Supplement of Geosci. Model Dev., 14, 1171–1193, 2021
https://doi.org/10.5194/gmd-14-1171-2021-supplement

Geoscientific Model Development
Open Access
EGU

Supplement of

Development of an atmospheric chemistry model coupled to the PALM model system 6.0: implementation and first applications

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This document is the supplement of the research article and comprises the additional data and information. The supplement contains emission factors (S1) used in the simulations as well as description of 8 preprocessed chemical mechanisms (S2-S9), that are shipped with PALM model system 6.0 source code. The terms and abbreviations used in this document are described below:

par_emis_time_factor: A Fortran array of the emission factors.
ph_t : Photolysis frequency of the photochemical compound.
arr2 : Rate law function that defines the rate of the chemical reaction. The rate law function also includes temperature.
temp : Temperature, Kpp4palm utilizes temperature field from the PALM model.

S1: Temporal profile of hourly emission factors:

```
par_emis_time_factor( : ) =  (/0.005, 0.002, 0.002, 0.004, 0.020,  0.050, &
                               0.060, 0.058, 0.052, 0.050, 0.050,  0.052, &
                               0.055, 0.060, 0.065, 0.070, 0.075,  0.075, &
                               0.060, 0.045, 0.035, 0.025, 0.020,  0.010 /)
```

Hourly emission factors for the entire diurnal course have been used in the "PARAMETERIZED" mode for the case study in Berlin and represents emissions factors for traffic sources only.

S2: PASSIVE1

```
{passive1.eqn
Current revisions
----------------
 $Id:
}
#EQUATIONS

{ passive1: no chemical reactions }
  { 1.}  PM10 = PM10 :                  1.0  ;
```

- A simple passive mechanism comprised of only one passive scalar of particulate diameter 10 μm.

S3: PASSIVE

```
{passive.eqn
Former revisions
----------------
 $Id:
}
#EQUATIONS

{ passive: no chemical reactions }
  { 1.}  PM10 = PM10 :                  1.0   ;
  { 2.}  PM25 = PM25 :                  1.0   ;
```

- A simple passive mechanism comprised of 2 passive scalars with particulate diameter 10 μm and 2.5 μm.

S4: PHSTAT

```
{phstat.eqn
Current revision
----------------
 $Id:
}
#EQUATIONS

  { 1.}  NO2 + hv = NO + O3: phot(j_no2)           ;
  { 2.}  NO  + O3 = NO2: arr2(1.8E-12,1370.0, temp);
```

- A steady state photostationary mechanism comprised of 3 species and 2 reactions.

S5: PHSTATP

```
{phstat.eqn
Current revision
----------------
 $Id:
}
#EQUATIONS

  { 1.}  NO2 + hv = NO + O3: phot(j_no2)           ;
  { 2.}  NO  + O3 = NO2: arr2(1.8E-12,1370.0, temp);
  { 3.}  PM10 = PM10:   1.0                        ;
```

- Same as PHSTAT mechanism but with additional passive PM10 tracer.

S6: SMOG

```
{smog.eqn
Current revisions
----------------
 $Id:
}
#EQUATIONS

{ Photochemical SMOG with photolysis}

  { 1.}  NO2 + hv = NO + O            :  phot(j_no2)                  ;
  { 2.}  O + O2 = O3                  :  arr2(3.2e-11 ,  -70.0 , temp) ;
  { 3.}  NO + O3 = NO2 + O2           :  arr2(1.8E-12 , 1370.0 , temp) ;
  { 4.}  RH + OH = RO2 + H2O          :  arr2(2.E-11  ,  500.0 , temp) ;
  { 5.}  RCHO + OH = RCOO2 + H2O      :  arr2(7.0E-12 , -250.0 , temp) ;
  { 6.}  RCHO + hv = RO2 + HO2 + CO   :  phot(j_rcho)                  ;
  { 7.}  HO2 + NO = NO2 + OH          :  arr2(3.7E-12 , -240.0 , temp) ;
  { 8.}  RO2 + NO = NO2 + RCHO + HO2  :  arr2(4.2E-12 , -180.0 , temp) ;
  { 9.}  RCOO2 + NO = NO2 + RO2 + CO2 :  arr2(5.4E-12 , -250.0 , temp) ;
  {10.}  OH + NO2 = HNO3              :  arr2(1.0E-12 , -713.0 , temp) ;
  {11.}  RCOO2 + NO2 = RCOO2NO2       :  arr2(1.2e-11 ,    0.0 , temp) ;
  {12.}  RCOO2NO2 = RCOO2 + NO2       :  arr2(9.4E+16 ,14000.0 , temp) ;
```

- A relatively simple chemistry mechanism comprised of 13 species and 12 reactions of NO_x-O_3-VOC chemistry.

S7: SIMPLE

```
{simple.eqn
Current revision
----------------
$Id:
}
#EQUATIONS

  { 1.}  NO2 + hv = NO + O3      :       phot(j_no2)                    ;
  { 2.}  O3 + H2O = 2OH          :       2.0 * 2.2E-10 * phot(j_o31d) /
                                        (arr2(1.9E+8   , -390.0 , temp));
  { 3.}  NO + O3 = NO2           :       arr2(1.8E-12  , 1370.0 , temp) ;
  { 4.}  RH + OH = RO2 + H2O     :       arr2(2.E-11   ,  500.0 , temp) ;
  { 5.}  RO2 + NO = NO2 + RCHO + HO2 :   arr2(4.2E-12  , -180.0 , temp) ;
  { 6.}  HO2 + NO = NO2 + OH     :       arr2(3.7E-12  , -240.0 , temp) ;
  { 7.}  NO2 + OH = HNO3         :       arr2(1.15E-11 ,    0.0 , temp) ;
```

- A more simplified version of SMOG mechanism comprised of 9 species and 7 reactions of NO_x-O_3-VOC chemistry.

S8: SIMPLEP

```
{simplep.eqn
Current revision
----------------
$Id:
}
#EQUATIONS

  { 1.}  NO2 + hv = NO + O3          :   phot(j_no2)                    ;
  { 2.}  O3 + H2O = 2OH              :   2.0  * 2.2E-10  * phot(j_o31d) /
                                        (arr2(1.9E+8 , -390.0 , temp))  ;
  { 3.}  NO + O3 = NO2               :   arr2(1.8E-12  , 1370.0 , temp) ;
  { 4.}  RH + OH = RO2 + H2O         :   arr2(2.E-11   ,  500.0 , temp) ;
  { 5.}  RO2 + NO = NO2 + RCHO + HO2 :   arr2(4.2E-12  , -180.0 , temp) ;
  { 6.}  HO2 + NO = NO2 + OH         :   arr2(3.7E-12  , -240.0 , temp) ;
  { 7.}  NO2 + OH = HNO3             :   arr2(1.15E-11 ,    0.0 , temp) ;
  { 8.}  PM10 = PM10                 :   1.0                            ;
```

- Same as SIMPLE mechanism but with the addition of PM10. SIMPLEP mechanism is comprised of 10 species and 8 reactions. Reaction 1-7 comprised of NO_x-O_3-VOC chemistry.

S9: CBM4

```
{cbm4.eqn
Current revision
----------------
$Id:
}
#EQUATIONS {CBM4}

{01:J01} NO2+hv=NO+O                          :  phot(j_no2)          ;
{02:J02} O3+hv=O                              :  phot(j_o33p)         ;
{03:J03} O3+hv=O1D_CB4                        :  phot(j_o31d)         ;
{04:J04} NO3+hv=0.89 NO2+0.89 O+0.11 NO       :  phot(j_no3o)+phot(j_no3o2);
{05:J05} HONO+hv=HO+NO                        :  phot(j_hono)         ;
{06:J06} H2O2+hv=2 HO                         :  phot(j_h2o2)         ;
{07:J07} HCHO+hv{+2 O2}= 2 HO2+CO             :  phot(j_ch2or)        ;
{08:J08} HCHO+hv=CO                           :  phot(j_ch2om)        ;
{09:J09} ALD2+hv{+ 2 O2}=HCHO+XO2+CO+ 2 HO2:  4.6E-4 *phot(j_no2) ;
{10:J10} OPEN+hv=C2O3+CO+HO2                  :  9.04 *phot(j_ch2or) ;
{11:J11} MGLY+hv=C2O3+CO+HO2                  :  9.64 *phot(j_ch2or) ;
{12:01} O{+O2+M}=O3                           :  arr2(1.4E+3 , -1175.0 , temp) ;
{13:02} O3+NO=NO2              :  arr2(1.8E-12 , +1370.0 , temp)   ;
{14:03} O+NO2=NO               :  9.3E-12  ;
{15:04} O+NO2=NO3              :  arr2(1.6E-13 , -687.0 , temp)    ;
{16:05} O+NO=NO2               :  arr2(2.2E-13 , -602.0 , temp)    ;
{17:06} O3+NO2=NO3             :  arr2(1.2E-13 , +2450.0 , temp)   ;
{18:07} O1D_CB4=O              :  arr2(1.9E+8 , -390.0 , temp)     ;
{19:08} O1D_CB4+H2O=2HO        :  2.2E-10  ;
{20:09} O3+HO=HO2              :  arr2(1.6E-12 , +940.0 , temp)    ;
{21:10} O3+HO2=HO              :  arr2(1.4E-14 , +580.0 , temp)    ;
{22:11} NO3+NO=2 NO2           :  arr2(1.3E-11 , -250.0 , temp)    ;
{23:12} NO3+NO2=NO+NO2         :  arr2(2.5E-14 , +1230.0 , temp)   ;
{24:13} NO3+NO2=N2O5           :  arr2(5.3E-13 , -256.0 , temp)    ;
{25:14} N2O5+H2O=2 HNO3        :  1.3E-21  ;
{26:15} N2O5=NO3+NO2           :  arr2(3.5E+14 , +10897.0 , temp)  ;
{27:16} 2 NO=2 NO2             :  arr2(1.8E-20 , -530.0 , temp)    ;
{28:17} NO+NO2+H2O=2 HONO      :  4.4E-40  ;
{29:18} HO+NO=HONO             :  arr2(4.5E-13 , -806.0 , temp)    ;
{30:19} HO+HONO=NO2            :  6.6E-12  ;
{31:20} 2 HONO=NO+NO2          :  1.0E-20  ;
{32:21} HO+NO2=HNO3            :  arr2(1.0E-12 , -713.0 , temp)    ;
{33:22} HO+HNO3=NO3            :  arr2(5.1E-15 , -1000.0 , temp)   ;
{34:23} HO2+NO=HO+NO2          :  arr2(3.7E-12 , -240.0 , temp)    ;
{35:24} HO2+NO2=PNA            :  arr2(1.2E-13 , -749.0 , temp)    ;
{36:25} PNA=HO2+NO2            :  arr2(4.8E+13 , +10121.0 , temp)  ;
{37:26} HO+PNA=NO2             :  arr2(1.3E-12 , -380.0 , temp)    ;
{38:27} 2 HO2=H2O2             :  arr2(5.9E-14 , -1150.0 , temp)   ;
{39:28} 2 HO2+H2O=H2O2         :  arr2(2.2E-38 , -5800.0 , temp)   ;
{40:29} HO+H2O2=HO2            :  arr2(3.1E-12 , +187.0 , temp)    ;
{40:29} HO+H2O2=HO2            :  arr2(3.1E-12 , +187.0 , temp)    ;
{41:30} HO+CO=HO2              :  2.2E-13  ;
{42:31} HCHO+HO=HO2+CO         :  1.0E-11  ;
{43:32} HCHO+O=HO+HO2+CO       :  arr2(3.0E-11 , +1550.0 , temp)   ;
{44:33} HCHO+NO3=HNO3+HO2+CO   :  6.3E-16  ;
{45:34} ALD2+O=C2O3+HO         :  arr2(1.2E-11 , +986.0 , temp) ;
```

```
{46:35} ALD2+HO=C2O3          :  arr2(7.0E-12 , -250.0 , temp) ;
{47:36} ALD2+NO3=C2O3+HNO3    :  2.5E-15  ;
{48:37} C2O3+NO=HCHO+XO2+HO2+NO2   :  arr2(5.4E-12 , -250.0   , temp) ;
{49:38} C2O3+NO2=PAN               :  arr2(8.0E-20 , -5500.0  , temp) ;
{50:39} PAN=C2O3+NO2               :  arr2(9.4E+16 , +14000.0 , temp) ;
{51:40} 2 C2O3=2 HCHO+2 XO2+2 HO2  :  2.0E-12  ;
{52:41} C2O3+HO2=0.79 HCHO+0.79 XO2
                 +0.79 HO2+0.79 HO  :  6.5E-12  ;
{53:42} HO=HCHO+XO2+HO2            :  arr2(1.1E+2 , +1710.0 , temp)   ;
{54:43} PAR+HO=0.87 XO2+0.13 XO2N
              +0.11 HO2+0.11 ALD2
              +0.76 ROR-0.11 PAR   :  8.1E-13  ;
{55:44} ROR=1.1 ALD2+0.96 XO2
           +0.94 HO2 +0.04 XO2N
           +0.02 ROR-2.10 PAR      :  arr2(1.0E+15 , +8000.0 , temp)  ;
{56:45} ROR=HO2                    :  1.6E+03  ;
{57:46} ROR+NO2= PROD              :  1.5E-11  ;
{58:47} O+OLE=0.63 ALD2+0.38 HO2
             +0.28 XO2+0.3 CO
             +0.2 HCHO+0.02 XO2N
             +0.22 PAR+0.2 HO        :  arr2(1.2E-11 , +324.0 , temp) ;
{59:48} HO+OLE=HCHO+ALD2+XO2+HO2-PAR :  arr2(5.2E-12 , -504.0 , temp) ;
{60:49} O3+OLE=0.5 ALD2+0.74 HCHO
              +0.33 CO+0.44 HO2
              +0.22 XO2+0.1 HO-PAR   :  arr2(1.4E-14 , +2105.0 , temp);
{61:50} NO3+OLE=0.91 XO2+HCHO
               +ALD2+0.09 XO2N
               +NO2-PAR              :  7.7E-15  ;
{62:51} O+ETH=HCHO+0.7 XO2
             +CO+1.7 HO2+0.3 HO      :  arr2(1.0E-11 , +792.0 , temp) ;
{63:52} HO+ETH=XO2+1.56 HCHO
              +HO2+0.22 ALD2         :  arr2(2.0E-12 , -411.0 , temp) ;
{64:53} O3+ETH=HCHO+0.42 CO+0.12 HO2 :  arr2(1.3E-14 , +2633.0 , temp);
{65:54} HO+TOL=0.08 XO2+0.36 CRES
              +0.44 HO2+0.56 TO2     :  arr2(2.1E-12 , -322.0 , temp) ;
{66:55} TO2+NO=0.9 NO2+0.9 OPEN+0.9 HO2  :  8.1E-12  ;
{67:56} TO2=HO2+CRES                     :  4.20  ;
{68:57} HO+CRES=0.4 CRO+0.6 XO2
               +0.6 HO2+0.3 OPEN         :  4.1E-11  ;
{69:58} NO3+CRES=CRO+HNO3                :  2.2E-11  ;
{70:59} CRO+NO2=PROD                     :  1.4E-11  ;
{71:60} HO+XYL=0.7 HO2+0.5 XO2
              +0.2 CRES+0.8 MGLY
              +1.10 PAR+0.3 TO2          :  arr2(1.7E-11 , -116.0 , temp) ;
{72:61} HO+OPEN=XO2+C2O3+2 HO2+2 CO+HCHO :  3.0E-11  ;
{73:62} O3+OPEN=0.03 ALD2+0.62 C2O3
               +0.7 HCHO+0.03 XO2
               +0.69 CO+0.08 HO
               +0.76 HO2+0.2 MGLY     :  arr2(5.4E-17 , +500.0 , temp)    ;
{74:63} HO+MGLY=XO2+C2O3               :  1.70E-11    ;
{75:64} O+ISOP=0.6 HO2+0.8 ALD2
              +0.55 OLE+0.5 XO2
              +0.5 CO+0.45 ETH
              +0.9 PAR                 :  1.80E-11    ;
```

```
{76:65} HO+ISOP=HCHO+XO2
               +0.67 HO2+0.4 MGLY
               +0.2 C2O3+ETH
               +0.2 ALD2+0.13 XO2N    :  9.6E-11  ;
{77:66} O3+ISOP=HCHO+0.4 ALD2
               +0.55 ETH+0.2 MGLY
               +0.06 CO+0.1 PAR
               +0.44 HO2+0.1 HO       :  1.2E-17  ;
{78:67} NO3+ISOP=XO2N                 :  3.2E-13  ;
{79:68} XO2+NO=NO2                    :  8.1E-12  ;
{80:69} 2 XO2=PROD                    :  arr2(1.7E-14 , -1300.0 , temp) ;
{81:70} XO2N+NO=PROD                  :  6.8E-13  ;
```

- A sufficiently detailed chemistry mechanism comprised of 32 chemical compounds and 81 reactions of NO_x-O_3-VOC chemistry.

--- Supplement ends here ---