



Chemical mechanisms and KPP

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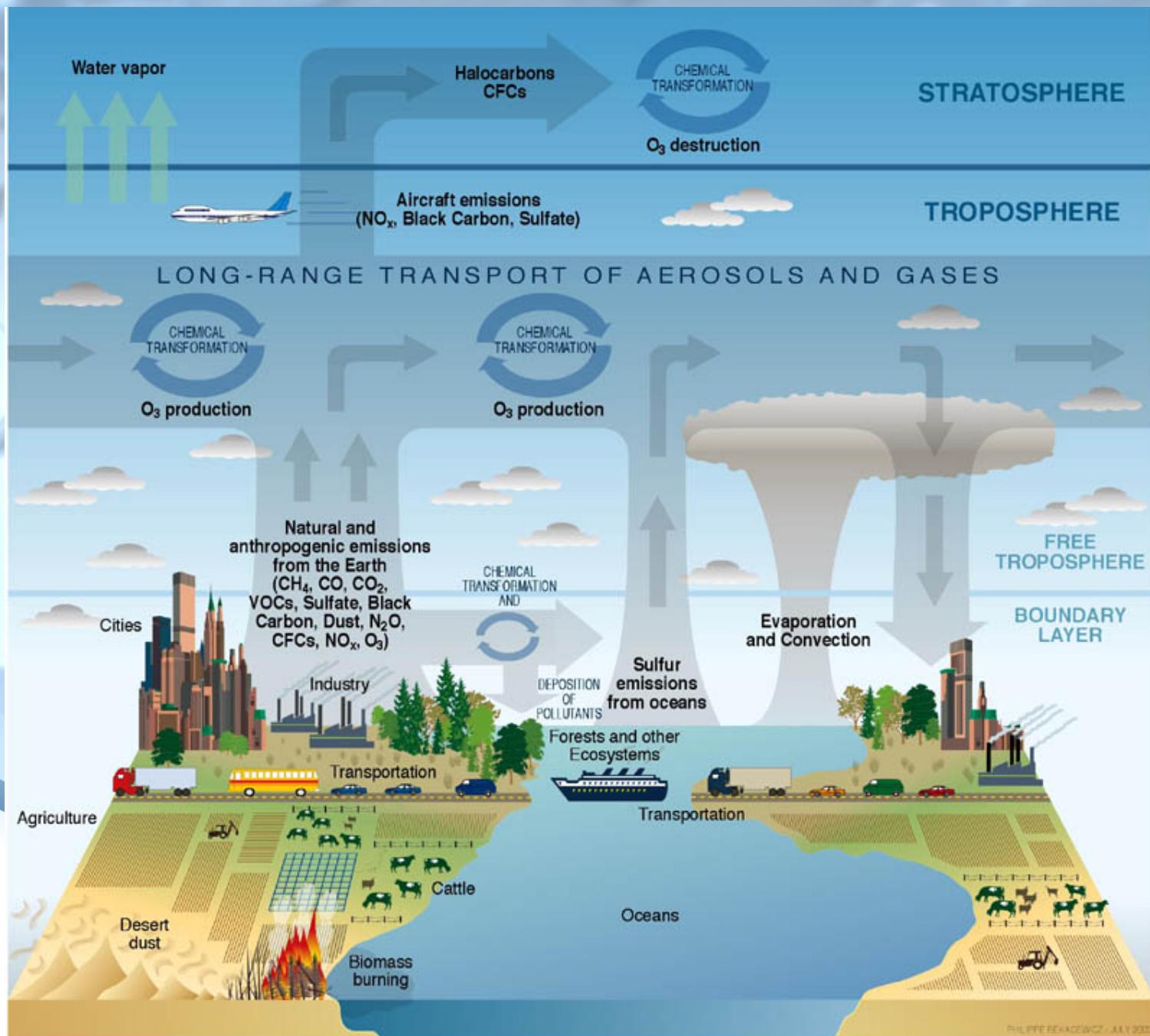
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Outline

- Chemical mechanisms in the WRF-Chem V3.5 model
- Kinetic PreProcessor (KPP) and WRF-Chem KPP Coupler (WKC)
- Adding chemical mechanisms to the WRF-Chem model using
KPP
- Additional notes



Main gas phase chemistry mechanisms in WRF-Chem3.5

- ❑ Regional Acid Deposition Model, 2nd generation (**RADM2**)
- ❑ Regional Atmospheric Chemistry Mechanism (**RACM**)
- ❑ RACM - Mainz Isoprene Mechanism (**RACM-MIM**)
- ❑ RACM - Earth System Research Laboratory (**RACM-ESRL**), *updated RACM-MIM*
- ❑ Carbon Bond Mechanism (**CB4**)
- ❑ Carbon-Bond Mechanism version Z (**CBMZ**)
- ❑ Model of Ozone and Related Chemical Tracers (**MOZART**)
- ❑ Nonmethane Hydrocarbons Chemistry (**NMHC9**)
- ❑ Statewide Air Pollution Research Center (**SAPRC99**)

different implementations, coupled to different aerosol schemes and aqueous chemistry, suitable for different applications ranging from regional air quality to global atmospheric chemistry simulations (no halogen chemistry yet!)

Some references

- Stockwell, W. R., et al. (1997), A new mechanism for regional atmospheric chemistry modeling, *J. Geophys. Res.-Atmos.*, 102(D22), 25847-25879.
- Stockwell, W. R., et al. (1990), The 2nd generation regional acid deposition model chemical mechanism for regional air-quality modeling, *J. Geophys. Res.-Atmos.*, 95(D10), 16343-16367.
- Horowitz, L. W., et al. (2003), A global simulation of tropospheric ozone and related tracers: Description and evaluation of MOZART, version 2, *J. Geophys. Res.*, 108(D24), 4784, doi:10.1029/2002JD002853.
- Gross, A., and W. R. Stockwell (2003), Comparison of the EMEP, RADM2 and RACM mechanisms, *Journal of Atmospheric Chemistry*, 44(2), 151-170.
- Geiger, H., et al. (2003), The tropospheric degradation of isoprene: an updated module for the regional atmospheric chemistry mechanism, *Atmos. Environ.*, 37(11), 1503-1519.
- Luecken, D. J., et al. (2008), Effects of using the CB05 vs. SAPRC99 vs. CB4 chemical mechanism on model predictions: Ozone and gas-phase photochemical precursor concentrations, *Atmos. Environ.*, 42(23), 5805-5820.
- Cai et al. (2011), Photochemical Modeling in California with Two Chemical Mechanisms: Model Intercomparison and Response to Emission Reductions, *J. Air & Waste Manage. Assoc.*
- Peckham S. et al. (2011), WRF-CHEM 3.3 User's Guide.

Chemistry mechanisms in WRF-Chem3.5

<i>Chemical mechanisms</i>	<i>Fixed versions</i>	<i>KPP</i>	<i>Coupled to the aerosol schemes</i>
RADM2	Yes	Yes	MADE/SORGAM, GOCART
RACM	None	Yes	MADE/SORGAM, GOCART
RACM-MIM	None	Yes	None
RACM-ESRL	None	Yes	MADE/SORGAM, MADE/ SOA_VBS
CB4	None	Yes	None
CBMZ	Yes	Yes	MOSAIC
MOZART	None	Yes	GOCART
SAPRC99	None	Yes	MOSAIC
NMHC9	None	Yes	None

Chemistry options in WRF-Chem3.5

chem_opt =0 no chemistry

= 1 RADM2 chemical mechanism - no aerosols

= 2 RADM2 chemical mechanism and MADE/SORGAM aerosols

No indirect effect To have radiative feed back with the chemistry/aerosols use `ra_sw_physics = 2` (Goddard shortwave scheme). For dust and sea salt use `dust_opt=2, seas_opt=2`

= 5 CBMZ chemical mechanism with Dimethylsulfide

= 6 CBMZ chemical mechanism without DMS

= 7 CBMZ chemical mechanism (`chem_opt=6`) and MOSAIC using 4 sectional aerosol bins

No indirect effect To have radiative feed back with the chemistry/aerosols use , `ra_sw_physics = 2`, for dust and seasalt use `dust_opt=2, seas_opt=2`

= 8 CBMZ chemical mechanism (`chem_opt=6`) and MOSAIC using 8 sectional aerosol bins.

No indirect effect To have radiative feed back with the chemistry/aerosols use, `ra_sw_physics = 2`, for dust and seasalt use `dust_opt=2, seas_opt=2`.

= 9 CBMZ chemical mechanism (`chem_opt=6`) and MOSAIC using 4 sectional aerosol bins) including some aqueous reactions

For direct and indirect effect use: `phot_opt=2; ra_sw_physics=2; progn=1; mp_physics=2; aer_ra_feedback=1; wetscav_onoff=1; cldchem_onoff=1`,

For dust and sea salt use `dust_opt=2, seas_opt=2`

= 10 CBMZ chemical mechanism (`chem_opt=6`) and MOSAIC using 8 sectional aerosol bins) including some aqueous reactions

For direct and indirect effect use: `phot_opt=2; ra_sw_physics=2; progn=1; mp_physics=2; aer_ra_feedback=1; wetscav_onoff=1; cldchem_onoff=1`

For dust and seasalt use `dust_opt=2, seas_opt=2`.

= 11 RADM2 chemical mechanism and MADE/SORGAM aerosols including some aqueous reactions

For direct and indirect effect use: `phot_opt=2; ra_sw_physics=2; progn=1; mp_physics=2; aer_ra_feedback=1; wetscav_onoff=1; cldchem_onoff=1`

For dust and seasalt use `dust_opt=2, seas_opt=2`.

KPP in WRF-Chem

Kinetic PreProcessor (KPP) reads chemical reactions and rate constants from ASCII input files and automatically generates code for chemistry integration using the Rosenbrok solver

No KPP for aerosols!

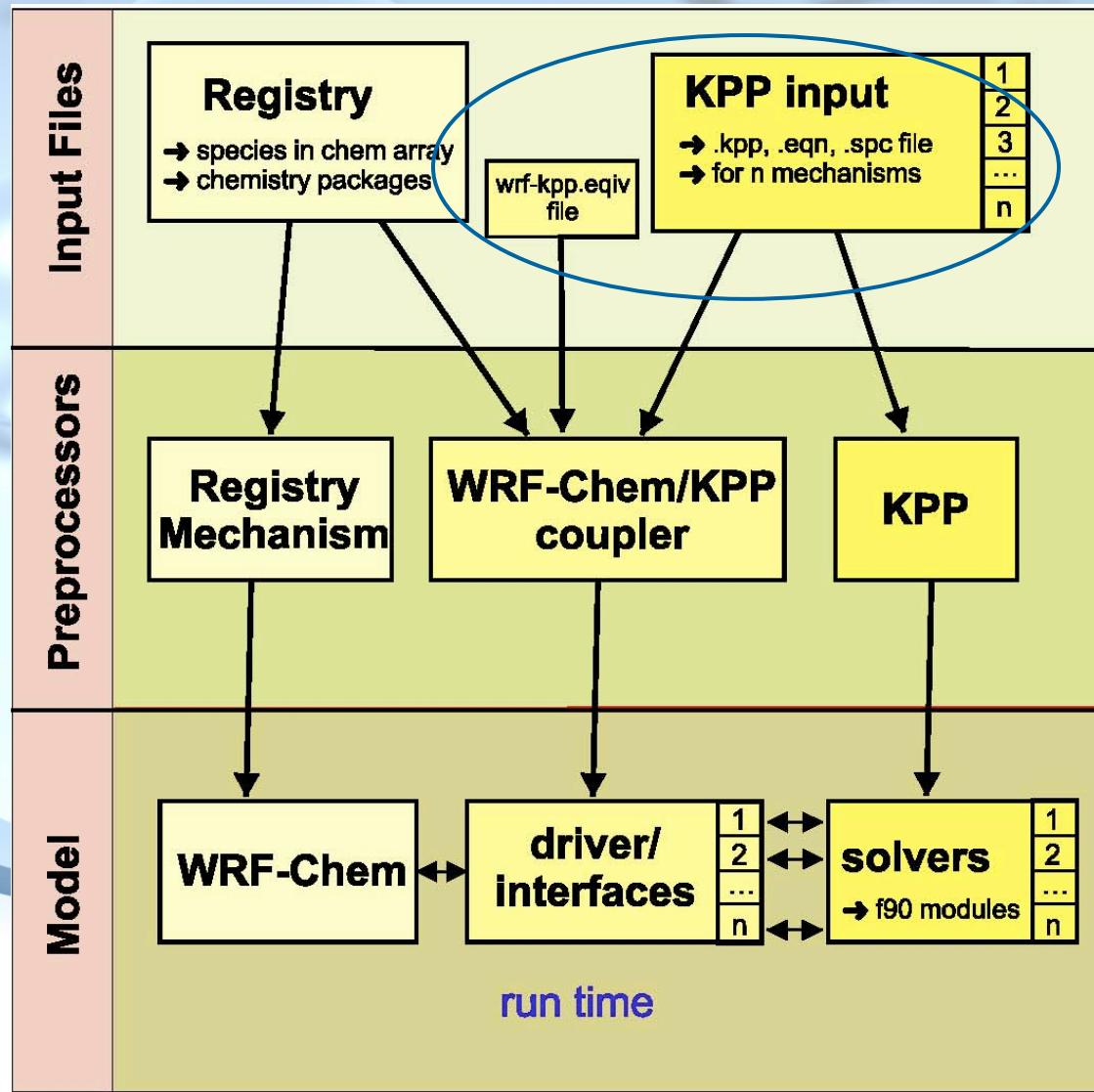
Advantages:

- less time consuming than manual coding**
- less error prone**
- numerically efficient**
- flexibility in updating mechanism with additional species and equations**
- suitable for adjoint code development**

References:

- Damian, V., et al. (2002), The kinetic preprocessor KPP - a software environment for solving chemical kinetics, *Comput. Chem. Eng.*, 26(11), 1567-1579.
- Sandu, A., and R. Sander (2006), Technical note: Simulating chemical systems in Fortran90 and Matlab with the Kinetic PreProcessor KPP-2.1, *Atmos. Chem. Phys.*, 6, 187-195.
- Verwer, J., Spee, E., Blom, J. G., and Hunsdorfer, W. (1999), A second order Rosenbrock method applied to photochemical dispersion problems, *SIAM Journal on Scientific Computing*, 20, 1456–1480.
- www.mpch-mainz.mpg.de/~salzmann/my_home/sub/wkc.html

WKC (WRF-Chem/KPP Coupler) (\$WRF-CHEM/chem/KPP/util/wkc/)



WRF-CHEM3.3 User's guide, 2012

racm_soa_vbs_wrfkpp.equiv file:

```
! use this file for species that have different
! names in WRF and KPP
!
! Currently case sensitive
!
! left column      right column
! name in WRF      name in KPP
rpho              pho
```

Input files of KPP

*.spc file

Definition of chemical species as variable or fixed value.

*.eqn file

Writing chemical reactions in kpp format

*.kpp file

Model description, computer language, precision, integrator (e.g. Rosenbrock solver)

etc.

*.def file

User defined functions

(also check \$WRF-CHEM/chem/KPP/kpp/kpp-2.1/util/ WRF_conform/ UserRateLaws.f90)

Pre-defined variables in WKC

	KPP equation file	Equation file units	Registry
Photolysis rate	J(Pj_no2)	s ⁻¹	ph_no2
Temperature	TEMP	K	t_phy
Third body concentration	C_M	(molecular moist air) cm ⁻³	Calculated from density
Water vapor concentration	C_H2O	Molecules cm ⁻³	Calculated from qvapor

WRF-CHEM3.4 User's guide, 2012

How to add a new KPP chemistry mechanism to WRF-Chem?

- 1) Add a new mechanism to \$WRF-CHEM/Registry/registry.chem
- 2) Add new variables to the registry if necessary (new species, namelist options etc.)
- 3) Create subdirectories in \$WRF-CHEM/chem/KPP/ “mechanisms” and “inc”
- 4) Create new KPP files with new reactions, rates and species
- 5) Modify some \$WRF-CHEM/chem/*.F (e.g. chem_driver.F) programs in order to include a new chemical mechanism
- 6) Modify \$WRF-CHEM/chem/convert_emiss.F for new species
- 7) Compile a new WRF-CHEM code and run using updated emission files

KPP requires some UNIX tools - flex, yacc, and sed to be installed on your system before compiling the code !

setenv FLEX_LIB_DIR = /usr/local/lib

setenv WRF_KPP =1

Example: Adding a new chemistry mechanism to WRF-Chem for the state of the art SOA parameterization

In order to implement the new SOA mechanism (chem_opt=108 in V3.5) we need to modify the RACM_ESRLSORG gas chemistry:

- Separate MBO from internal alkenes - OLI species
- Add SESQ (biogenic VOC) reactions

Adding the new chemistry package and species to \$WRF-CHEM/Registry/registry.chem

```
state real sesq ikjftb chem 1 - irhusdf=(bdy_interp:dt) "sesq" "SESQ concentration" "ppmv"  
state real mbo ikjftb chem 1 - irhusdf=(bdy_interp:dt) "mbo" "MBO concentration" "ppmv"
```

The new package RACM_SOA_VBS_KPP chem_opt==108

Chem array:

G a s e s :
so2,sulf,no2,no,o3,hno3,h2o2,ald,hcho,op1,op2,paa,ora1,ora2,n2o5,no3,pan,hc3,hc5,hc8,eth,co,ete,
olt,oli,tol,xyl,aco3,tpan,hono,hno4,ket,gly,mgly,dcb,onit,csl,iso,co2,ch4,udd,hket,api,lim,dien,macr,hac
e, ishp,ison,mahp,mpan,nald, **sesq,mbo**, cvasoa1,cvasoa2,cvasoa3,cvasoa4,
cvbsoa1,cvbsoa2,cvbsoa3, cvbsoa4,ho,ho2,

Aerosols:

so4aj,so4ai,nh4aj,nh4ai,no3aj,no3ai, asoa1j,aso1i,aso2j,aso2i,aso3j,aso3i,aso4j,aso4i,
bsoa1j,bsoa1i,bsoa2j,bsoa2i,bsoa3j,bsoa3i,bsoa4j,bsoa4i,
orgpaj,orgpai,ecj,eci,p25j,p25i,antha,seas,soila,nu0,ac0,corn

All species within “chem” array are advected and mixed by WRF-CHEM!

Some species are part of the “misc” array (not advected)

\$WRF-CHEM/Registry/registry.chem:

non-transported radical species for the RACM mechanism

state	real addt	ikj	misc	1	-	r	"addt"	"Radicals" "ppm"
state	real addx	ikj	misc	1	-	r	"adx"	"Radicals" "ppm"
state	real addc	ikj	misc	1	-	r	"adc"	"Radicals" "ppm"
state	real etep	ikj	misc	1	-	r	"etep"	"Radicals" "ppm"
state	real oltp	ikj	misc	1	-	r	"oltp"	"Radicals" "ppm"
state	real olip	ikj	misc	1	-	r	"olip"	"Radicals" "ppm"
state	real cslp	ikj	misc	1	-	r	"cslp"	"Radicals" "ppm"
state	real limp	ikj	misc	1	-	r	"limp"	"Radicals" "ppm"
state	real hc5p	ikj	misc	1	-	r	"hc5p"	"Radicals" "ppm"
state	real hc8p	ikj	misc	1	-	r	"hc8p"	"Radicals" "ppm"
state	real tolp	ikj	misc	1	-	r	"tolp"	"Radicals" "ppm"
state	real xylp	ikj	misc	1	-	r	"xylp"	"Radicals" "ppm"
state	real apip	ikj	misc	1	-	r	"apip"	"Radicals" "ppm"
state	real isop	ikj	misc	1	-	r	"isop"	"Radicals" "ppm"
state	real hc3p	ikj	misc	1	-	r	"hc3p"	"Radicals" "ppm"

Make a new subdirectory in **\$WRFV-CHEM/chem/KPP/mechanisms/**

The name of this directory should be the same as the package name in the Registry without the “_kpp” suffix.

\$WRF-CHEM/chem/KPP/mechanisms/racm_soa_vbs

Copy these files from chem/KPP/mechanisms/racm_esrlsorg to the new subdirectory and rename them except “atoms_red”:

atoms_red

racm_soa_vbs.def

racm_soa_vbs.eqn

racm_soa_vbs.kpp

racm_soa_vbs.spc

racm_soa_vbs_wrfkpp.equiv

racm_soa_vbs.def file

If necessary update equation sets and rate constants etc.

```
#include atoms_red
#include ./racm_soa_vbs.spc
#include ./racm_soa_vbs.eqn

#INLINE F90_RATES
REAL(KIND=dp) FUNCTION k46( TEMP, C_M )
    REAL(KIND=dp), INTENT(IN) :: temp, c_m
    REAL(KIND=dp) :: k0, k2, k3

    k0=2.4E-14_dp * EXP(460._dp/TEMP)
    k2=2.7E-17_dp * EXP(2199._dp/TEMP)
    k3=6.5E-34_dp * EXP(1335._dp/TEMP) * c_m

    k46=k0+k3/(1+k3/k2)

END FUNCTION k46
```

racm_soa_vbs.spc file:

```
#DEFVAR  
  
O3 =IGNORE ;  
  
H2O2 =IGNORE ;  
  
.....  
  
SESQ =IGNORE ;  
  
MBO =IGNORE ;
```

racm_soa_vbs.kpp file:

```
#MODEL racm_soa_vbs  
  
#LANGUAGE Fortran90  
  
#DOUBLE ON  
  
#INTEGRATOR WRF_conform/rosenbrock  
  
.....
```

racm_soa_vbs.eqn file:

#EQUATIONS {} ;

photolysis:

{001:J01} NO2+hv=O3P+NO : j(Pj_no2) ;

{002:J02} O3+hv=O1D{+O2} : j(Pj_o31d) ;

{003:J03} O3+hv=O3P{+O2} : j(Pj_o33p)

{004:J04} HONO+hv=HO+NO : j(Pj_hno2) ;

{005:J05} HNO3+hv=HO+NO2 : j(Pj_hno3) ;

chemical reactions:

{024:001} O3P+M{O2}=O3 : (C_M *6.00D-34*(TEMP/300.0)**(-2.4)) ;

{025:002} O3P+O3=M {2O2} : ARR2(8.00D-12 , 2060.0_dp, TEMP) ;

{026:003} O1D + M = O3P : .78084*ARR2(2.15D-11 , -110.0_dp, TEMP) +
.20946*ARR2(3.30D-11 , -55.0_dp , TEMP) ;

{027:004} O1D+H2O=HO+HO : ARR2(1.63D-10 , -60.0_dp, TEMP) ;

{028:005} O3+HO=HO2{+O2} : ARR2(1.70D-12 , 940.0_dp, TEMP) ;

Adding new reactions to racm_soa_vbs.eqn file

- {245:222} SESQ+HO=0.36 KET+0.3 HCHO+0.05 ORA1+0.19 OLIP : 2.52D-10 ;
- {246:223} SESQ+O3=0.51 HCHO+0.85 ALD+0.039 ORA1+0.23 KET+0.053 ORA2
+0.63 HO : 5.60D-16 ;
- {247:224} SESQ+NO3=0.9 OLNN+0.10 OLND+0.9 MACR : 2.20D-11 ;
- {248:225} MBO+HO=OLIP : ARR2(1.33D-11 , -500.0_dp, TEMP) ;
- {249:226} MBO+NO3=0.11 OLNN+0.89 OLND : ARR2(8.64D-13 , -450.0_dp, TEMP) ;
- {250:227} MBO+O3=0.02 HCHO+0.99 ALD+0.16 KET+0.30 CO+0.011 H2O2
+0.14 ORA2+0.07 CH4+0.22 HO2+0.63 HO+0.23 MO2
+0.12 KETP+0.06 ETH+0.18 ETPH :ARR2(4.40D-15 , 845.0_dp,
TEMP) ;

Reference:

Papiez, M. R., et al. (2009), The impacts of reactive terpene emissions from plants on air quality in Las Vegas, Nevada, *Atmos. Environ.*, 43(27), 4109-4123

Update some \$WRF-CHEM/chem/ subroutines

In order to call necessary subroutines for the new chemical mechanism, e.g. SO₂->SO₄ conversion

chem_driver.F:

```
.....  
so2so4_select: SELECT CASE(config_flags%chem_opt)  
CASE (RADM2SORG,RADM2SORG_KPP,RACMSORG_KPP, RACM_SOA_VBS_KPP)  
CALL wrf_debug(15,'gocart so2-so4 conversion')  
call so2so4(chem,p_so2,p_sulf,p_h2o2,p_QC,T_PHY,MOIST,      &  
.....
```

Also the following subroutines in chem/

chemics_init.F

module_input_chem_data.F

mechanism_driver.F

cloudchem_driver.F

module_wetscav_driver.F

aerosol_driver.F

dry_dep_driver.F

emissions_driver.F

module_bioemi_megan2.F

module_add emiss_burn.F

module_ftuv_driver.F

optical_driver.F

module_optical_averaging.F

...

Update chem/convert_emiss.F and generate new anthropogenic and biogenic emissions input (wrfchemi_* and wrfbiochemi* files)

```
.....  
#ifdef DM_PARALLEL  
    IF (wrf_dm_on_monitor()) THEN  
        READ(26,'(12E9.2)') dumc1(ids:ide-1,jds:jde-1)  
    ENDIF  
    DM_BCAST_MACRO(dumc1)  
#else  
    READ(26,'(12E9.2)') dumc1(ids:ide-1,jds:jde-1)  
#endif  
    grid%sebio_sesq(ips:ipe ,jps:jpe ) = dumc1(ips:ipe ,jps:jpe )  
ENDIF  
.....
```

After compiling WRF-CHEM with KPP option

\$WRF-CHEM/chem/KPP/mechanisms/racm_soa_vbs:

Makefile -> ../../util/Makefile_kpp	racm_soa_vbs_Main.f90
Makefile_racm_soa_vbs	racm_soa_vbs_Model.f90
atoms_red	racm_soa_vbs_Monitor.f90
racm_soa_vbs.def	racm_soa_vbs_Parameters.f90
racm_soa_vbs.eqn	racm_soa_vbs_Precision.f90
racm_soa_vbs.kpp	racm_soa_vbs_Rates.f90
racm_soa_vbs.spc	racm_soa_vbs_Update_Rconst.f90
racm_soa_vbs_wrfkpp.equiv	racm_soa_vbs_Util.f90
racm_soa_vbs.map	racm_soa_vbs_mex_Fun.f90
racm_soa_vbs_Function.f90	racm_soa_vbs_mex_Jac_SP.f90
racm_soa_vbs_Global.f90	
racm_soa_vbs_Initialize.f90	
racm_soa_vbs_Integrator.f90	
racm_soa_vbs_Jacobian.f90	
racm_soa_vbs_JacobianSP.f90	
racm_soa_vbs_LinearAlgebra.f90	

WKC generated racm_soa_vbs.map file

Variable species

1 = SULF (n) 32 = HKET (r) 63 = LIMP (r)

2 = CO2 (n) 33 = O3P (r) 64 = HC5P (r)

3 = ORA1 (n) 34 = PHO (r) 65 = HC8P (r)

4 = ORA2 (n) 35 = H2O2 (r) 66 = HCHO (r)

5 = CVASOA1 (n) 36 = ADDT (r) 67 = TOLP (r)

6 = CVASOA2 (r) 37 = ADDX (r) 68 = XYLP (r)

7 = CVASOA3 (r) 38 = ETE (r) 69 = OLIP (r)

8 = CVASOA4 (r) 39 = ADDC (r) 70 = ONIT (r)

9 = CVBSOA1 (n) 40 = PAA (r) 71 = DCB (r)

10 = CVBSOA2 (r) 41 = ISON (r) 72 = XO2 (r)

11 = CVBSOA3 (r) 42 = SESQ (r) 73 = OLI (r)

18 = HC5 (r) 49 = MBO (r) 80 = HC3P (r)

Additional notes

- 1) Always run “clean -a” command after you change any of KPP files
- 2) When you add chemical species for a new chem_opt to registry.chem, place the gases between “so2 ... ho2” and if you add aerosols then place them after “so4aj...”
- 3) Only species within “chem” array (not “misc”!) are used to initialize from previous simulation data when chem_in_opt=1
- 4) Check if the added mechanisms work with pre-existing initial and boundary conditions, emissions, photolysis rates, aerosol modules, dry and wet deposition rates: e.g. check module_dep_simple.F
- 5) You can also simulate some species as passive tracers such as chem_opt=13-15 (prescribed emissions only), e.g. CO
- 6) chem_opt=16,17 (with modeled fluxes and prescribed emissions for CO2 and CH4)



QUESTIONS ?

+O (CH₃)

Table 1. RACM Mechanism Species List

No.	Species	Definition	Carbon Number	Molecular Weight
<i>Stable Inorganic Compounds</i>				
<i>Oxidants</i>				
1	O ₃	ozone		48
2	H ₂ O ₂	hydrogen peroxide		34
<i>Nitrogenous compounds</i>				
3	NO	nitric oxide		30
4	NO ₂	nitrogen dioxide		46
5	NO ₃	nitrogen trioxide		62
6	N ₂ O ₅	dinitrogen pentoxide		108
7	HONO	nitrous acid		47
8	HNO ₃	nitric acid		63
9	HNO ₄	pernitric acid		79
<i>Sulfur compounds</i>				
10	SO ₂	sulfur dioxide		64
11	SULF	sulfuric acid		98
<i>Carbon oxides</i>				
12	CO	carbon monoxide	1	28
13	CO ₂	carbon dioxide	1	44
<i>Abundant Stable Species</i>				
14	N ₂	nitrogen		28
15	O ₂	oxygen		32
16	H ₂ O	water		18
17	H ₂	hydrogen		2
<i>Inorganic Short-Lived Intermediates</i>				
18	O ^{3P}	ground state oxygen atom, O(^{3P})		16
19	O ^{1D}	excited state oxygen atom, O(^{1D})		16
<i>Odd hydrogen</i>				
20	HO	hydroxy radical		17
21	HO ₂	hydroperoxy radical		33

STOCKWELL ET AL.: REGIONAL ATMOSPHERIC CHEMISTRY MECHANISM

Table 2b. The RACM Mechanism

Reaction No.	Reaction	A, cm ³ s ⁻¹	E/R, K	k ^a
<i>Inorganic Reactions</i>				
(R24)	O ³ P + O ₂ → O ₃	Table 2f		1.50 × 10 ⁻¹⁴
(R25)	O ³ P + O ₃ → 2 O ₂	8.00 × 10 ⁻¹²	2060	7.96 × 10 ⁻¹⁵
(R26)	O ¹ D + N ₂ → O ³ P + N ₂	1.80 × 10 ⁻¹¹	-110	2.60 × 10 ⁻¹¹
(R27)	O ¹ D + O ₂ → O ³ P + O ₂	3.20 × 10 ⁻¹¹	-70	4.05 × 10 ⁻¹¹
(R28)	O ¹ D + H ₂ O → HO + HO	2.20 × 10 ⁻¹⁰		2.20 × 10 ⁻¹⁰
(R29)	O ₃ + HO → HO ₂ + O ₂	1.60 × 10 ⁻¹²	940	6.83 × 10 ⁻¹⁴
(R30)	O ₃ + HO ₂ → HO + 2 O ₂	1.10 × 10 ⁻¹⁴	500	2.05 × 10 ⁻¹⁵
(R31)	HO + HO ₂ → H ₂ O + O ₂	4.80 × 10 ⁻¹¹	-250	1.11 × 10 ⁻¹⁰
(R32)	H ₂ O ₂ + HO → HO ₂ + H ₂ O	2.90 × 10 ⁻¹²	160	1.70 × 10 ⁻¹²
(R33)	HO ₂ + HO ₂ → H ₂ O ₂ + O ₂	Table 2f		2.92 × 10 ⁻¹²
(R34)	HO ₂ + HO ₂ + H ₂ O → H ₂ O ₂ + O ₂ + H ₂ O	Table 2f		6.58 × 10 ⁻³⁰
(R35)	O ³ P + NO → NO ₂	Table 2d		1.66 × 10 ⁻¹²
(R36)	O ³ P + NO ₂ → NO + O ₂	6.50 × 10 ⁻¹²	-120	9.72 × 10 ⁻¹²
(R37)	O ³ P + NO ₂ → NO ₃	Table 2d		1.58 × 10 ⁻¹²
(R38)	HO + NO → HONO	Table 2d		4.87 × 10 ⁻¹²
(R39)	HO + NO ₂ → HNO ₃	Table 2d		1.15 × 10 ⁻¹¹
(R40)	HO + NO ₃ → NO ₂ + HO ₂	2.20 × 10 ⁻¹¹		2.20 × 10 ⁻¹¹
(R41)	HO ₂ + NO → NO ₂ + HO	3.70 × 10 ⁻¹²	-250	8.56 × 10 ⁻¹²
(R42)	HO ₂ + NO ₂ → HNO ₄	Table 2d		1.39 × 10 ⁻¹²
(R43)	HNO ₄ → HO ₂ + NO ₂	Table 2e		8.62 × 10 ⁻²
(R44)	HO ₂ + NO ₃ → 0.3 HNO ₃ + 0.7 NO ₂ + 0.7 HO + O ₂	3.50 × 10 ⁻¹²		3.50 × 10 ⁻¹²
(R45)	HO + HONO → NO ₂ + H ₂ O	1.80 × 10 ⁻¹¹	390	4.86 × 10 ⁻¹²
(R46)	HO + HNO ₃ → NO ₃ + H ₂ O	Table 2f		1.47 × 10 ⁻¹³
(R47)	HO + HNO ₄ → NO ₂ + O ₂ + H ₂ O	1.30 × 10 ⁻¹²	-380	4.65 × 10 ⁻¹²
(R48)	O ₃ + NO → NO ₂ + O ₂	2.00 × 10 ⁻¹²	1400	1.82 × 10 ⁻¹⁴
(R49)	O ₃ + NO ₂ → NO ₃ + O ₂	1.20 × 10 ⁻¹³	2450	3.23 × 10 ⁻¹⁷
(R50)	NO + NO + O ₂ → NO ₂ + NO ₂	3.30 × 10 ⁻³⁹	-530	1.95 × 10 ⁻³⁸
(R51)	NO ₃ + NO → NO ₂ + NO ₂	1.50 × 10 ⁻¹¹	-170	2.65 × 10 ⁻¹¹
(R52)	NO ₃ + NO ₂ → NO + NO ₂ + O ₂	4.50 × 10 ⁻¹⁴	1260	6.56 × 10 ⁻¹⁶
(R53)	NO ₃ + NO ₂ → N ₂ O ₅	Table 2d		1.27 × 10 ⁻¹²
(R54)	N ₂ O ₅ → NO ₂ + NO ₃	Table 2e		4.36 × 10 ⁻²
(R55)	NO ₃ + NO ₃ → NO ₂ + NO ₂ + O ₂	8.50 × 10 ⁻¹³	2450	2.29 × 10 ⁻¹⁶
(R56)	HO + H ₂ → H ₂ O + HO ₂	5.50 × 10 ⁻¹²	2000	6.69 × 10 ⁻¹⁵
(R57)	HO + SO ₂ → SULF + HO ₂	Table 2d		8.89 × 10 ⁻¹³
(R58)	CO + HO → HO ₂ + CO ₂	Table 2f		2.40 × 10 ⁻¹³