Automatic coding of chemistry solvers in WRF-Chem using KPP

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Marriage

VRF Chem

KPP

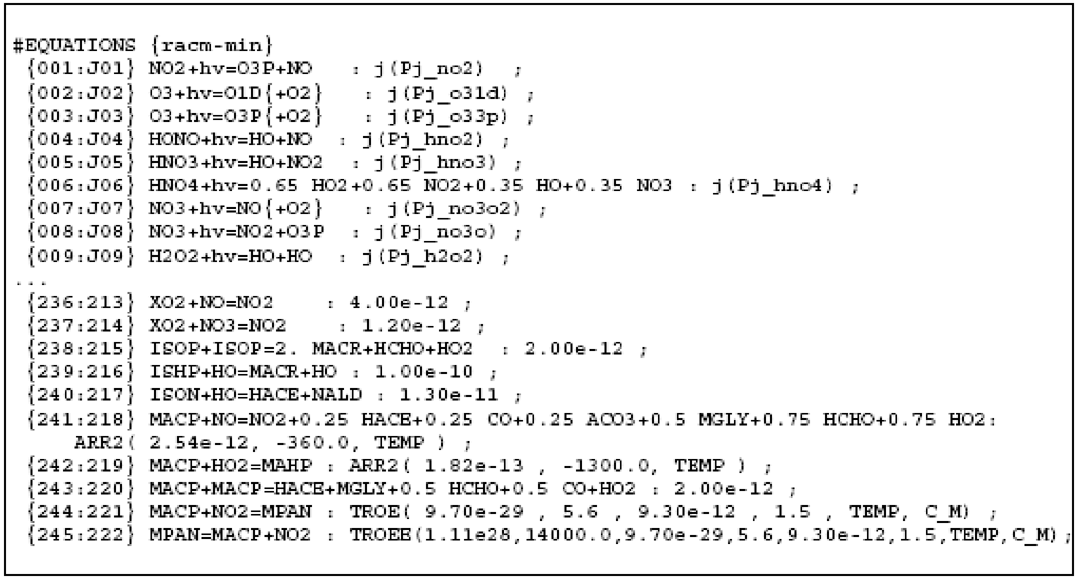
Why KPP?

KPP: Kinetic PreProcessor (Damian et al, 2002, Sandu et al, 2003, Sandu and Sander 2006)

- well documented
- well tested
- widely used

Why KPP?

- KPP reads ASCII files containing chemical equations and automatically generates Fortran 90 code for integrating the corresponding differential equations.



```
#EQUATIONS {racm-min}
 {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) ;
 {006:J06} HNO4+hv=0.65 HO2+0.65 NO2+0.35 HO+0.35 NO3 : j(Pj_hno4) ;
 {007:J07} NO3+hv=NO{+O2}    : j(Pj_no3o2) ;
 {008:J08} NO3+hv=NO2+O3P   : j(Pj_no3o) ;
 {009:J09} H2O2+hv=HO+HO   : j(Pj_h2o2) ;
...
 {236:213} XO2+NO=NO2     : 4.00e-12 ;
 {237:214} XO2+NO3=NO2     : 1.20e-12 ;
 {238:215} ISOP+ISOP=2. MACR+HCHO+HO2   : 2.00e-12 ;
 {239:216} ISHP+HO=MACR+HO : 1.00e-10 ;
 {240:217} ISON+HO=HACE+NALD : 1.30e-11 ;
 {241:218} MACP+NO=NO2+0.25 HACE+0.25 CO+0.25 ACO3+0.5 MGLY+0.75 HCHO+0.75 HO2:
     ARR2( 2.54e-12, -360.0, TEMP ) ;
 {242:219} MACP+HO2=MAHP : ARR2( 1.82e-13 , -1300.0, TEMP ) ;
 {243:220} MACP+MACP=HACE+MGLY+0.5 HCHO+0.5 CO+HO2 : 2.00e-12 ;
 {244:221} MACP+NO2=MPAN : TROE( 9.70e-29 , 5.6 , 9.30e-12 , 1.5 , TEMP, C_M) ;
 {245:222} MPAN=MACP+NO2 : TROEE(1.11e28,14000.0,9.70e-29,5.6,9.30e-12,1.5,TEMP,C_M);
```

Why KPP?

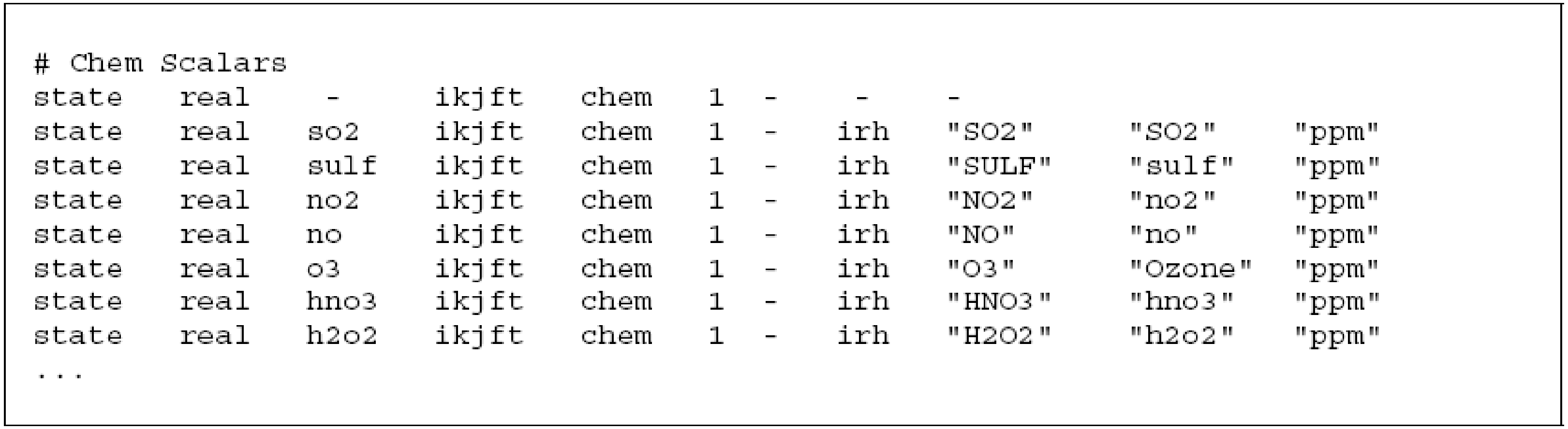
Advantages

- much less time consuming than manual coding
- less error prone
- numerically efficient

- results in greater flexibility
  - updating mechanisms by additional equations
  - sensitivity studies

WRF-Chem Registry

Excerpt: chemistry array



```
# Chem Scalars
state    real    -     ikjft    chem    1  -    -       -
state    real   so2    ikjft    chem    1  -   irh   "SO2"     "SO2"     "ppm"
state    real   sulf   ikjft    chem    1  -   irh   "SULF"    "sulf"    "ppm"
state    real   no2    ikjft    chem    1  -   irh   "NO2"     "no2"     "ppm"
state    real   no     ikjft    chem    1  -   irh   "NO"      "no"      "ppm"
state    real   o3     ikjft    chem    1  -   irh   "O3"      "Ozone"   "ppm"
state    real   hno3   ikjft    chem    1  -   irh   "HNO3"    "hno3"    "ppm"
state    real   h2o2   ikjft    chem    1  -   irh   "H2O2"    "h2o2"    "ppm"
...
```

+ arrays for radicals

+ arrays for photolysis rates

+ package declaration for each mechanism

WRF-Chem/KPP Coupler

Written in C and in parts based on the Registry mechanism

Writes f90 interfaces between WRF-Chem and KPP generated code

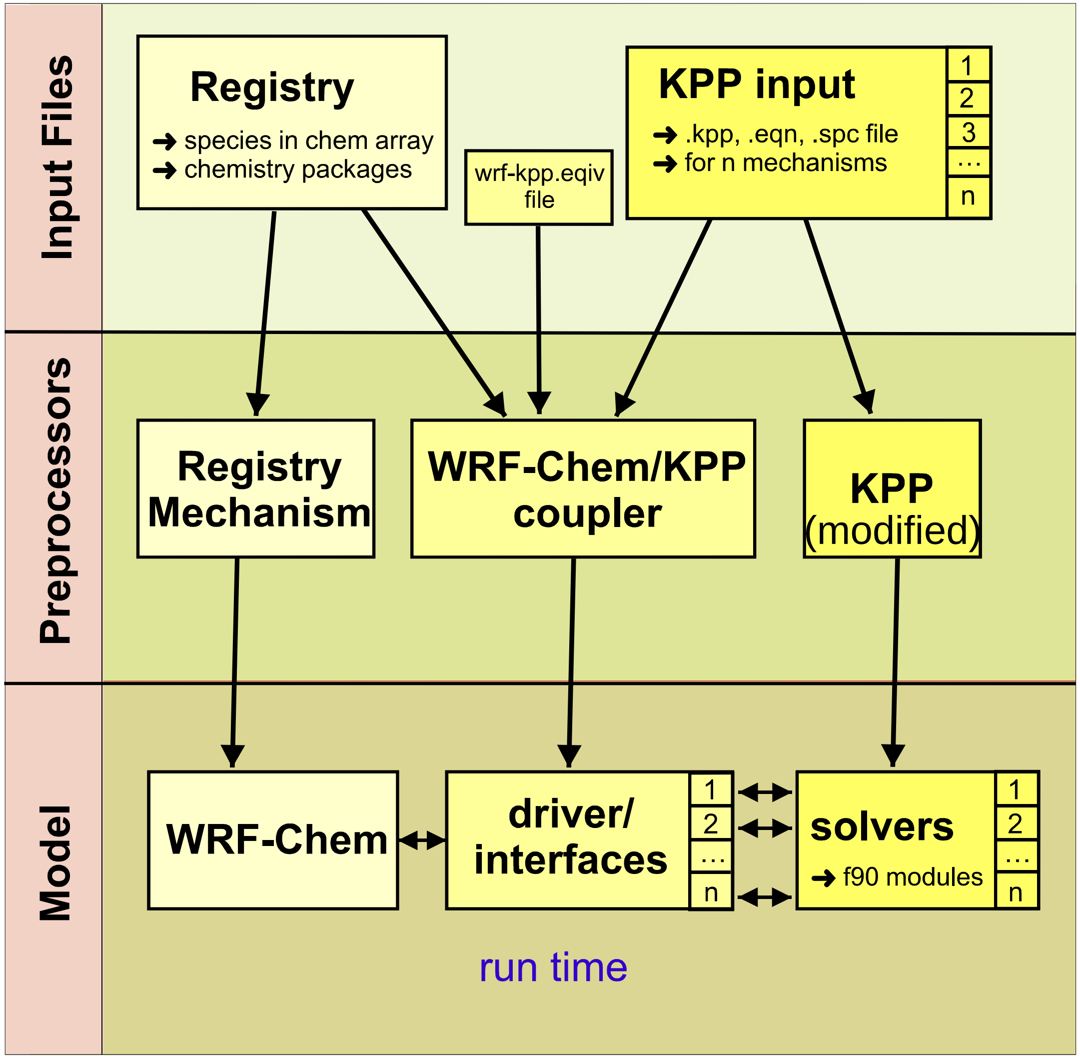
Layout: still open for suggestions

A few modifications to KPP (switch)

not all features available

currently only Rosenbrock type solvers

WRF-Chem/KPP coupler



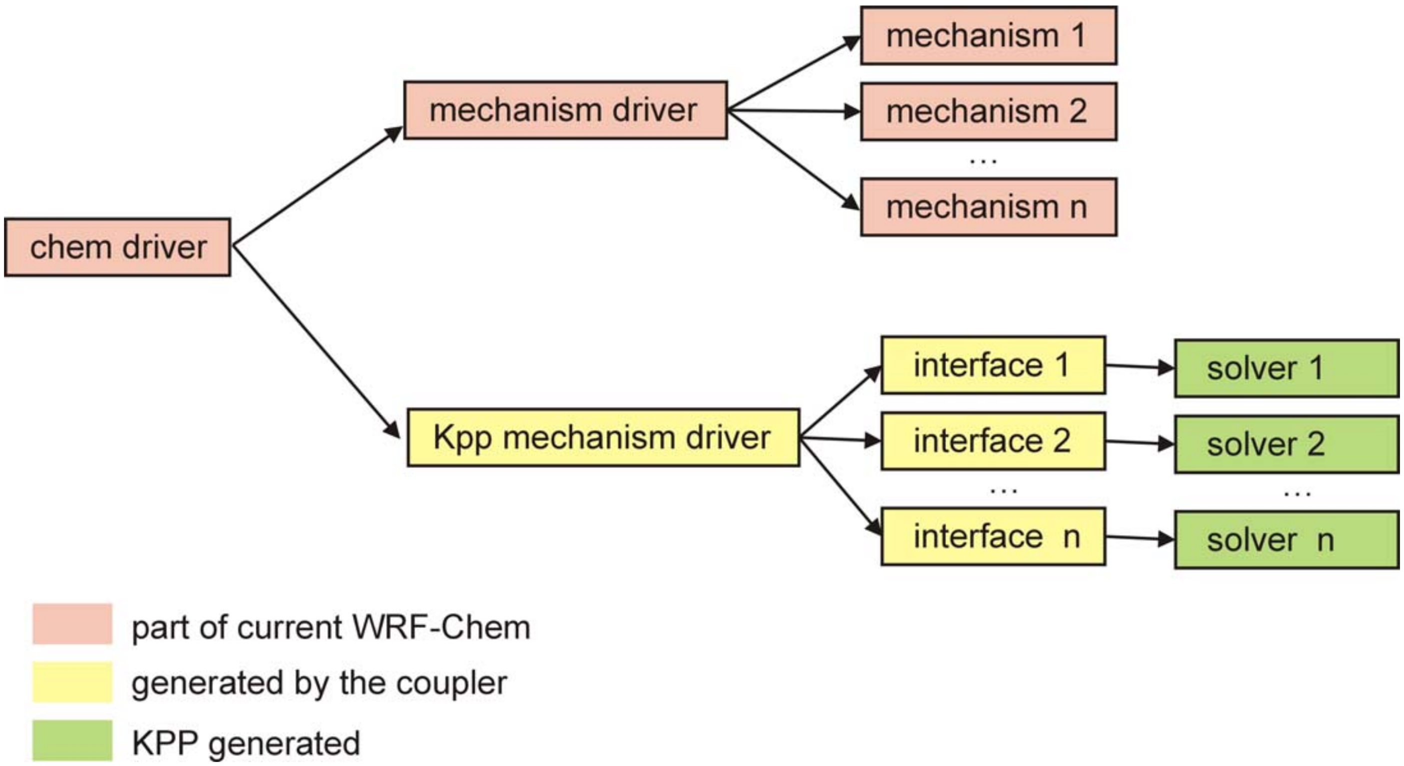
Layout of the coupler

„Non-destructive“

Located in one directory: chem/KPP

- compile_kpp script, clean_kpp script and Makefiles
- modified KPP (latest version, v2.1)
- the coupler
- mechanisms directory
- module_wkppc_constants.F
- documentation (work in progress)
- can be called from compile script

Call tree for the generated code

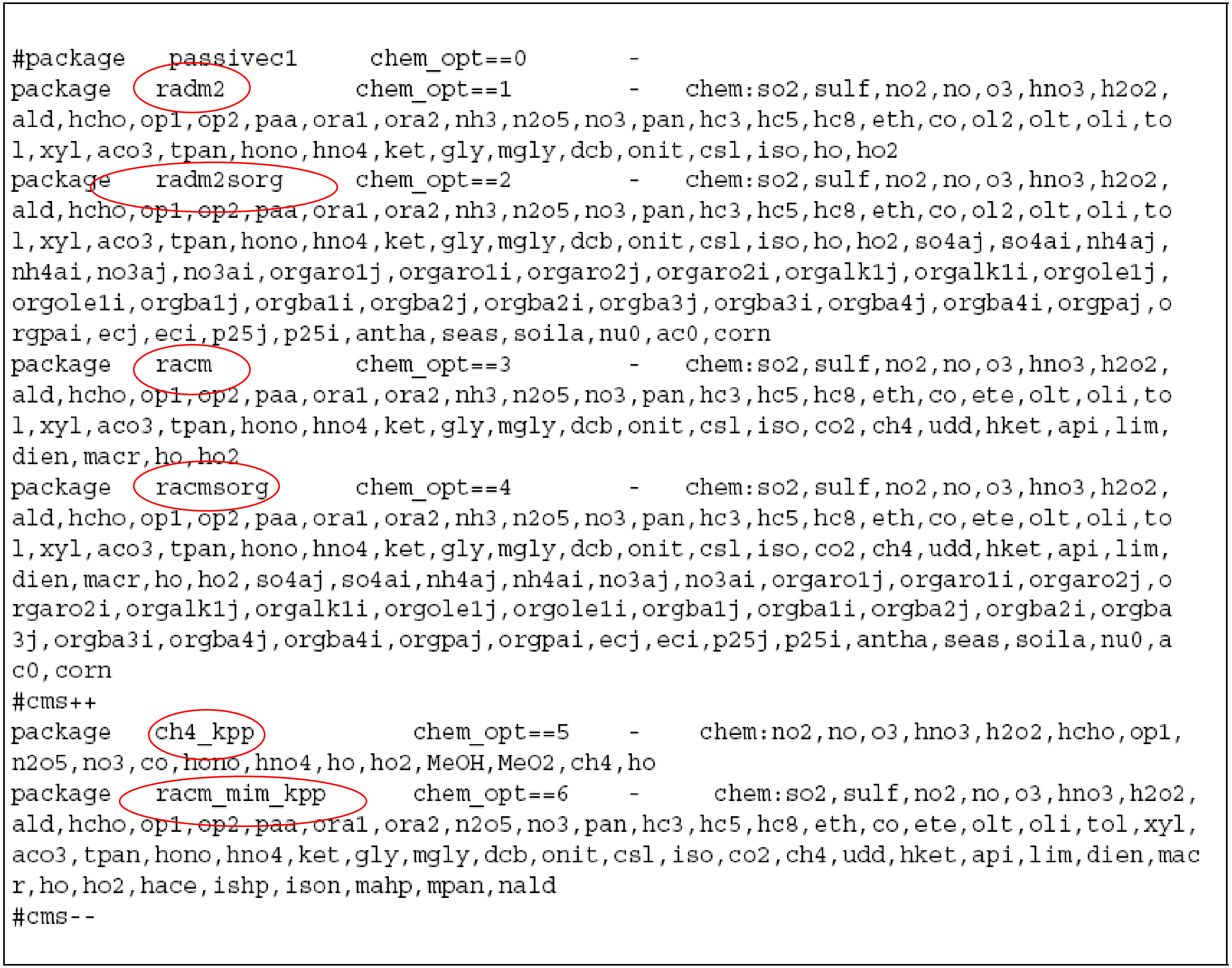


chem driver
mechanism driver
mechanism 1
mechanism 2
…
mechanism n
Kpp mechanism driver
interface 1
interface 2
…
interface n
solver 1
solver 2
…
solver n

🟥 part of current WRF-Chem
🟨 generated by the coupler
🟩 KPP generated

Adding mechanisms I

1. Edit the WRF-Chem Registry (currently Registry.EM_CHEM)
    - add additional species to chem array
    - add a package (=a mechanism) with a name ending with _kpp



```
#package   passivec1     chem_opt==0        -
package    radm2          chem_opt==1        -    chem:so2,sulf,no2,no,o3,hno3,h2o2,
ald,hcho,op1,op2,paa,ora1,ora2,nh3,n2o5,no3,pan,hc3,hc5,hc8,eth,co,ol2,olt,oli,to
l,xyl,aco3,tpan,hono,hno4,ket,gly,mgly,dcb,onit,csl,iso,ho,ho2
package    radm2sorg      chem_opt==2        -    chem:so2,sulf,no2,no,o3,hno3,h2o2,
ald,hcho,op1,op2,paa,ora1,ora2,nh3,n2o5,no3,pan,hc3,hc5,hc8,eth,co,ol2,olt,oli,to
l,xyl,aco3,tpan,hono,hno4,ket,gly,mgly,dcb,onit,csl,iso,ho,ho2,so4aj,so4ai,nh4aj,
nh4ai,no3aj,no3ai,orgaro1j,orgaro1i,orgaro2j,orgaro2i,orgalk1j,orgalk1i,orgole1j,
orgole1i,orgba1j,orgba1i,orgba2j,orgba2i,orgba3j,orgba3i,orgba4j,orgba4i,orgpaj,o
rgpai,ecj,eci,p25j,p25i,antha,seas,soila,nu0,ac0,corn
package    racm           chem_opt==3        -    chem:so2,sulf,no2,no,o3,hno3,h2o2,
ald,hcho,op1,op2,paa,ora1,ora2,nh3,n2o5,no3,pan,hc3,hc5,hc8,eth,co,ete,olt,oli,to
l,xyl,aco3,tpan,hono,hno4,ket,gly,mgly,dcb,onit,csl,iso,co2,ch4,udd,hket,api,lim,
dien,macr,ho,ho2
package    racmsorg       chem_opt==4        -    chem:so2,sulf,no2,no,o3,hno3,h2o2,
ald,hcho,op1,op2,paa,ora1,ora2,nh3,n2o5,no3,pan,hc3,hc5,hc8,eth,co,ete,olt,oli,to
l,xyl,aco3,tpan,hono,hno4,ket,gly,mgly,dcb,onit,csl,iso,co2,ch4,udd,hket,api,lim,
dien,macr,ho,ho2,so4aj,so4ai,nh4aj,nh4ai,no3aj,no3ai,orgaro1j,orgaro1i,orgaro2j,o
rgaro2i,orgalk1j,orgalk1i,orgole1j,orgole1i,orgba1j,orgba1i,orgba2j,orgba2i,orgba
3j,orgba3i,orgba4j,orgba4i,orgpaj,orgpai,ecj,eci,p25j,p25i,antha,seas,soila,nu0,a
c0,corn
#cms++
package    ch4_kpp            chem_opt==5    -     chem:no2,no,o3,hno3,h2o2,hcho,op1,
n2o5,no3,co,hono,hno4,ho,ho2,MeOH,MeO2,ch4,ho
package    racm_mim_kpp       chem_opt==6    -      chem: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,mac
r,ho,ho2,hace,ishp,ison,mahp,mpan,nald
#cms--
```

Adding mechanisms I

1. Edit the WRF-Chem Registry (currently Registry,EM_CHEM)
    - add additional species to chem array
    - add a package (=a mechanism) with a name ending with _kpp

2. Provide input files (.eqn, .spc, .kpp) for KPP in a subdirectory of chem/KPP/mechanisms named after the package

3. Optionally provide a file (wrfkpp.equiv) for mapping variable names in WRF-Chem to variable names in KPP

Adding mechanisms II (the hard part)

Possibly calculate additional photolysis rates

Emissions

Initial and boundary conditions

Dry deposition rates

Wet deposition

Deep convection

…

Future Perspectives/Availability

Currently under evaluation for the WRF-Chem Repository

One step towards generalizing WRF-Chem

Suggestions are welcome!

Acknowledgements

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Cloud resolving studies of trace gas scavenging and photochemistry

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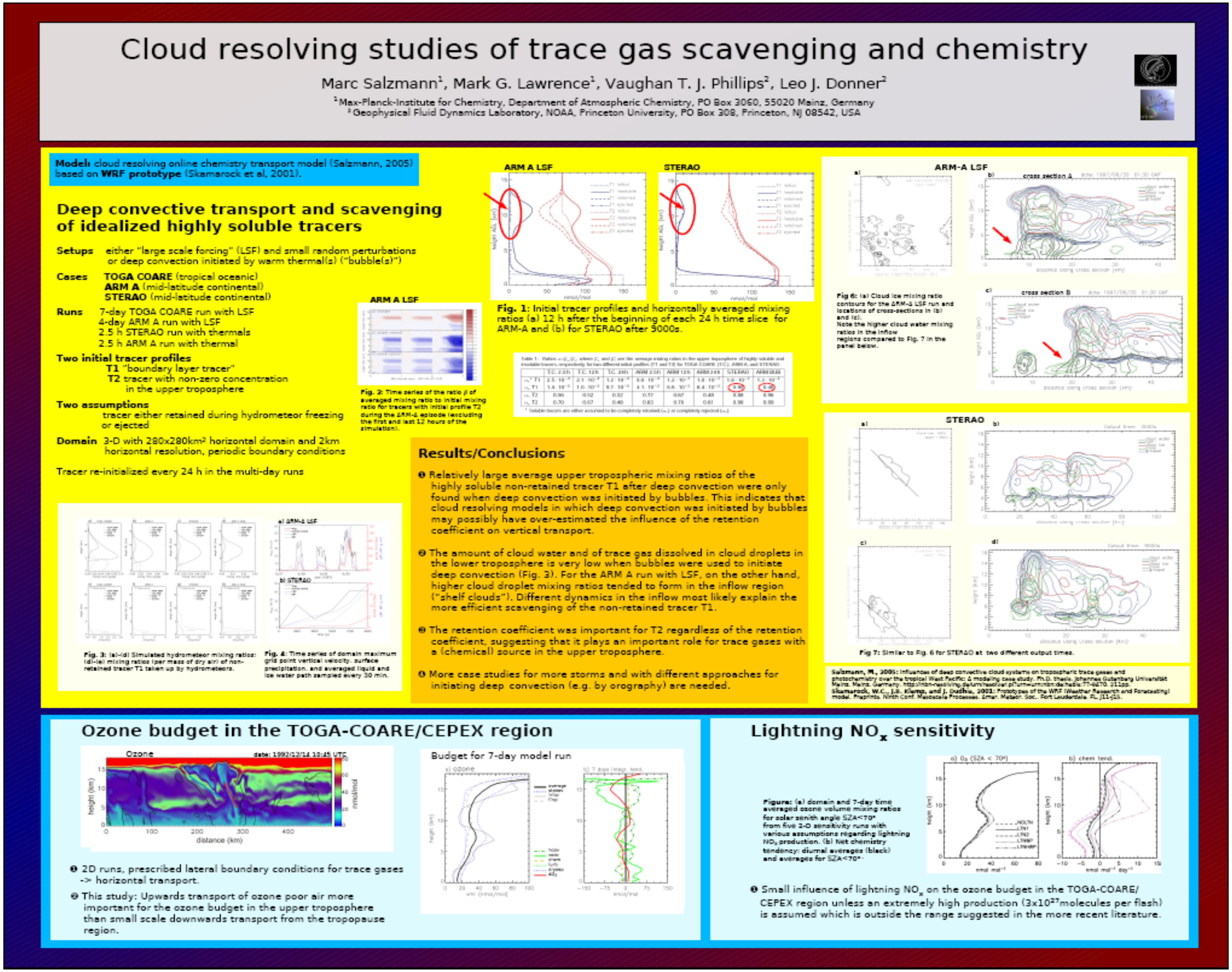
Poster

Image courtesy of Image Science & Analysis Laboratory, NASA on Space Center

Shameless self-advertising



Cloud resolving studies of trace gas scavenging and chemistry

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Model: cloud resolving online chemistry transport model (Salzmann, 2005) based on **WRF prototype** (Skamarock et al, 2001).

Deep convective transport and scavenging of idealized highly soluble tracers

Setups either "large scale forcing" (LSF) and small random perturbations or deep convection initiated by warm thermal(s) ("bubble(s)")

Cases
TOGA COARE (tropical oceanic)
ARM A (mid-latitude continental)
STERAO (mid-latitude continental)

Runs
7-day TOGA COARE run with LSF
4-day ARM A run with LSF
2.5 h STERAO run with thermals
2.5 h ARM A run with thermal

Two initial tracer profiles
T1 "boundary layer tracer"
T2 tracer with non-zero concentration in the upper troposphere

Two assumptions
tracer either retained during hydrometeor freezing or ejected

Domain 3-D with 280x280km² horizontal domain and 2km horizontal resolution, periodic boundary conditions

Tracer re-initialized every 24 h in the multi-day runs

ARM A LSF

Fig. 2: Time series of the ratio β of averaged mixing ratio to initial mixing ratio for tracers with initial profile T2 during the ARM-A episode (excluding the first and last 12 hours of the simulation).

Fig. 3: (a)-(d) Simulated hydrometeor mixing ratios: (d)-(e) mixing ratios (per mass of dry air) of non-retained tracer T1 taken up by hydrometeors.

Fig. 4: Time series of domain maximum grid point vertical velocity, surface precipitation, and averaged liquid and ice water path sampled every 30 min.

ARM A LSF STERAO

Fig. 1: Initial tracer profiles and horizontally averaged mixing ratios (a) 12 h after the beginning of each 24 h time slice for ARM-A and (b) for STERAO after 9000s.

Results/Conclusions

❶ Relatively large average upper tropospheric mixing ratios of the highly soluble non-retained tracer T1 after deep convection were only found when deep convection was initiated by bubbles. This indicates that cloud resolving models in which deep convection was initiated by bubbles may possibly have over-estimated the influence of the retention coefficient on vertical transport.

❷ The amount of cloud water and of trace gas dissolved in cloud droplets in the lower troposphere is very low when bubbles were used to initiate deep convection (Fig. 3). For the ARM A run with LSF, on the other hand, higher cloud droplet mixing ratios tended to form in the inflow region ("shelf clouds"). Different dynamics in the inflow most likely explain the more efficient scavenging of the non-retained tracer T1.

❸ The retention coefficient was important for T2 regardless of the retention coefficient, suggesting that it plays an important role for trace gases with a (chemical) source in the upper troposphere.

❹ More case studies for more storms and with different approaches for initiating deep convection (e.g. by orography) are needed.

ARM-A LSF

Fig 6: (a) Cloud ice mixing ratio contours for the ARM-A LSF run and locations of cross-sections in (b) and (c).
Note the higher cloud water mixing ratios in the inflow regions compared to Fig. 7 in the panel below.

STERAO

Fig 7: Similar to Fig. 6 for STERAO at two different output times.

Salzmann, M., 2005: Influences of deep convective cloud systems on tropospheric trace gases and photochemistry over the tropical West Pacific: A modeling case study. Ph.D. thesis, Johannes Gutenberg Universität Mainz, Mainz, Germany. http://nbn-resolving.de/urn/resolver.pl?urn=urn:nbn:de:hebis:77-9870. 211pp.
Skamarock, W.C., J.B. Klemp, and J. Dudhia, 2001: Prototypes of the WRF (Weather Research and Forecasting) model. Preprints, Ninth Conf. Mesoscale Processes, Amer. Meteor. Soc., Fort Lauderdale, FL, J11-J15.

Ozone budget in the TOGA-COARE/CEPEX region

Ozone date: 1992/12/14 10:45 UTC

Budget for 7-day model run

❶ 2D runs, prescribed lateral boundary conditions for trace gases -> horizontal transport.

❷ This study: Upwards transport of ozone poor air more important for the ozone budget in the upper troposphere than small scale downwards transport from the tropopause region.

Lightning NO_x sensitivity

Figure: (a) domain and 7-day time averaged ozone volume mixing ratios for solar zenith angle SZA<70° from five 2-D sensitivity runs with various assumptions regarding lightning NO_x production. (b) Net chemistry tendency: diurnal averages (black) and averages for SZA<70°.

❶ Small influence of lightning NO_x on the ozone budget in the TOGA-COARE/CEPEX region unless an extremely high production (3×10^{27} molecules per flash) is assumed which is outside the range suggested in the more recent literature.

Tasks of the coupler

- Gather information from the WRF-Chem Registry:
  - chem array species names (from package lines)
  - names of radicals from radical arrays
  - photolysis rates

- Read KPP species files (from chem/KPP/mechanisms/*/*.spc)
- Read wrfkpp.equiv files
- Perform consistency checks and issue warnings if necessary
- Write a mechanism driver for KPP mechanisms (called from chem/mechanism_driver.F)
- Write a solver interface module for each KPP mechanism

- Take care of running KPP (make) and later compiling the generated code together with WRF-Chem

Preliminary benchmarks