Supplemental Material:

An example of the MECCA-TAG configuration file

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This document is part of the electronic supplement of the article "A kinetic chemistry tagging technique and its application to modelling the stable isotopic composition of atmospheric trace gases." in Geosci. Model Dev. (2010), available at: http://www.geosci-model-dev.net

Date: 08/06/2010

Example of the tagging configuration file

The tagging/doubling configuration file contains dedicated sections (each starts with a section name framed with the squared braces, an example is presented below). Each section provides specific input data:

[TAG] lists general tagging information including the unique tagging name, the number of classes and their names, the selection of the tagging integrator, and the units for the species initial compositions given in [SPC] section (both fraction and δ-permil values are supported). When the isotopic tagging is performed, this section includes also the reference name of the tagged isotope element and the atomic masses of considered isotopes.

[SPC] contains the list of species intended to be tagged, including the number of atoms of the tagged isotope element constituting the molecule. The latter, if not set to unity, indicates that the tagging should be performed accounting for the isotope transfer, otherwise the molecular tagging is performed. Optionally one can specify the initial distribution of classes or initial isotope ratios.

[SRC] includes the optional information on particular composition transfer (see Sect. 4 of the main manuscript) in selected reactions, referring to the corresponding reaction numbers in the MECCA equation file. The particular entry describing educt-to-product exchange is given in a form of an equation; one can specify the arbitrary branching ratio coefficients ($\eta_r^{e\to p}$) for the products. During the parsing, all branching ratios are normalized to unity for each pair of products in a selected reaction.

[KIE] lists the kinetic isotope effects included in the setup. The syntax is similar to that in the [SRC] section, *i.e.* includes the reaction number, the isotopologue and the rate modifier (*e.g.* an expression that is to modify the reaction rate, for example, in form of '* α' where α is the fractionation factor).

[IEX] lists the additional reactions to be introduced to account for the isotope exchange in the mechanism. The new reactions will be added to the MECCA equations list in case of doubling. The record for each reaction (syntax is depicted below) includes the reaction number, two exchanging species names and the reaction rate. The kinetic isotope effects for the forward and backward reactions must be listed in the [KIE] section.

An example of the tagging/doubling configuration file for stable oxygen isotopes is presented below. It includes 3 isotopes, 16 tagged species, 2 isotope exchange reactions, 2 KIEs and 4 composition transfer records. Note that this is only an illustrative example but not the setup used for the simulations presented.

```
; tagging/doubling configuration file
;
; #N# STABLE ISOTOPIC OXYGEN 16/17/18
; #K# o
;
; semicolon denotes the start of a commentary
;
; === general tagging information ================================================
[TAG]
  classes=I16 I17 I18                    ; tagging classes (for isotopologues: masses)
  iatom=O                                ; atom name: optional
  imasses=15.994915 16.999133 17.999160  ; isotope masses

; units in delta-permil, RKA integrator   (INT_LINMAX is for (Bloch 1991))
  parameters=ISO INIUNIT_DELTAPM INT_RKA xINT_CG1 xINT_LINMAX

; === list of species to tag =====================================================
[SPC]
; syntax: SPEC [atoms] = set of δ-values for minor isotopologues
;                   or = set fractions for tagging classes
;
; - optional [atoms] value overrides those picked from MECCA SPC file
; - for molecular/fractional tagging all atomic quantities
;   should be set to 1 (suppresses specific isotopic transfer)
;
; species initial composition
;
; species  O-atoms      d17O    d18O  (permil)
  O1D      1 =          0.00    0.00
  O3P      1 =          0.00    0.00
  O2       2 =         12.41   23.50
  O3       3 =         50.52   95.50
  H2O      1 =          0.00    0.00
  H2O2     2 =         21.16   40.00
  N2O      1 =         12.41   23.50
  NO       1 =         12.41   23.50
  NO2      2 =         12.41   23.50
  NO3      3 =         12.41   23.50
  N2O5     5 =         12.41   23.50
  HNO3     3 =         12.41   23.50
  CH3OH    1 =          7.92   15.00
  CH3OOH   2 =          7.92   15.00
  HCHO     1 =          7.92   15.00
  CO       1 =          0.00    0.00     ; zeroed intentionally
...

; === composition transfer/source specification section ========================
[SRC]
; syntax: REAC source species = list of destination species
;
; <G2104>  OH + O3 = HO2 + O2
  G2104 OH = HO2
  G2104 O3 = HO2 O2
...

; <G3106> NO2 + O3  = NO3 + O2
; NO2 accounts for 2/3 of NO3
; O3              1/3 of NO3
  G3106 NO2 = 2 NO3
  G3106 O3  = 1 NO3 O2
...
```

```
; ------------------------------------------------------------
; <G4101> CH4 + OH = CH3O2 + H2O
;  [Weston, 2001]: CH4 + OH     -> CH3 + H2O
;                  CH3 + O2 + M -> CH3O2 + M
  G4101 O2 = CH3O2
  G4101 OH = H2O
...
; ------------------------------------------------------------
; isoprene ozonolysis in lumped r-n G4500
; <G4500>  ISOP  + O3 = .28 HCOOH + .65 MVK + .1 MVKO2  + .1 PA +
;                       .14 CO + .58 HCHO + .09 H2O2 + .08 CH3O2 +
;                       .25 OH + .25 HO2 : {%TrGC} 7.86E-15*EXP(-1913./temp); {&1614}
  G4500  O3 = 1 HCOOH MVK 1 MVKO2 1 PA CO 0.081 HCHO 1 H2O2       OH
  G4500  O2 =             2 MVKO2 2 PA    0.919 HCHO        CH3O2    HO2
  G4500 H2O = 1 HCOOH                                  1 H2O2

; === kinetic isotope effect section ========================================
[KIE]
; syntax: REAC isotopologue = expression (*-like)
;         G1000 I18O2       = *1.001
;
; --- O3 -----------------------------------------------------------------
; Johnston et al. (2000)
;
; <G1001> O2 + O3P = O3 : {%StTrG} 6.E-34*((temp/300.)**(-2.4))*cair; {&1555}
  G1001  I18O2 = *1.1775
  G1001  I17O2 = *1.1575
...
; isotope exchange
;
  IOE07  I17O2  = *0.9611
  IOE07  I18O2  = *0.9235

; === isotope exchange reactions section ====================================
[IEX]
; syntax: REAC = exchanging species : {%Spec} rate ; (syntax after ":" follows MECCA)
;
; --- Lyons (2001) and references therein
;
; QH + H2O <-> OH + H2Q    () -> Greenblatt and Howard (1989)
  IOE01 = OH H2O : {%StTrG} 1.6E-13*EXP(-2100./temp);
...
; --- Johnston et al. (2000)
; Q + OO --> O + OQ        (R10a-d)
  IOE07 = O3P O2 : {%StTrG} 2.9E-12;
;
```