The expressions for state-specific single-quantum rates of V-T and V-V energy transfer in nitrogen, taken from Ref. [37], are as follows:

** (1)

** (2)

In Eqs. (1,2),  and *w* are vibrational quantum numbers, and are “radii” for V-T and V-V energy transfer,

, (3)

, (4)

*T* is the rotational-translational temperature (“gas temperature”), and  and  are the rates of V-T and V-V energy transfer processes

 (5)

and

 , (6)

respectively. Temperature-dependent rates of V-T relaxation of nitrogen by N2, O2­, N, and O, used in the present model, , were taken from Ref. [38], which provides curve fits to the available experimental data. Specifically, the room temperature rate coefficient for N2 V-T relaxation by O atoms is =3.5∙10-15 cm3/s [39]. The rates of N2 V-T relaxation by N atoms were taken the same as relaxation rates by O atoms. Note that this is an upper bound estimate since theoretically predicted low-temperature V-T rates for N2-N are very slow [40]. The same assumption was made for N2 V-T relaxation by H atoms. This use of this assumption, however, is unlikely to affect the model predictions significantly, since both N atom and H atom number densities at the present conditions are significantly lower compared to that of O atoms (predicted peak number density of [O] ≈ 9∙1015 cm-3), such that vibrational relaxation of nitrogen occurs primarily in collisions with oxygen atoms. V-T relaxation rates of nitrogen by H2 were calculated using  from Ref. [41], with temperature dependence suggested in Ref. [42]. The rate coefficient of N2-N2 V-V relaxation, cm3/s, was taken from Refs. [43,44].

Ting, ChemKin does not allow rate expressions given by Eqs. (2,4), so I have modified it to be consistent with the generalized Landau-Teller rate expression, as follows:

** (2′)

** (2′′)

** (2′′′)

This should make it clear how to program the V-V rate expressions using the keywords DUP (to accommodate two terms in the sum in Eq .(2′)) and LT (for Landau-Teller rate expression).