species (through the SP suffix), in addition to the mixture, which is always mandatory, through the MX suffix, the overall reaction rate would be:

Please remember that 3rd body efficiencies for all the bath species must be necessarily equal to 1. The OS++ checks for this.

**Extended PLOG Reactions**

Same ideas are applied to PLOG reactions with multiple bath species. This is an example with only 1 bath species:

H2O2 = 2OH 1.0 0. 0. ! Dummy k

PLOGMX / 1. 1.0e14 0. 50000./ ! k at 1 atm for [M]

PLOGMX / 100. 1.0e15 0. 51000./ ! k at 100 atm for [M]

PLOGSP / H2O 1. 1.0e14 0. 50000./ ! k at 1 atm for [H2O]

PLOGSP / H2O 10. 1.0e14 0. 50000./ ! k at 10 atm for [H2O]

The reaction rate is given by:

Of course, it is possible to specify any number of pressures for the mixture and for each bath species. The pressure levels do not necessarily have to be the same for all the species and mixture. This is a more complex example, with 2 bath species and different pressure levels (numbers are random!):

H2O2 = 2OH 1.0 0. 0. ! Dummy k

PLOGMX / 1. 1.0e10 2. 53000./ ! k at 1 atm for [M]

PLOGMX / 10. 1.0e11 -1. 51000./ ! k at 10 atm for [M]

PLOGSP / H2O 1. 1.0e12 0.1 72000./ ! k at 1 atm for [H2O]

PLOGSP / H2O 10. 1.0e13 0.3 45000./ ! k at 10 atm for [H2O]

PLOGSP / H2O 100. 1.0e14 0.2 25000./ ! k at 100 atm for [H2O]

PLOGSP / CO2 1. 1.0e12 0.5 34000./ ! k at 1 atm for [CO2]

PLOGSP / CO2 20. 1.0e13 0.4 47000./ ! k at 20 atm for [CO2]

In this case, the overall reaction rate would be:

More in general, if you specify N bath species (through the SP suffix), in addition to the mixture, which is always mandatory, through the MX suffix, the overall reaction rate would be: