Supplement of :

Development of an atmospheric chemistry model coupled to the PALM model systems 6.0: Implementation and first applications

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This document is the supplement of the paper and comprised of the additional data and information. 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 um.

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 um and 2.5 um.

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 a 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 ---