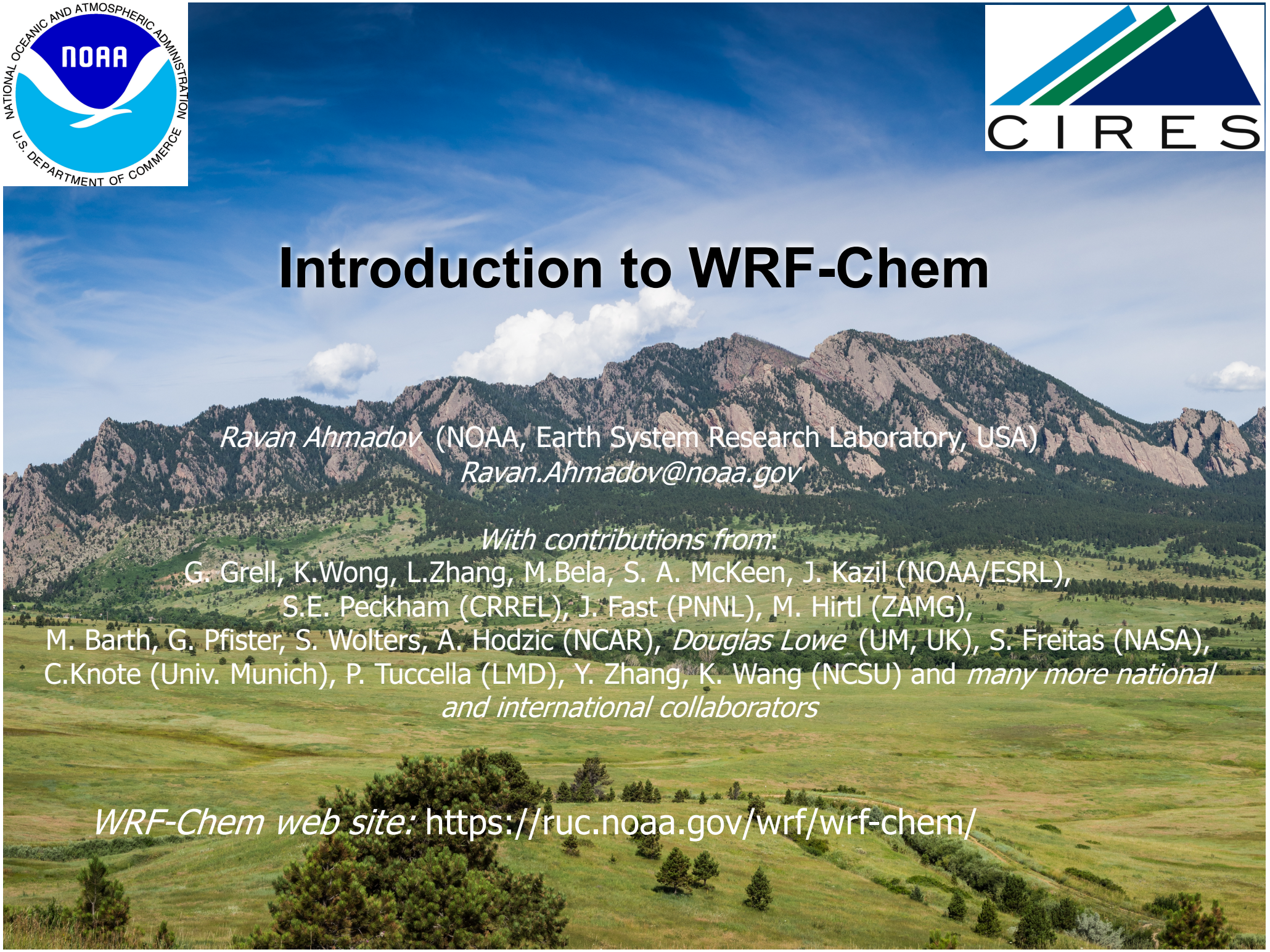
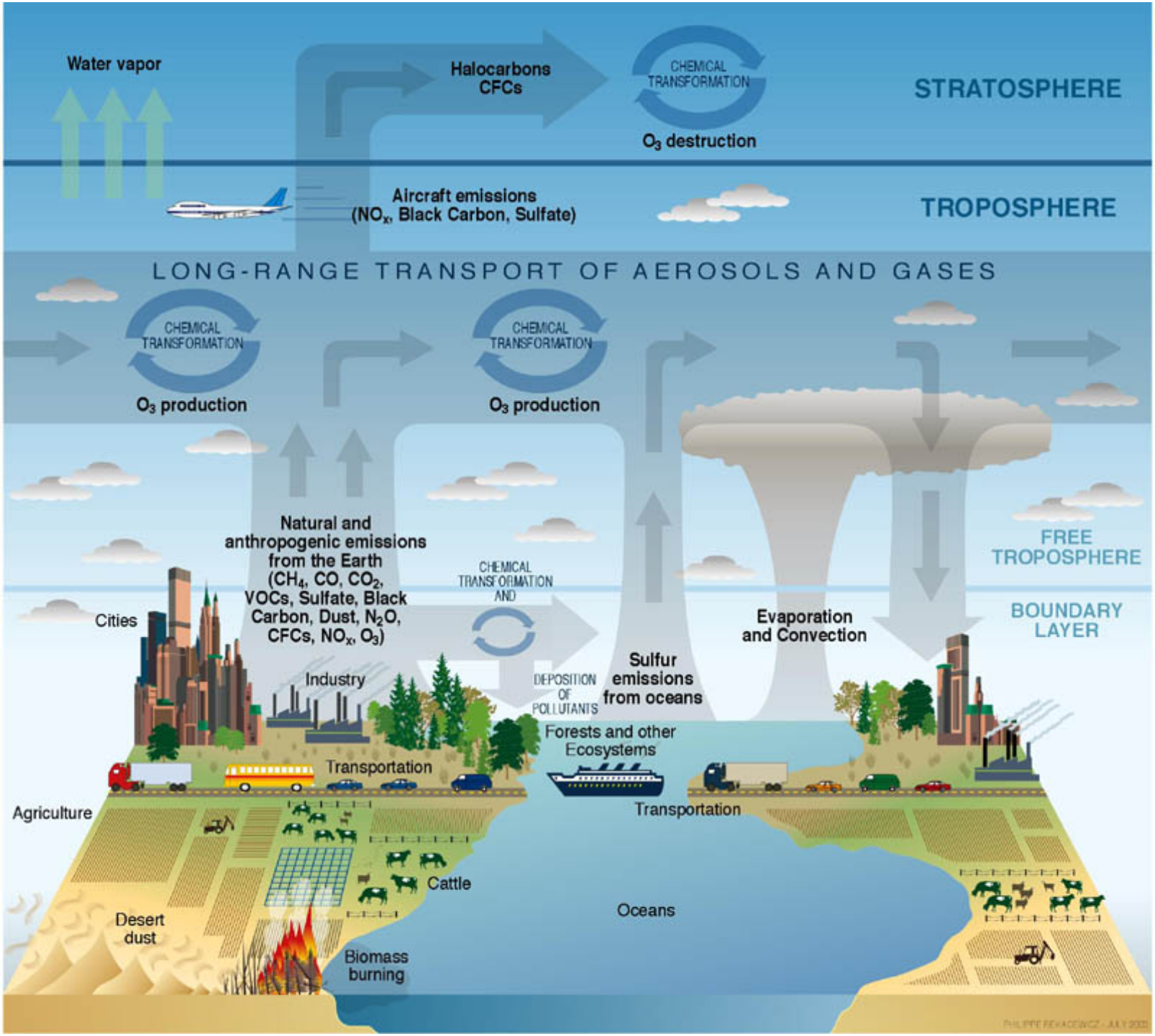


Introduction to WRF-Chem

Ravan Ahmadov (NOAA, Earth System Research Laboratory, USA)
Ravan.Ahmadov@noaa.gov

With contributions from:
G. Grell, K.Wong, L.Zhang, M.Bela, S. A. McKeen, J. Kazil (NOAA/ESRL),
S.E. Peckham (CRREL), J. Fast (PNNL), M. Hirtl (ZAMG),
M. Barth, G. Pfister, S. Wolters, A. Hodzic (NCAR), *Douglas Lowe* (UM, UK), S. Freitas (NASA),
C.Knote (Univ. Munich), P. Tuccella (LMD), Y. Zhang, K. Wang (NCSU) and *many more national and international collaborators*

WRF-Chem web site: https://ruc.noaa.gov/wrf/wrf-chem/


Water vapor
Halocarbons
CFCs
CHEMICAL TRANSFORMATION
O_3 destruction
STRATOSPHERE
Aircraft emissions
(NO_x, Black Carbon, Sulfate)
TROPOSPHERE
LONG-RANGE TRANSPORT OF AEROSOLS AND GASES
CHEMICAL TRANSFORMATION
O_3 production
CHEMICAL TRANSFORMATION
O_3 production
Natural and anthropogenic emissions from the Earth (CH_4, CO, CO_2, VOCs, Sulfate, Black Carbon, Dust, N_2O, CFCs, NO_x, O_3)
CHEMICAL TRANSFORMATION AND
FREE TROPOSPHERE
BOUNDARY LAYER
Cities
Industry
DEPOSITION OF POLLUTANTS
Sulfur emissions from oceans
Evaporation and Convection
Forests and other Ecosystems
Transportation
Transportation
Agriculture
Cattle
Oceans
Desert dust
Biomass burning

WRF-Chem

- Chemistry is online, completely embedded within the WRF code infrastructure
- Consistent: all transport done by the meteorological model
  - Same vertical and horizontal coordinates (no horizontal and vertical interpolation)
  - Same physics parameterization for subgrid scale transport
  - No interpolation in time
- Easy handling (Data management)
- Ideally suited to study feedbacks between chemistry and meteorology
- Ideally suited for tracer (e.g. dust, pollen) and air quality forecasting on regional to cloud resolving scales

Some WRF-Chem facts and news

- WRF-Chem is a fully coupled meteorology-chemistry model.
- Current version of WRF-Chem (V4.1.3) contains multiple parameterizations to simulate greenhouse gases, dust, fires, volcanoes, gas and aerosol chemistry (ranging from simple to more complex schemes), photolysis, removal processes, meteorology-chemistry interactions and so on.
- Many national and international collaborators from NOAA, NCAR, PNNL, NASA, universities still contribute and support the WRF-Chem developments.
- Among the registered WRF users about 3000 have selected chemistry as their main area of interest.
- The WRF-Chem web-site has been updated (https://ruc.noaa.gov/wrf/wrf-chem/)
- The WRF-Chem discussions group has been set up to reach out to the large WRF-Chem and air quality modeling community, to inform users about ongoing and future developments, new features and bug fixes in WRF-Chem: https://list.woc.noaa.gov/cgi-bin/mailman/listinfo/wrf-chem-discussions

Haagen-Smit Prize 2016 awarded to the WRF-Chem paper

1238 citations (Google Scholar)

ELSEVIER

Available online at www.sciencedirect.com

SCIENCE DIRECT®

Atmospheric Environment 39 (2005) 6957–6975

ATMOSPHERIC ENVIRONMENT

www.elsevier.com/locate/atmosenv

Fully coupled "online" chemistry within the WRF model

Georg A. Grell[a,*], Steven E. Peckham[a], Rainer Schmitz[c], Stuart A. McKeen[b], Gregory Frost[b], William C. Skamarock[d], Brian Eder[e]

The Executive Editors and the Publisher of Atmospheric Environment take great pleasure in announcing the 2016 "Haagen-Smit Prize", designed to recognize *outstanding papers published in Atmospheric Environment*. The Prize is named in honor of Prof. Arie Jan Haagen-Smit, a pioneer in the field of air pollution and one of the first editors of the International Journal of Air Pollution, a predecessor to Atmospheric Environment.

What is needed for this type of modeling system?

- Advection and diffusion (all done by WRF)
- Sub-grid scale transport (WRF parameterizations, PBL, convection)
- Some processes that are specific for chemical constituents, but need meteorology: emissions (biogenic, fire, sea salt, dust, volcanic, anthropogenic), dry deposition, wet scavenging
- Treatment of chemical reactions, aqueous phase chemistry, gas phase species and aerosols
- "Chemical" radiation routines (photolysis routines) that provide photolysis rates necessary for the gas chemistry schemes
- Capability of feedback from chemistry to meteorology (meteorological radiation and microphysics parameterizations, possibly also convective parameterizations)

The passive tracer chemistry options in WRF-Chem

- **Passive tracer options (chem_opt=13-15): no chemistry, transport only, anthropogenic or any other assigned emissions can be used**
- **Passive tracer options for greenhouse gases (chem_opt=16, 17): no chemistry, transport only, anthropogenic emissions and biospheric fluxes of CO_2 and CH_4**
- **You can run the chemistry options as passive tracer simulations by setting gaschem_onoff=0 in namelist.input**
- **In passive tracer type of simulation all the tracers are advected (chem_adv_opt in namelist.input), vertically mixed (vertmix_onoff) and also mixed by cumulus parameterization (chem_conv_tr)**
- **Passive tracer transport simulations are very useful to evaluate the transport and mixing of chemicals, emissions and for other tasks; Computationally very efficient!**
- **In WRF-Chem the meteorological and chemical variables share the same model grid and advection scheme**

The gas phase chemistry mechanisms in WRF-Chem

- **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)**
- **Carbon Bond mechanism (CB05)**
- **Carbon-Bond Mechanism version Z (CBMZ)**
- **Model of Ozone and Related Chemical Tracers (MOZART)**
- **Statewide Air Pollution Research Center (SAPRC99)**
- **Common Representative Intermediates Mechanism (CRIMech)**

different implementations, coupled to different aerosol schemes and aqueous chemistry, suitable for different applications ranging from regional air quality to global atmospheric chemistry simulations

Table 1. RACM Mechanism Species List

No.	Species	Definition	Carbon Number	Molecular Weight
		Stable Inorganic Compounds		
	Oxidants			
1	O_3	ozone		48
2	H_2O_2	hydrogen peroxide		34
	Nitrogenous compounds			
3	NO	nitric oxide		30
4	NO_2	nitrogen dioxide		46
5	NO_3	nitrogen trioxide		62
6	N_2O_5	dinitrogen pentoxide		108
7	HONO	nitrous acid		47
8	HNO_3	nitric acid		63
9	HNO_4	pernitric acid		79
	Sulfur compounds			
10	SO_2	sulfur dioxide		64
11	SULF	sulfuric acid		98
	Carbon oxides			
12	CO	carbon monoxide	1	28
13	CO_2	carbon dioxide	1	44
		Abundant Stable Species		
14	N_2	nitrogen		28
15	O_2	oxygen		32
16	H_2O	water		18
17	H_2	hydrogen		2
		Inorganic Short-Lived Intermediates		
18	O^3P	ground state oxygen atom, $O(^3P)$		16
19	O^1D	excited state oxygen atom, $O(^1D)$		16
	Odd hydrogen			
20	HO	hydroxy radical		17
21	HO_2	hydroperoxy radical		33

$$k = A \exp[(-E/R)/T]$$

Table 2b. The RACM Mechanism

Reaction No.	Reaction	A, $cm^3\ s^{-1}$	E/R, K	k^a
	Inorganic Reactions			
(R24)	$O^3P + O_2 \rightarrow O_3$	Table 2f		1.50×10^{-14}
(R25)	$O^3P + O_3 \rightarrow 2\ O_2$	8.00×10^{-12}	2060	7.96×10^{-15}
(R26)	$O^1D + N_2 \rightarrow O^3P + N_2$	1.80×10^{-11}	−110	2.60×10^{-11}
(R27)	$O^1D + O_2 \rightarrow O^3P + O_2$	3.20×10^{-11}	−70	4.05×10^{-11}
(R28)	$O^1D + H_2O \rightarrow HO + HO$	2.20×10^{-10}		2.20×10^{-10}
(R29)	$O_3 + HO \rightarrow HO_2 + O_2$	1.60×10^{-12}	940	6.83×10^{-14}
(R30)	$O_3 + HO_2 \rightarrow HO + 2\ O_2$	1.10×10^{-14}	500	2.05×10^{-15}
(R31)	$HO + HO_2 \rightarrow H_2O + O_2$	4.80×10^{-11}	−250	1.11×10^{-10}
(R32)	$H_2O_2 + HO \rightarrow HO_2 + H_2O$	2.90×10^{-12}	160	1.70×10^{-12}
(R33)	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	Table 2f		2.92×10^{-12}
(R34)	$HO_2 + HO_2 + H_2O \rightarrow H_2O_2 + O_2 + H_2O$	Table 2f		6.58×10^{-30}
(R35)	$O^3P + NO \rightarrow NO_2$	Table 2d		1.66×10^{-12}
(R36)	$O^3P + NO_2 \rightarrow NO + O_2$	6.50×10^{-12}	−120	9.72×10^{-12}
(R37)	$O^3P + NO_2 \rightarrow NO_3$	Table 2d		1.58×10^{-12}
(R38)	$HO + NO \rightarrow HONO$	Table 2d		4.87×10^{-12}
(R39)	$HO + NO_2 \rightarrow HNO_3$	Table 2d		1.15×10^{-11}
(R40)	$HO + NO_3 \rightarrow NO_2 + HO_2$	2.20×10^{-11}		2.20×10^{-11}
(R41)	$HO_2 + NO \rightarrow NO_2 + HO$	3.70×10^{-12}	−250	8.56×10^{-12}
(R42)	$HO_2 + NO_2 \rightarrow HNO_4$	Table 2d		1.39×10^{-12}
(R43)	$HNO_4 \rightarrow HO_2 + NO_2$	Table 2e		8.62×10^{-2}
(R44)	$HO_2 + NO_3 \rightarrow 0.3\ HNO_3 + 0.7\ NO_2 + 0.7\ HO + O_2$	3.50×10^{-12}		3.50×10^{-12}
(R45)	$HO + HONO \rightarrow NO_2 + H_2O$	1.80×10^{-11}	390	4.86×10^{-12}
(R46)	$HO + HNO_3 \rightarrow NO_3 + H_2O$	Table 2f		1.47×10^{-13}
(R47)	$HO + HNO_4 \rightarrow NO_2 + O_2 + H_2O$	1.30×10^{-12}	−380	4.65×10^{-12}
(R48)	$O_3 + NO \rightarrow NO_2 + O_2$	2.00×10^{-12}	1400	1.82×10^{-14}
(R49)	$O_3 + NO_2 \rightarrow NO_3 + O_2$	1.20×10^{-13}	2450	3.23×10^{-17}
(R50)	$NO + NO + O_2 \rightarrow NO_2 + NO_2$	3.30×10^{-39}	−530	1.95×10^{-38}
(R51)	$NO_3 + NO \rightarrow NO_2 + NO_2$	1.50×10^{-11}	−170	2.65×10^{-11}
(R52)	$NO_3 + NO_2 \rightarrow NO + NO_2 + O_2$	4.50×10^{-14}	1260	6.56×10^{-16}
(R53)	$NO_3 + NO_2 \rightarrow N_2O_5$	Table 2d		1.27×10^{-12}
(R54)	$N_2O_5 \rightarrow NO_2 + NO_3$	Table 2e		4.36×10^{-2}
(R55)	$NO_3 + NO_3 \rightarrow NO_2 + NO_2 + O_2$	8.50×10^{-13}	2450	2.29×10^{-16}
(R56)	$HO + H_2 \rightarrow H_2O + HO_2$	5.50×10^{-12}	2000	6.69×10^{-15}
(R57)	$HO + SO_2 \rightarrow SULF + HO_2$	Table 2d		8.89×10^{-13}
(R58)	$CO + HO \rightarrow HO_2 + CO_2$	Table 2f		2.40×10^{-13}

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

Photolysis in WRF-Chem

- Several radiative transfer options:
  - phot_opt = 1 : TUV (140 λs, delta-Eddington)
  - phot_opt = 2 : Fast-J (17 λs, 8-str Feautrier)
  - phot_opt = 3 : F-TUV (17 λs, correction factor, delta-Eddington)

  New option in WRF-Chem v3.9:

  ⇒ phot_opt = 4: updated TUV (140 λs, delta-Eddington)

  ⇒ only works with MOZART_MOSAIC_4BIN_KPP, MOZART_MOSAIC_4BIN_AQ_KPP, and MOZCART_KPP chemical options

- Limitations & advantages
  - Cross section and quantum yield data are hard-coded and not up to date in older schemes;

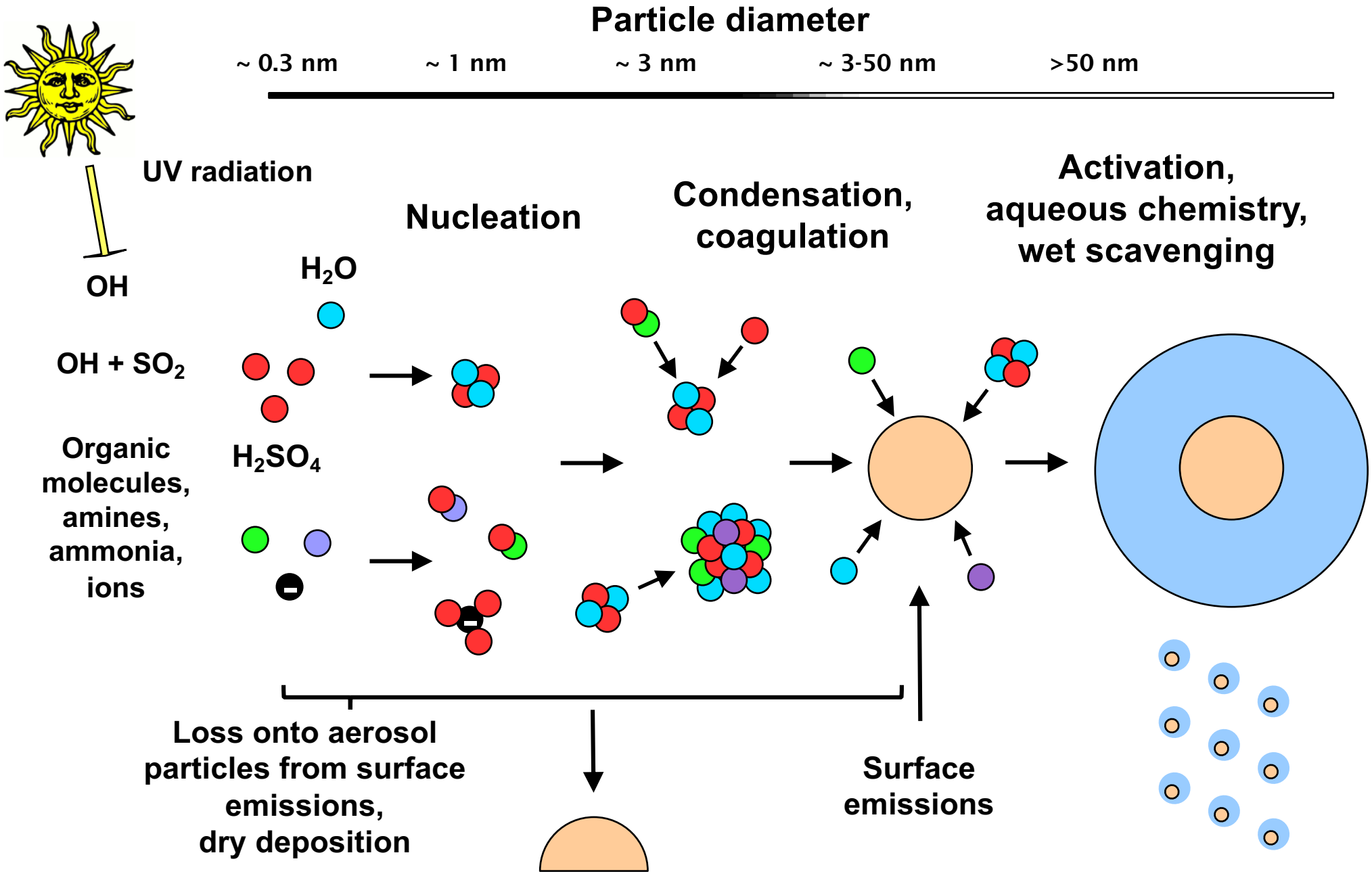
  ⇒ updated database to the latest TUV model (V5.3, Oct. 2016)

  - Difficult to add new reactions (typically available ~ 20)

  ⇒ 109 reactions relevant for tropo & strato chemistry (e.g. halogens)

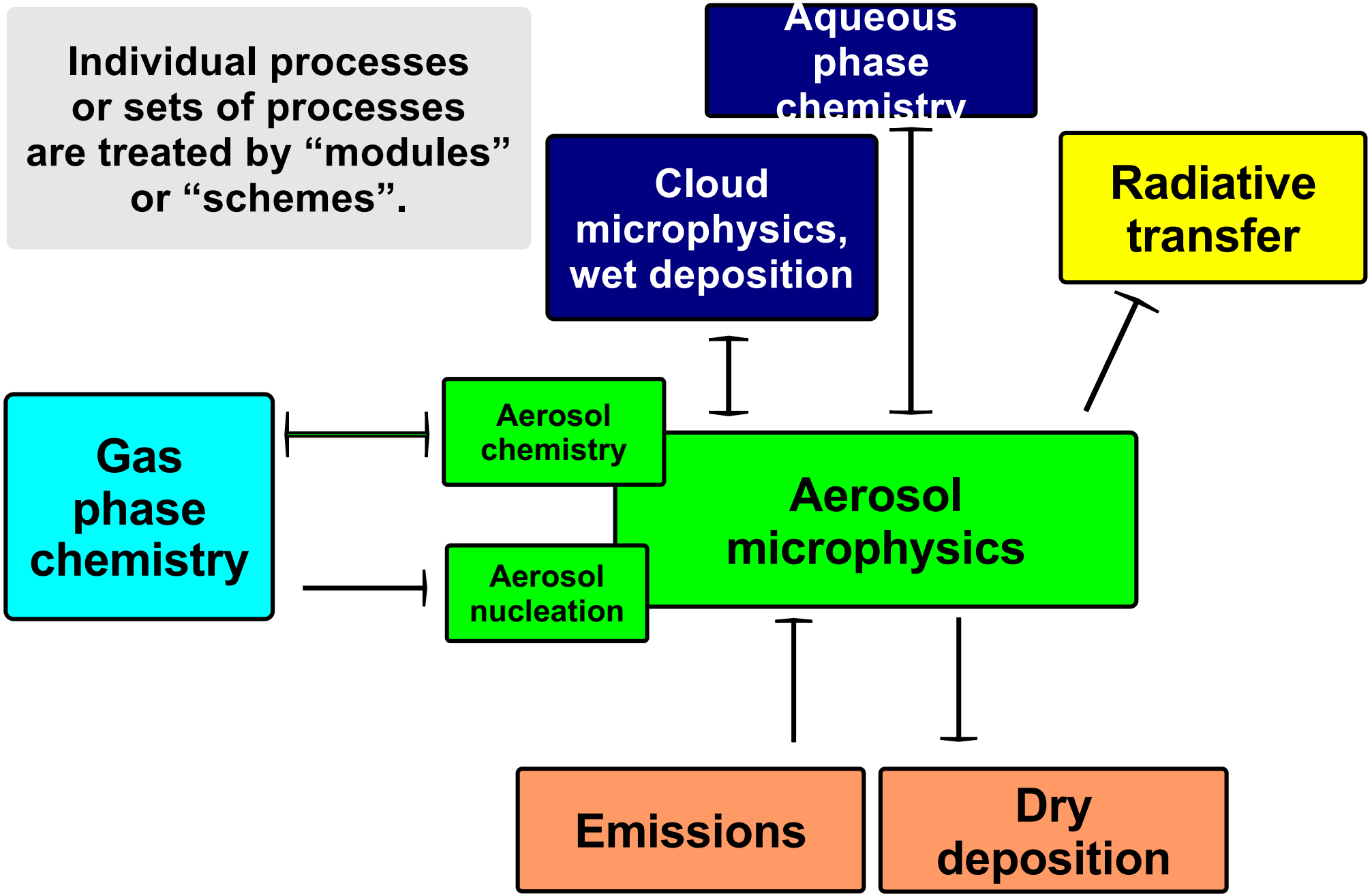
Madronich and Hodzic, WRF-Chem tutorial, 2017

Aerosol life cycle and processes



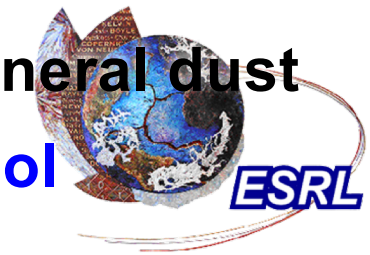
Model treatment of aerosols

Individual processes or sets of processes are treated by "modules" or "schemes".



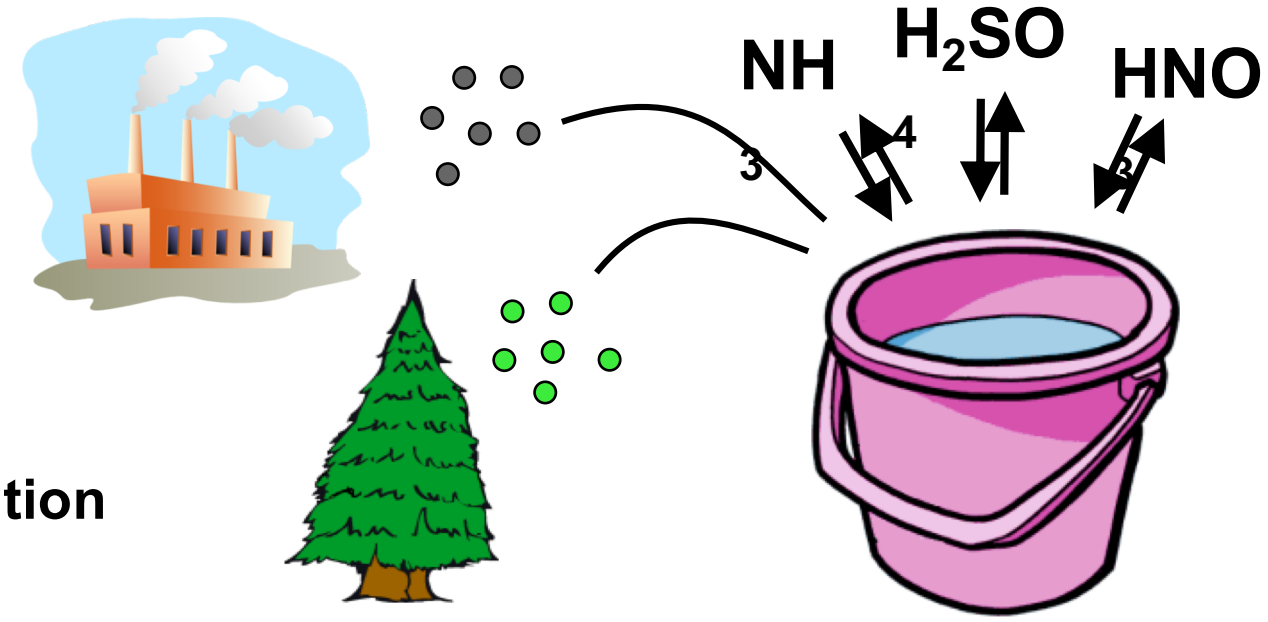
WRF-Chem aerosol schemes

- **An efficient aerosol scheme from the GOCART model**
  - No size information for sulfate, BC, OC
  - Size information for dust and sea salt
  - No secondary organic aerosol (SOA)
- **Modal Aerosol Dynamics Model for Europe – MADE**
  - 3 log-normal modes
  - Inorganic, organic aerosols, SOA
- **Model for Simulating Aerosol Interactions and Chemistry (MOSAIC)**
  - Sectional aerosol scheme, 4 or 8 bins
  - Inorganic, organic aerosols, SOA
- **MAM – Modal Aerosol Model from CAM5**
  - 3 or 7 log-normal modes
  - Inorganic, organic aerosols, SOA, sea salt, BC, mineral dust
- **Simple sectional (bin) scheme for volcanic ash aerosol**



Bulk aerosol schemes

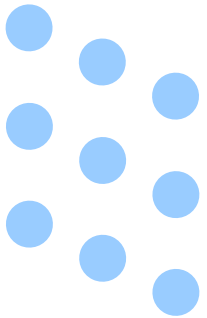
- Only total mass of aerosol compounds is known



- No information on
  - Particle number
  - Aerosol size distribution

Aerosol size distribution needs to be assumed for:

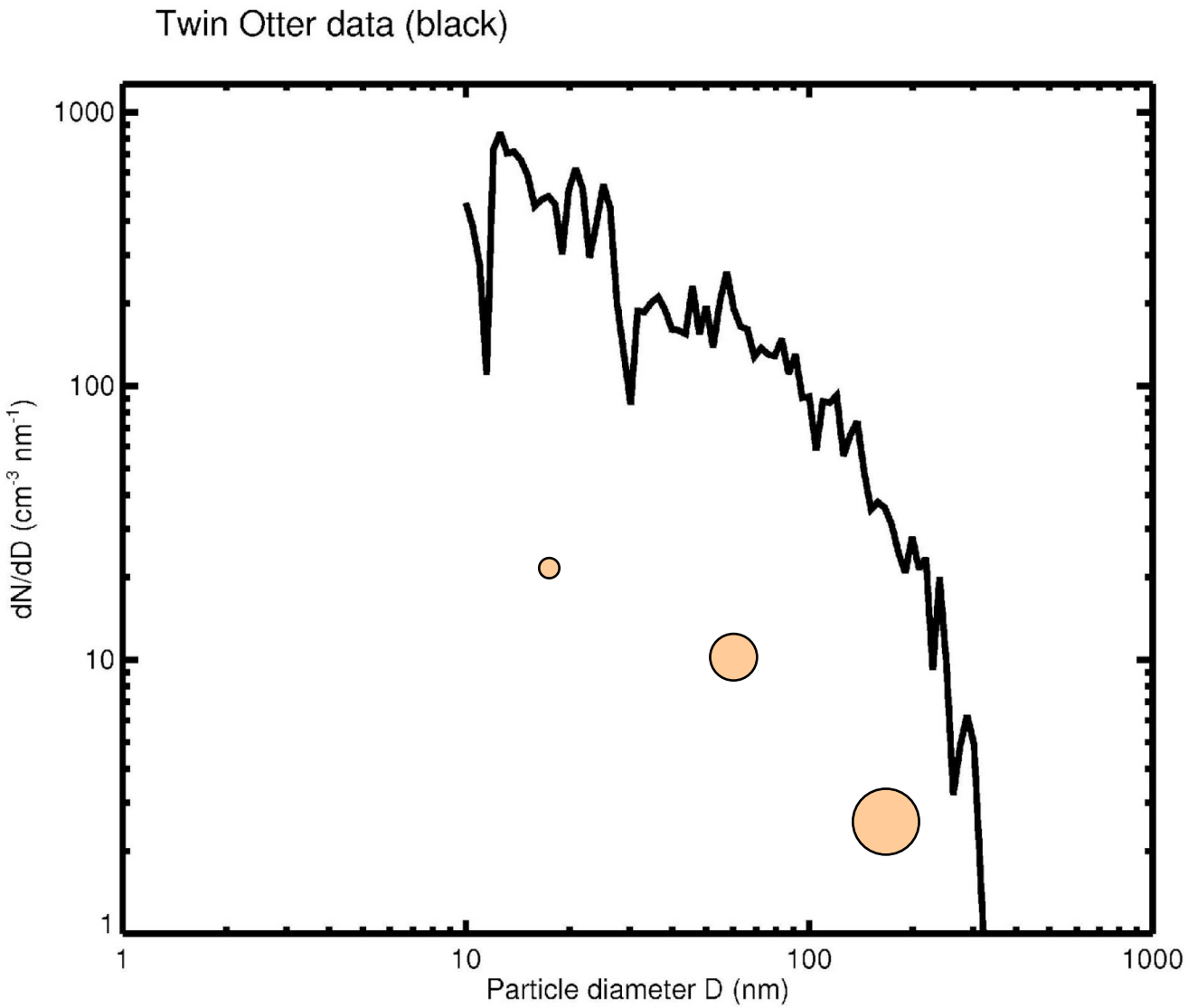
- radiative transfer
- response of cloud properties to aerosol number



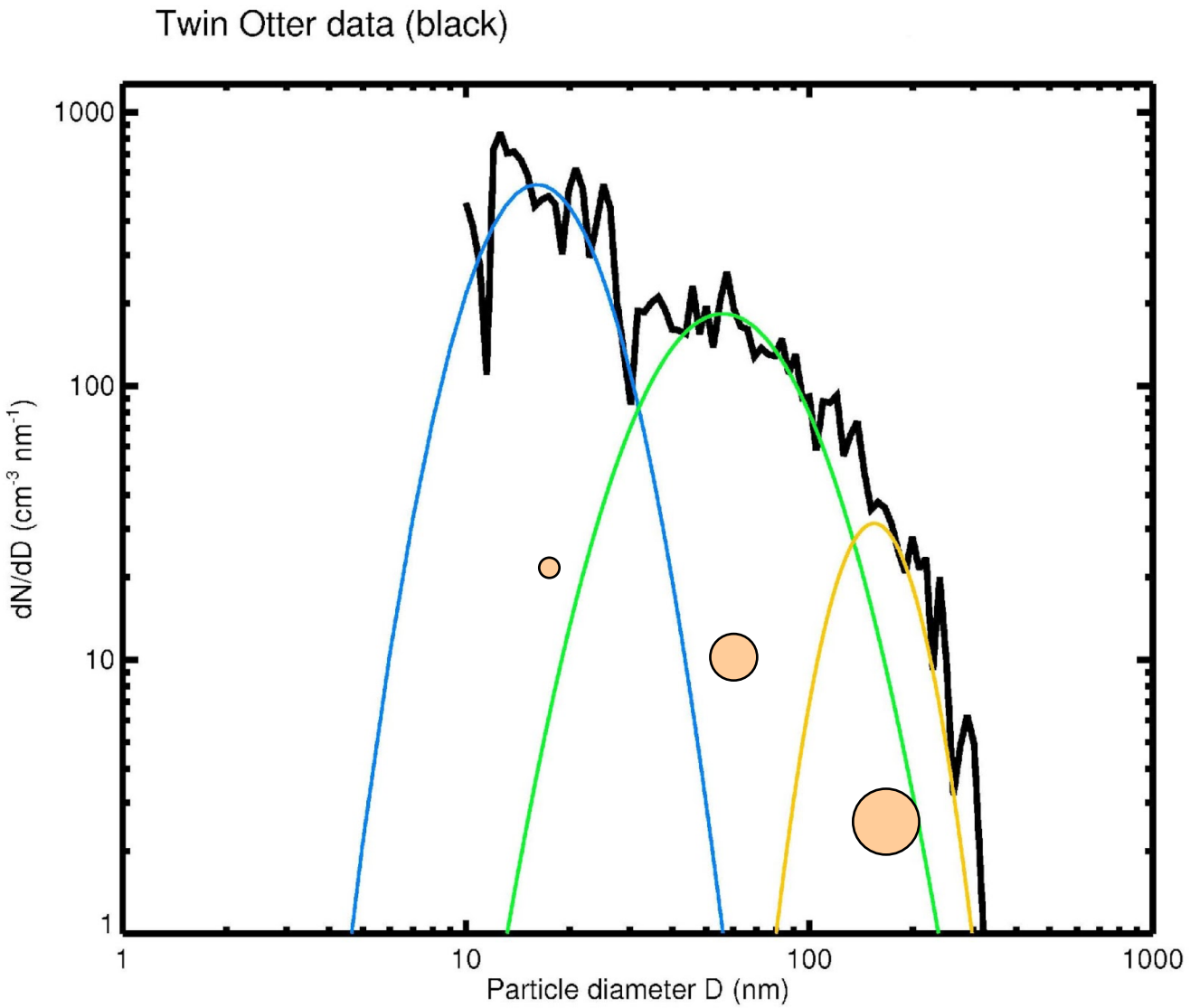
- Numerically efficient
- Useful when focus is on complex gas phase chemistry e.g.

→ **GOCART (+ size resolved dust and sea salt)**

Modal aerosol schemes



Modal aerosol schemes

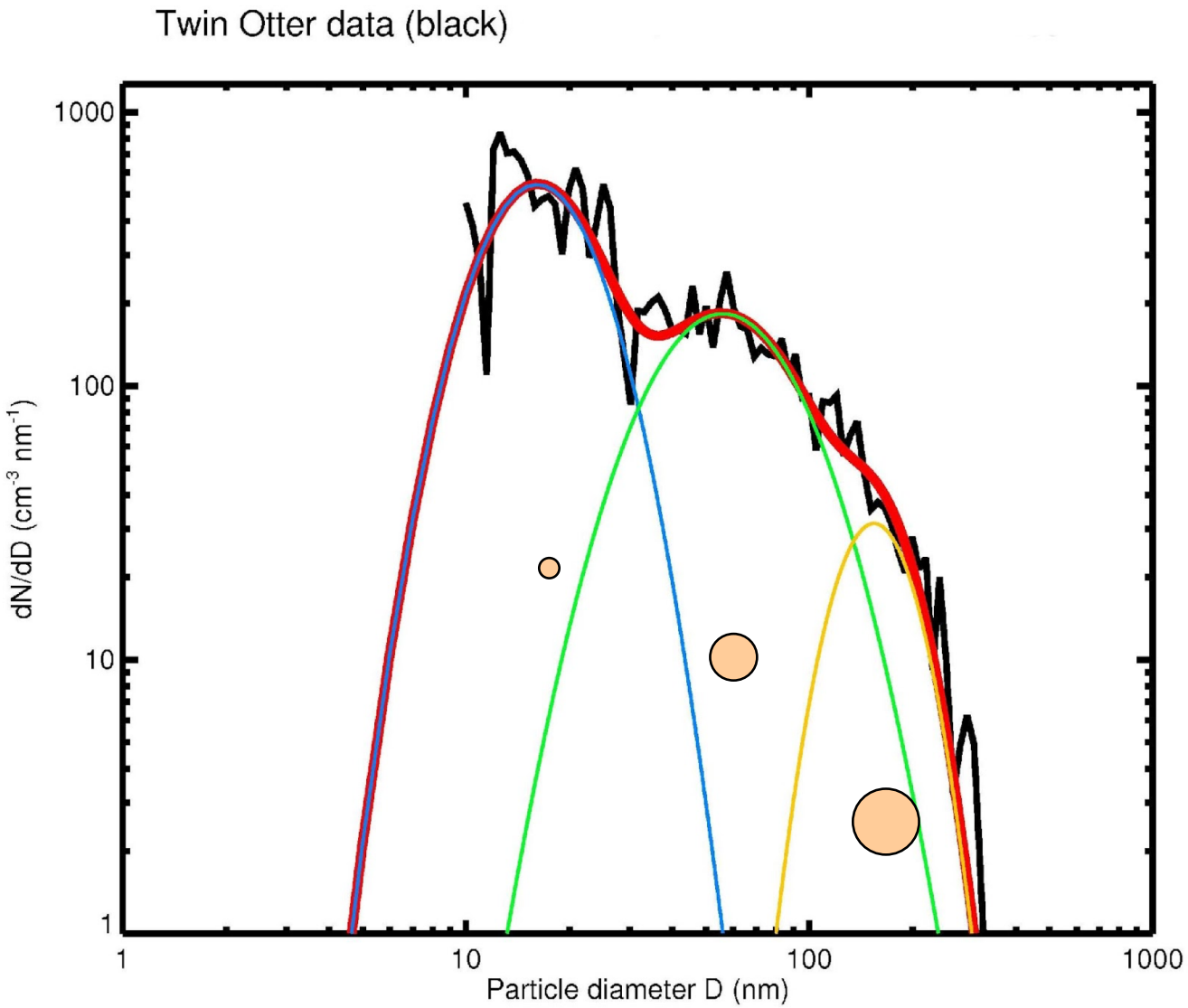


$\frac{dN}{dD}$ → $N = 8195\ cm^{-3}$
$\mu = 18.22\ nm$
$\sigma = 1.42$

$\frac{dN}{dD}$ → $N = 12732\ cm^{-3}$
$\mu = 68.44\ nm$
$\sigma = 1.57$

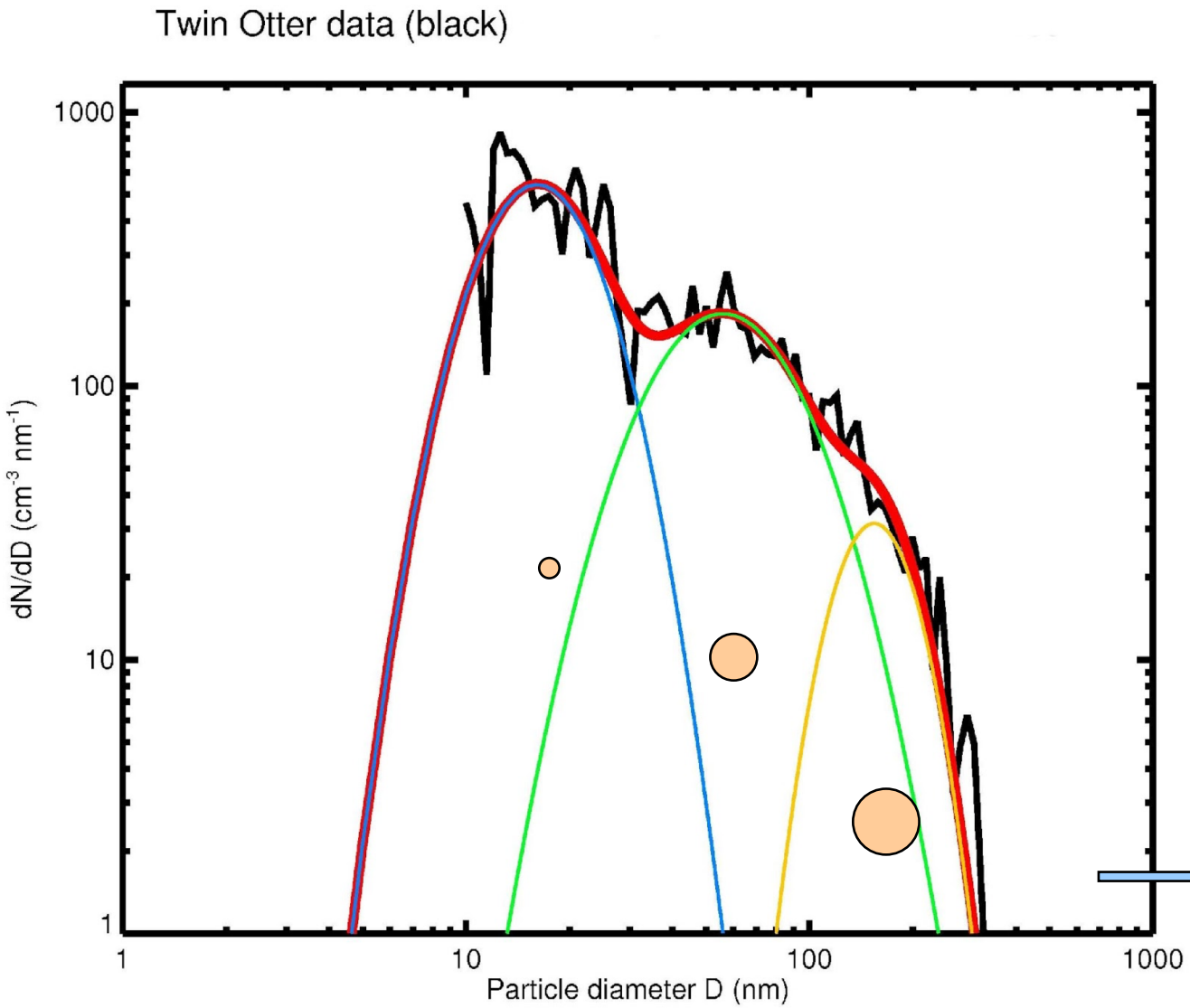
$\frac{dN}{dD}$ → $N = 3140\ cm^{-3}$
$\mu = 164.41\ nm$
$\sigma = 1.28$

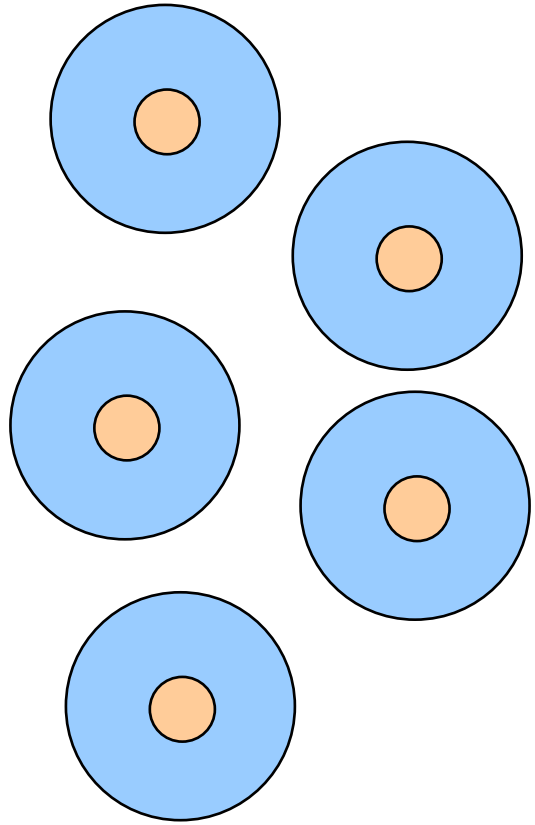
Modal aerosol schemes



$$\frac{dN}{dD} = \frac{dN}{dD} + \frac{dN}{dD} + \frac{dN}{dD}$$

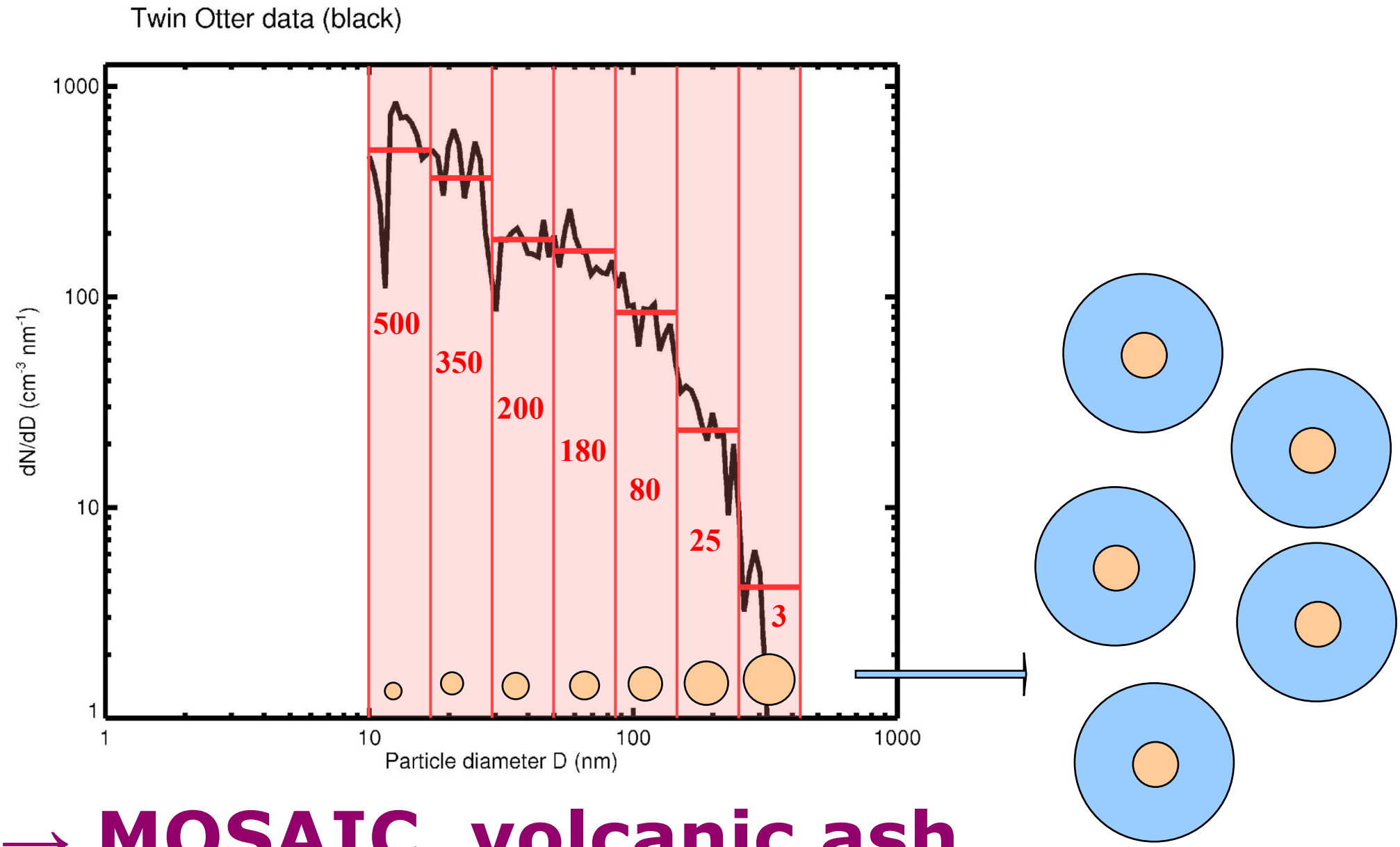
Modal aerosol schemes





→ **MADE and MAM**

Sectional aerosol schemes



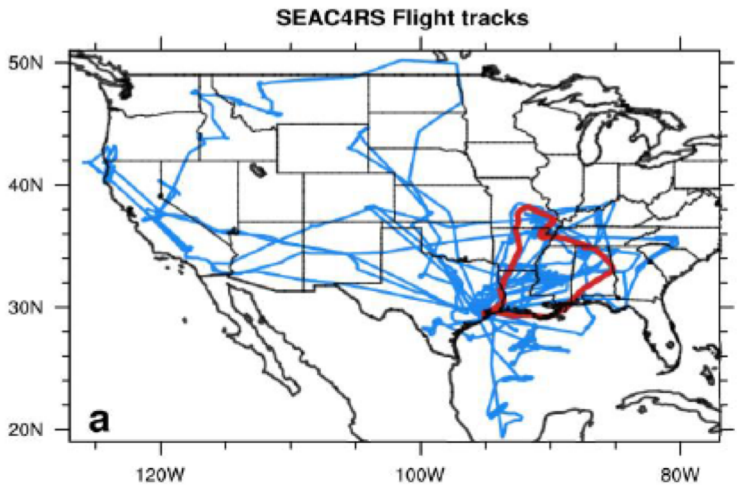
→ **MOSAIC, volcanic ash,**

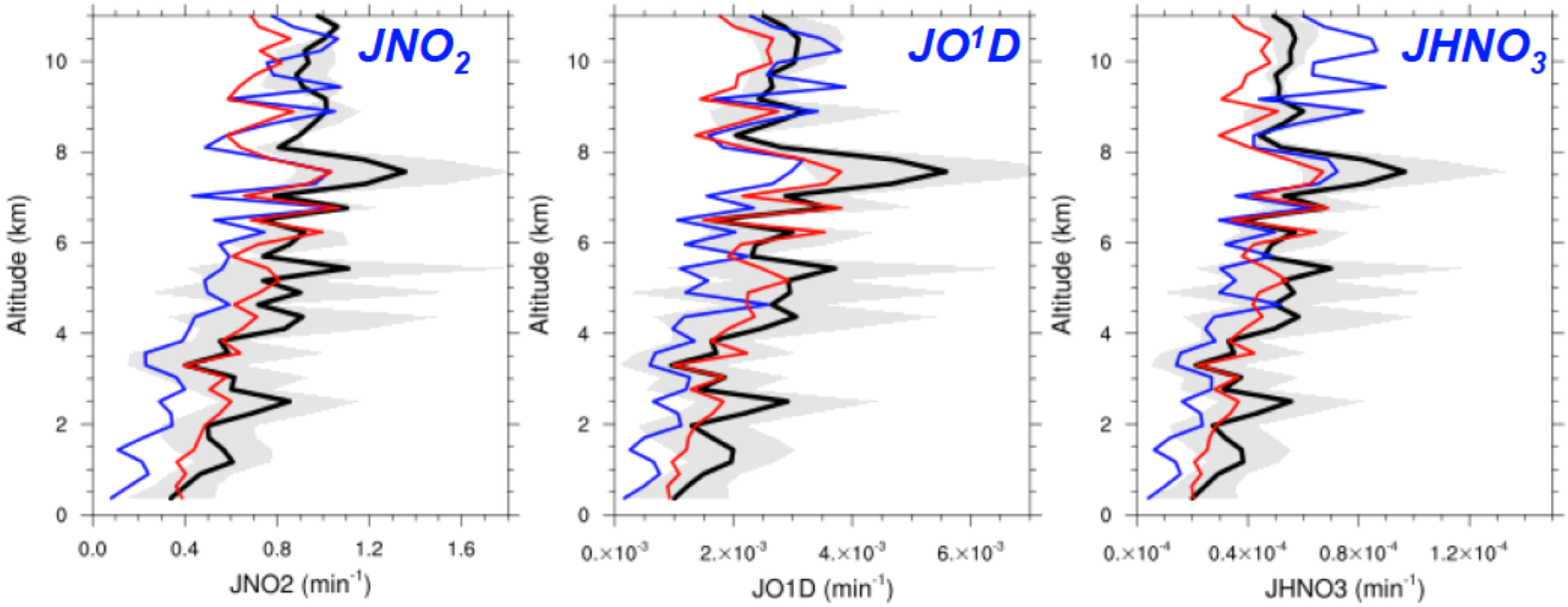
Comparison with the 2013 SEAC^{4}RS flights

OBS SEAC4RS

Old TUV (phot_opt=1)

New TUV (phot_opt=4)





Madronich and Hodzic, WRF-Chem tutorial, 2017

Parameterization of O_3 boundary conditions according to Potential Vorticity (PV)

Courtesy of Stu McKeen (NOAA/ESRL)

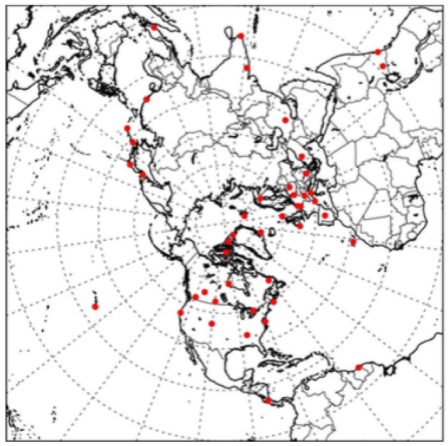
$$PV = \frac{1}{\rho}\left[\nabla\times\vec{v} + Coriolis\right]\cdot\nabla\theta$$

1 PV unit = 10^{-6}·°K·m^2/kg-s

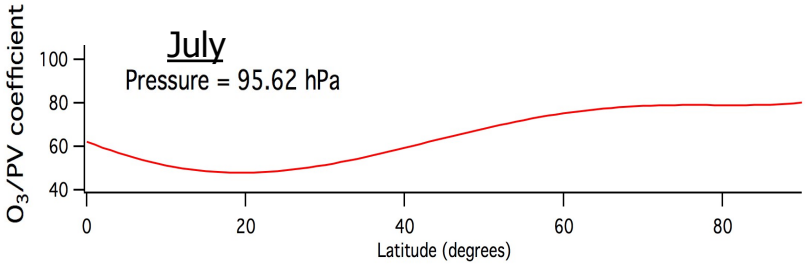
Danielsen (1968): $\boldsymbol{O_3 \propto PV}$ In stratospheric folds and cut-off lows

Literature values: O_3/PV from 35 to 130 ppbv/PVU

Xing et al. (ACP, 2016) – A global climatology of O_3/PV ratios:



- 21 years of data (1990-2010)
- WRF with NCEP reanalysis nudging
- 44 O_3 sonde locations from WOUDC
- Latitude, Month, Pressure dependent



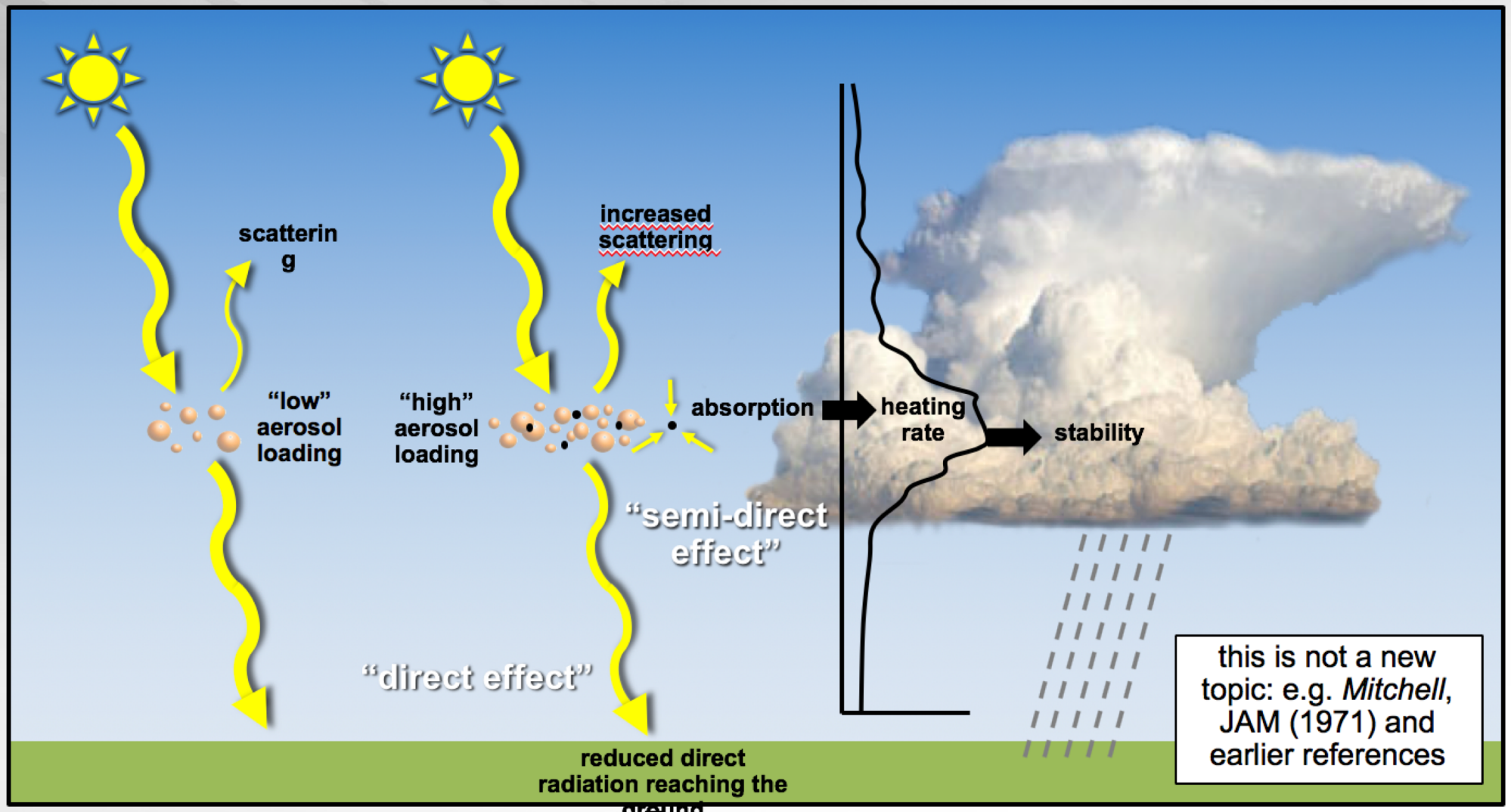
WRF-Chem Stratospheric Tracers:

1) IC/BC O_3 above 500 mb from O_3/PV
2) O_3/PV = 100 – upper limit

J.Fast (PNNL)

Pacific Northwest
NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965

Part 1: Aerosol Direct Effects

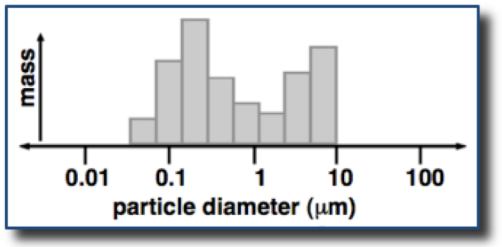


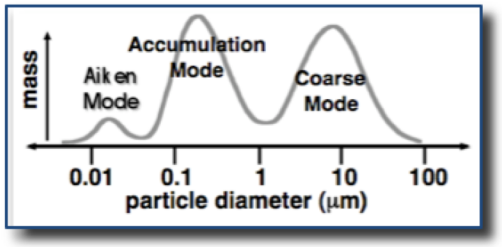
In additions to water vapor, carbon dioxide, ozone, and other trace gases, aerosols can also affect the radiation budget, and atmospheric stability

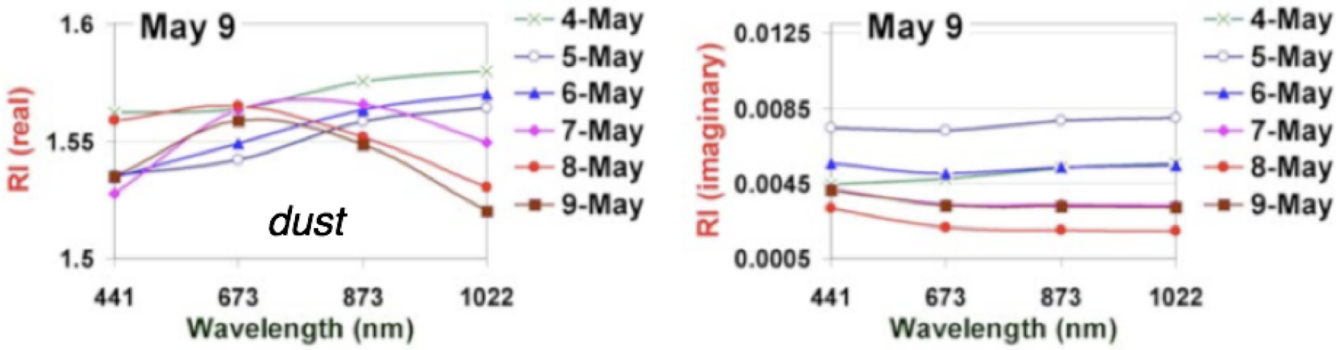
surface heat and latent heat fluxes → boundary layer temperature and moisture → clouds

Assumptions of Optical Property Module

- Interfaces with GOCART, MADE/SORGAM, MAM, and MOSAIC, but linking to other aerosol models should be relatively easy
- **Sectional** (MOSAIC): tested only with 4 and 8 size bins should work if additional size bins are specified
- **Modal** (MADE/SORGAM, MAM): maps the used size modes into 8 sections
- **Bulk** (GOCART): converts bulk mass into assumed distribution, then divides mass into 8 sections
- Note: Refractive indices may need updating
  - Range of values reported in the literature
  - Wavelength dependence of refractive indices for some species





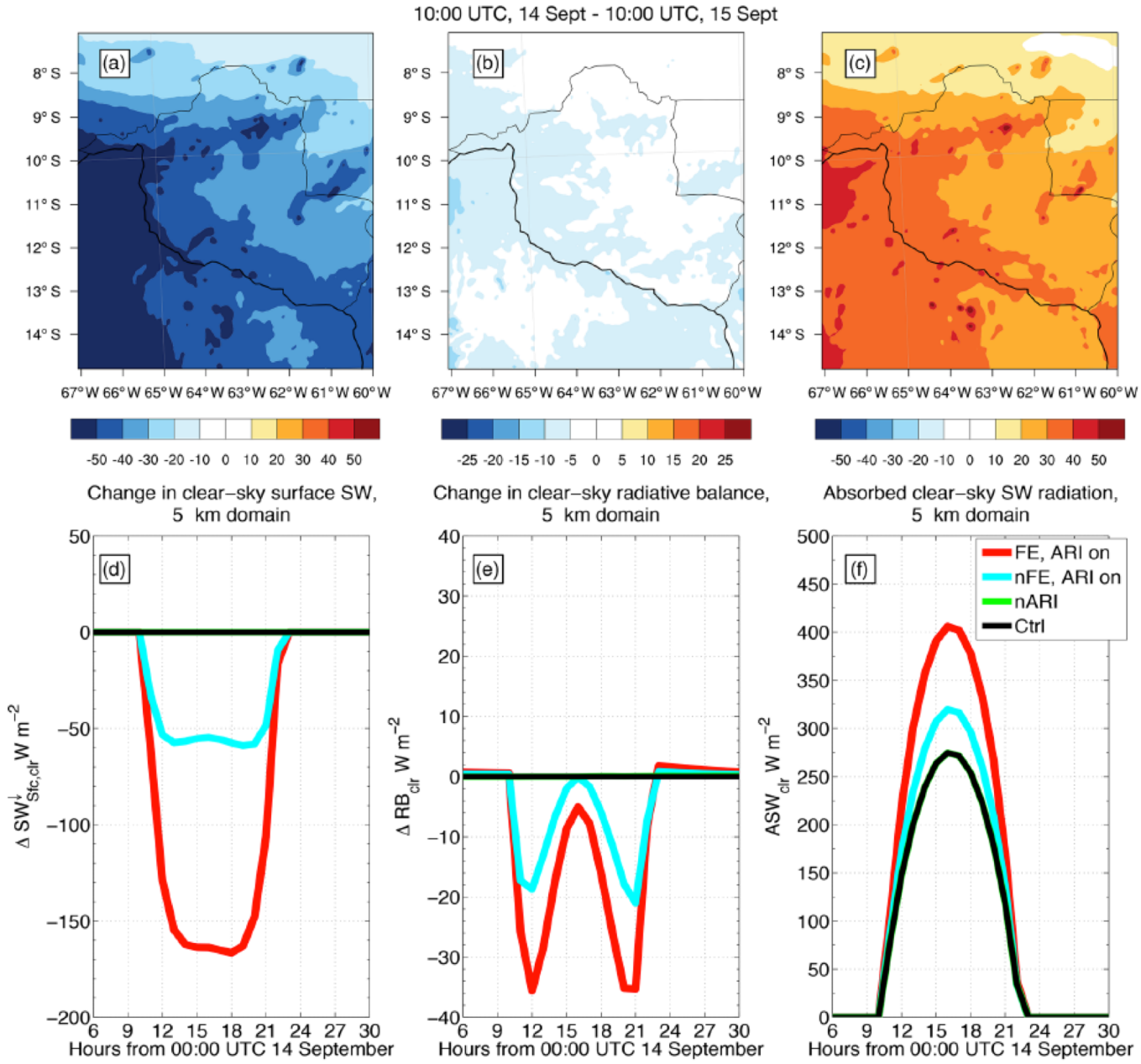


from Prasad and Singh, JGR, 2007

Dust refractive indices for SW constant by default – need to modify code to turn on

J.Fast (PNNL)

Diagnostics option for the aerosol-radiation feedback within the radiation driver of WRF-Chem V4 (*clean_atm_diag* namelist option)

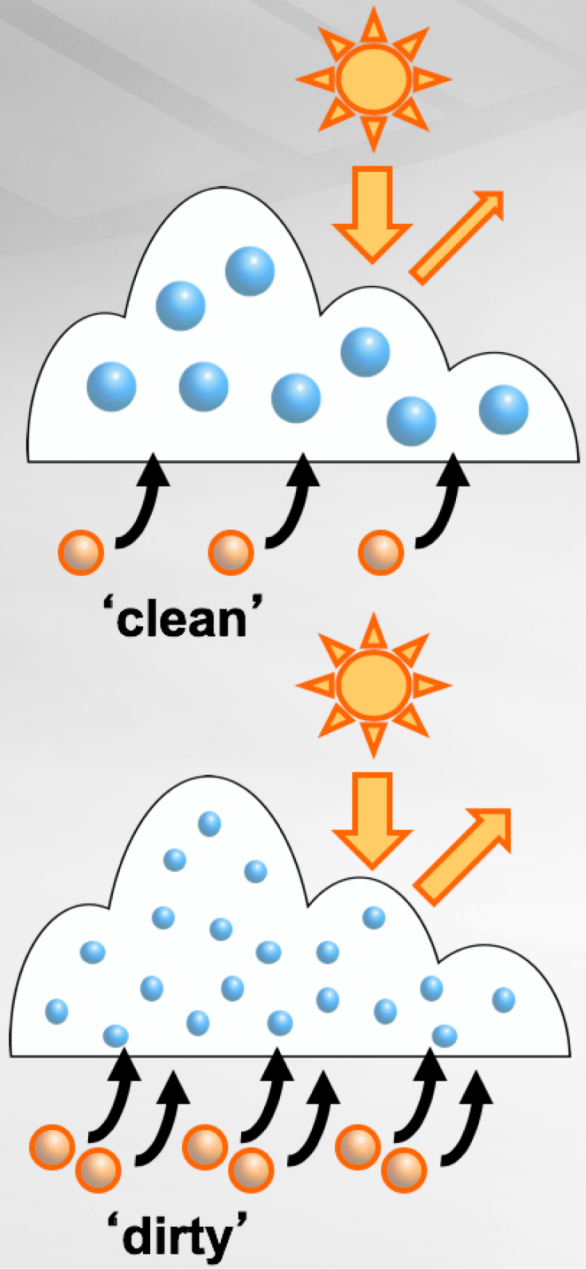


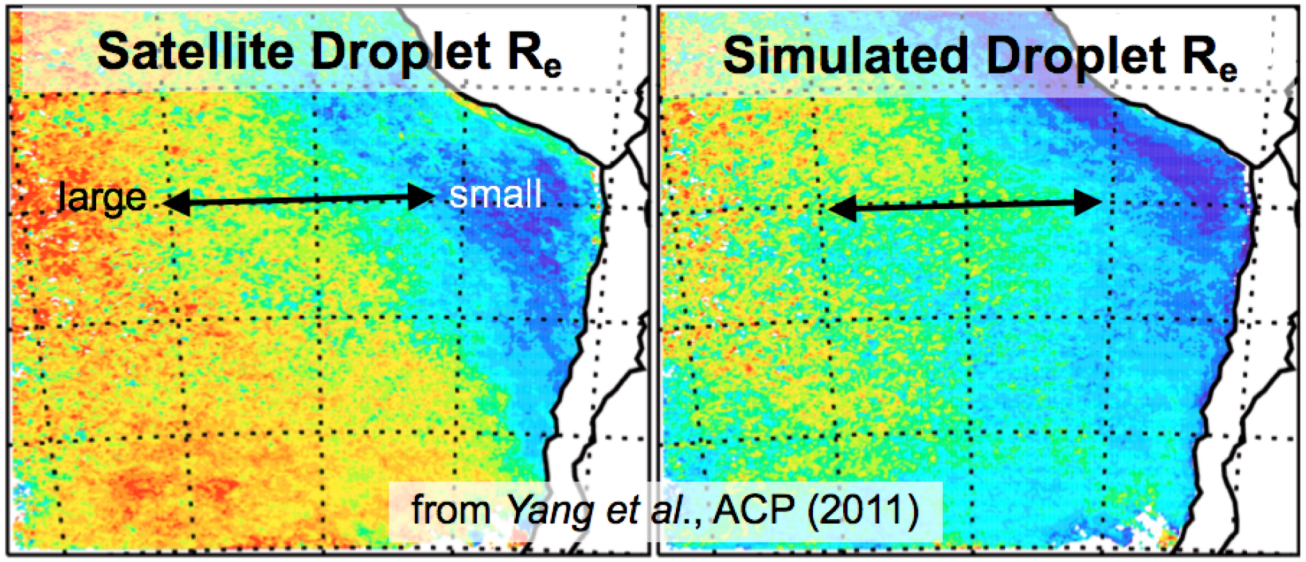
Archer-Nicholls S. et al., ACP, 16, 5573–5594, 2016

J.Fast (PNNL)

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965

Part 2: Aerosol Indirect Effects





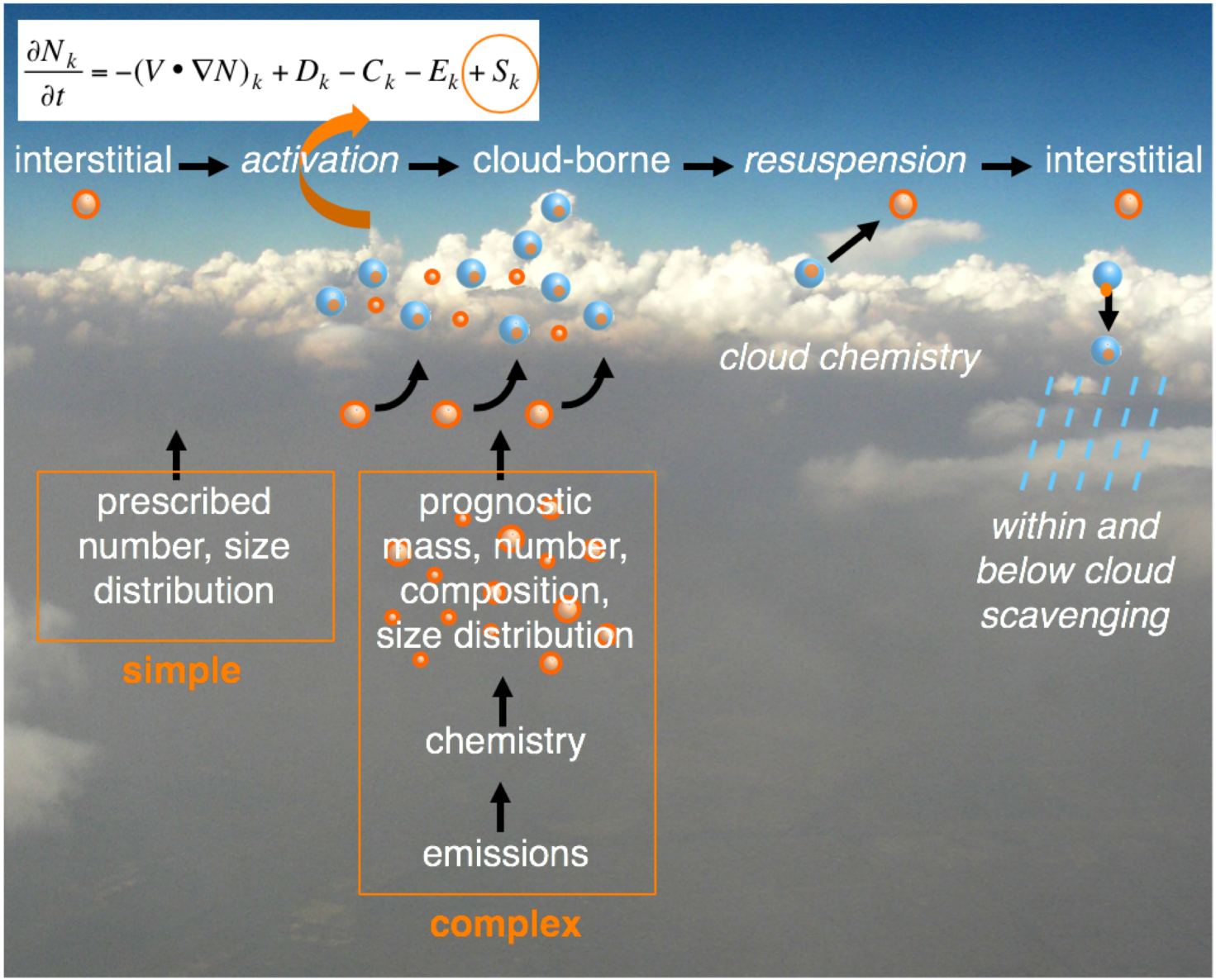
The number of activated aerosols affects the cloud drop size distribution, and consequently cloud albedo and radiation budget

Aerosol-Cloud Interactions in grid-scale clouds

J.Fast (PNNL)

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965

General Description and Assumptions



Simple:

- chem_opt=0
- progn = 1
- naer = specified

Complex:

- chem_opt = 9-12, 32, 34, 35, 41-43, 132, 202, 203, 503, 504, 601, 611
- progn = 1
- naer = ignored

coupled to 2 microphysics schemes: Lin and Morrison

Coupling Aerosols and Parameterized Convection For "Large" Dx

from Jerome Fast (

Cloud-aerosol interactions are a source of uncertainty in climate simulations, but most convective parameterizations lack these processes

New KF-CuP Chemistry package

- cu_opt=10 (KF+CuP), chem_opt=203 (SAPRC+MOSAIC)
- Modified Kain-Fritsch (deep convection) coupled with Cumulus Potential (CuP) (shallow convection) – both cloud types affect radiation

Berg et al., GMD, 2015

- Aerosol activation
- Transport
- Aqueous chemistry
- Wet removal

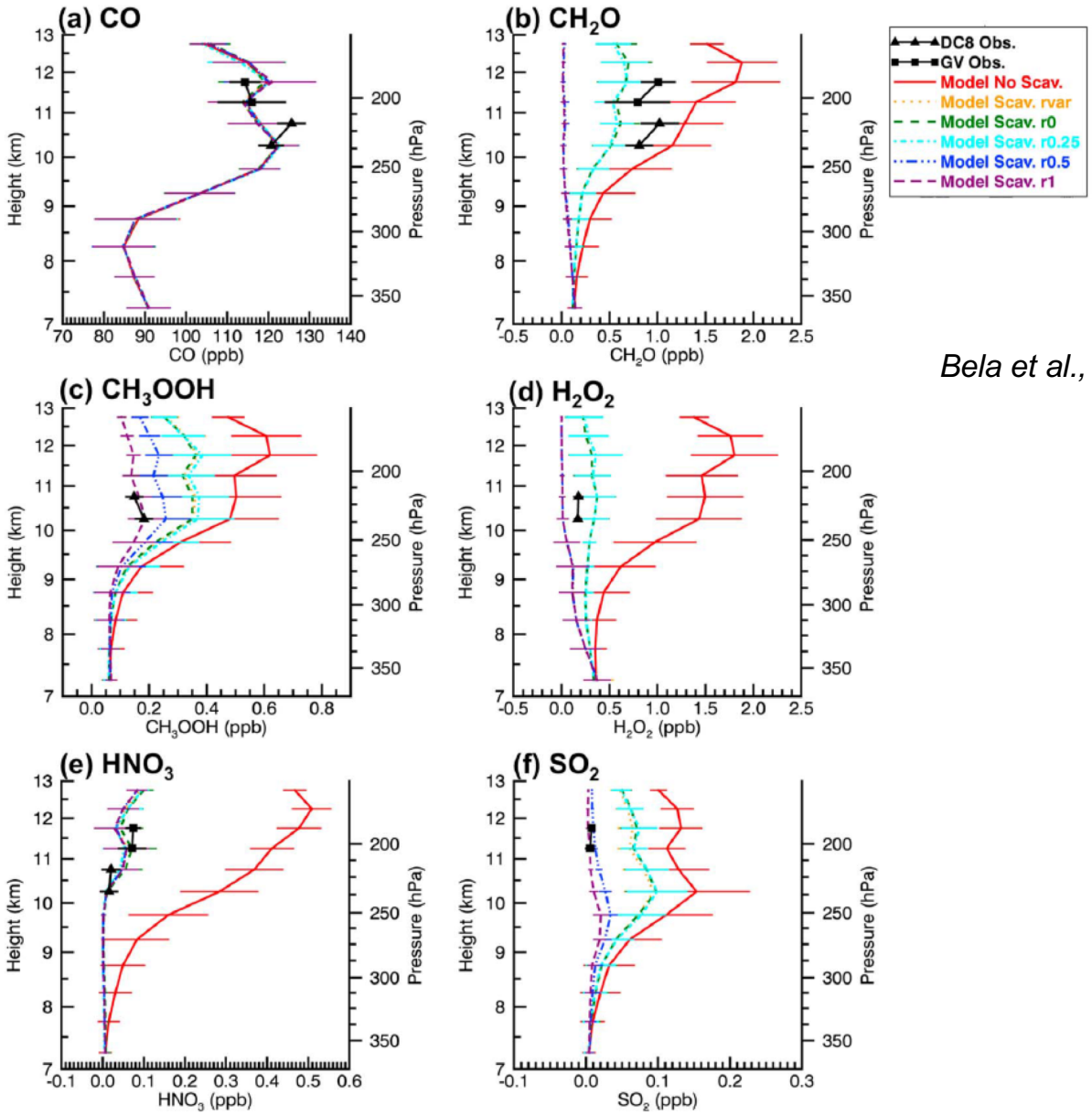
in parameterized clouds

Studies using KF-CuP:
Fast et al., JGR, 2016
Raut et al., ACPD, 2017
Marelle et al., GMDD, 2017
Thomas et al., GRL, 2017

Not Included Yet:

- Feedbacks to radiation, precipitation, etc.

Wet removal for the MOZART based chemistry options in WRF-Chem3.9



Bela et al., JGR, 2016

Figure 4. Mean outflow chemical profiles from the Oklahoma 29–30 May 2012 storm as observed by the DC-8 (black triangles and solid lines) and GV (black squares and solid lines) aircraft and mean profiles within the aircraft outflow sampling latitude-longitude region and vertical extent of anvil cloud as simulated by WRF-Chem without (solid red) and with wet removal (Rvar = dot orange; R0 = dash green; R0.25 = dash-dotted cyan; R0.5 = dash dot dot dot blue; and R1 = long dash purple), for (a) CO, (b) CH_2O, (c) CH_3OOH, (d) H_2O_2, (e) HNO_3, and (f) SO_2. The error bars indicate one

WRF-Chem Developments by PNNL (Not in Public Version) Fast J. et al.

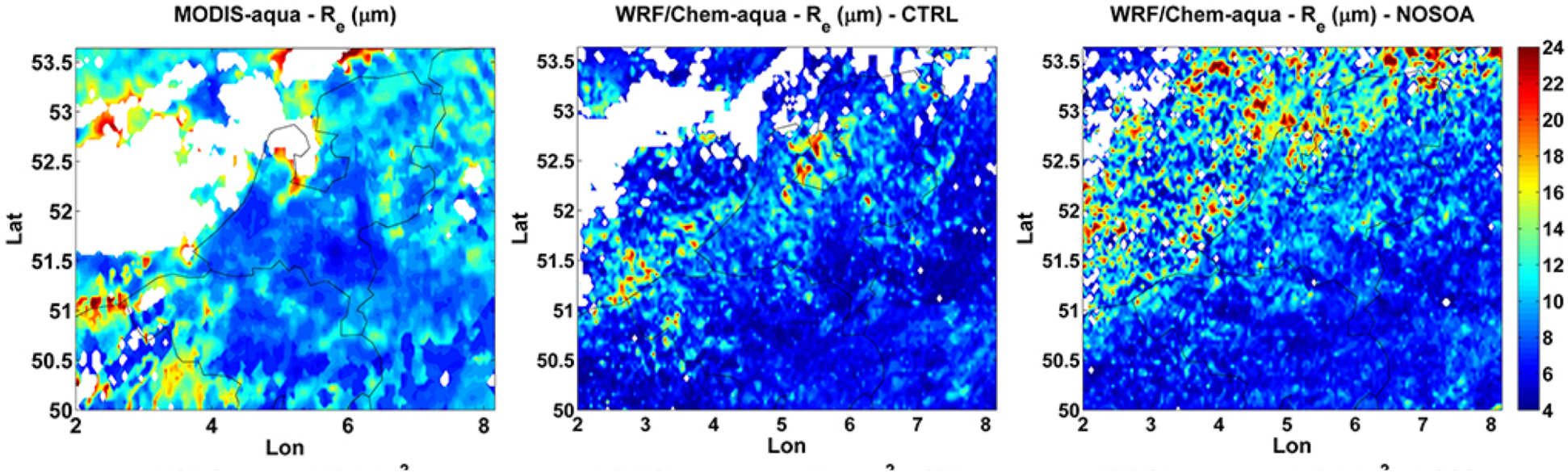
Not currently planned for upcoming releases:

- **Secondary Activation:** Permitting activation above cloud base, shown to be significant for deep convection (Yang et al. JGR 2015)
- **Ice-Borne Aerosols** (Yang et al., JGR 2015)
- **Explicit Nucleation and Ultrafine Particles:** 20-size bin version of MOSAIC, 1 nm – 10 μm (Lupascu et al., ACP 2015)
- **Secondary Organic Aerosol:** Isoprene epoxydiol (IEPOX) and other explicit biogenic chemistry (Shrivastava et al., in preparation)
- **Cloud-Aerosol Interactions with Spectral Bin Microphysics:** Coupling of MOSAIC aerosol model with spectral bin microphysics for cloud-resolving scales (Gao et al. JAMES, 2016)

(available upon request)

Simulating aerosol-meteorology feedback by using the modal aeosol scheme in WRF-Chem

- The chemistry option (#109, since V3.8) with secondary organic aerosol parameterization based on the volatility basis set approach, with direct and indirect cloud feedback, evaluated in Europe with data from a field campaign (*Tuccella et al., GMD, 2015*)



The 17–19 May 2008 averages of droplet effective radius at cloud top (first row), retrieved using MODIS-aqua observations (first column), predicted by model in the references run (CTRL, second columns) and sensitivity test without SOA (NOSOA, third column).

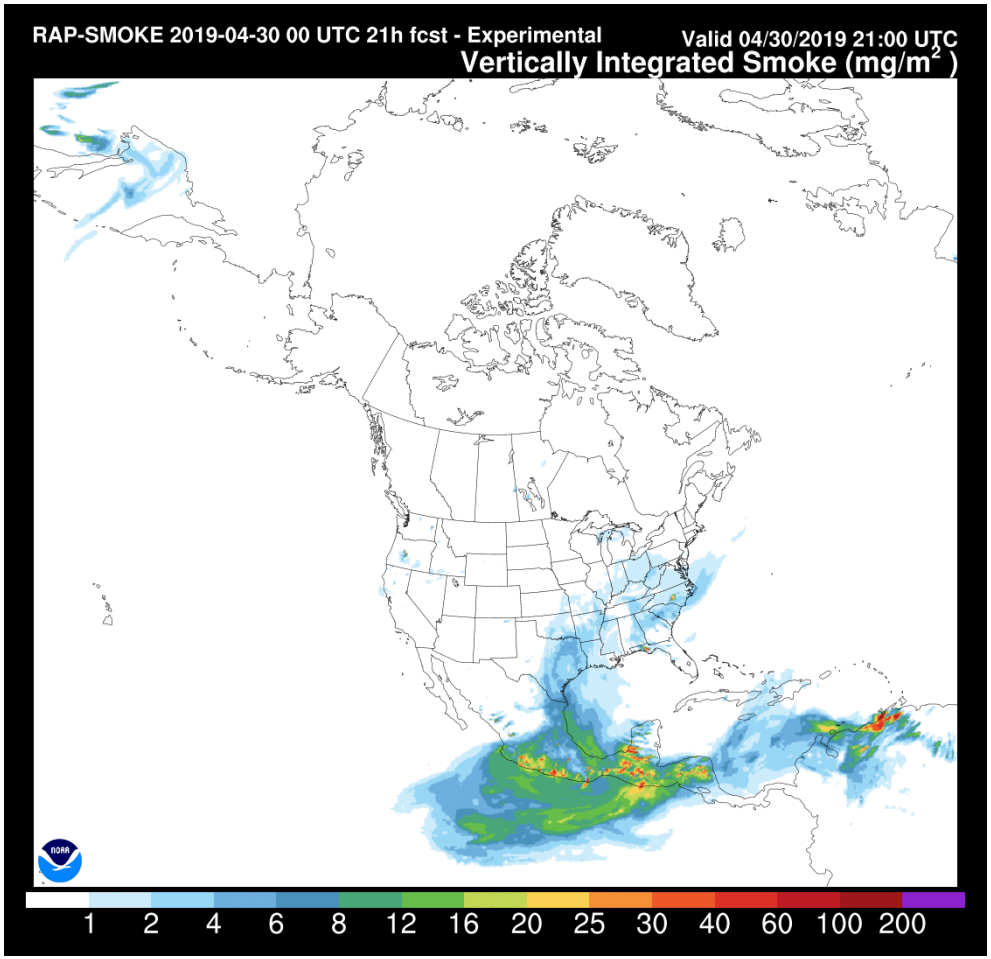
Updates in the WRF-Chem model in recent years

- Potential Vorticity based stratospheric ozone calculation (NOAA/ESRL)
- An updated version of the Model for Simulating Aerosol Interactions and Chemistry scheme (MOSAIC II) (PNNL)
- An updated gas phase chemistry scheme Model for Ozone and Related Tracers (MOZART) version T1 from (NCAR/ACOM)
- A new heterogeneous gas chemistry (based on the Regional Atmospheric Chemistry Mechanism) option coupled with the ISORROPIA II aerosol thermodynamic model (Hong Kong Polytechnic University)
- A Henry's Law Constant table to use the same constants across different chemistry parameterizations, e.g. dry/wet deposition schemes (NCAR)
- An integrated reaction rate diagnostics option (NCAR)
- Diagnostics for WRF-Chem aerosol-radiation feedback in the radiation driver (Universities of Cambridge and Manchester)
- A number of minor bug fixes and enhancements;

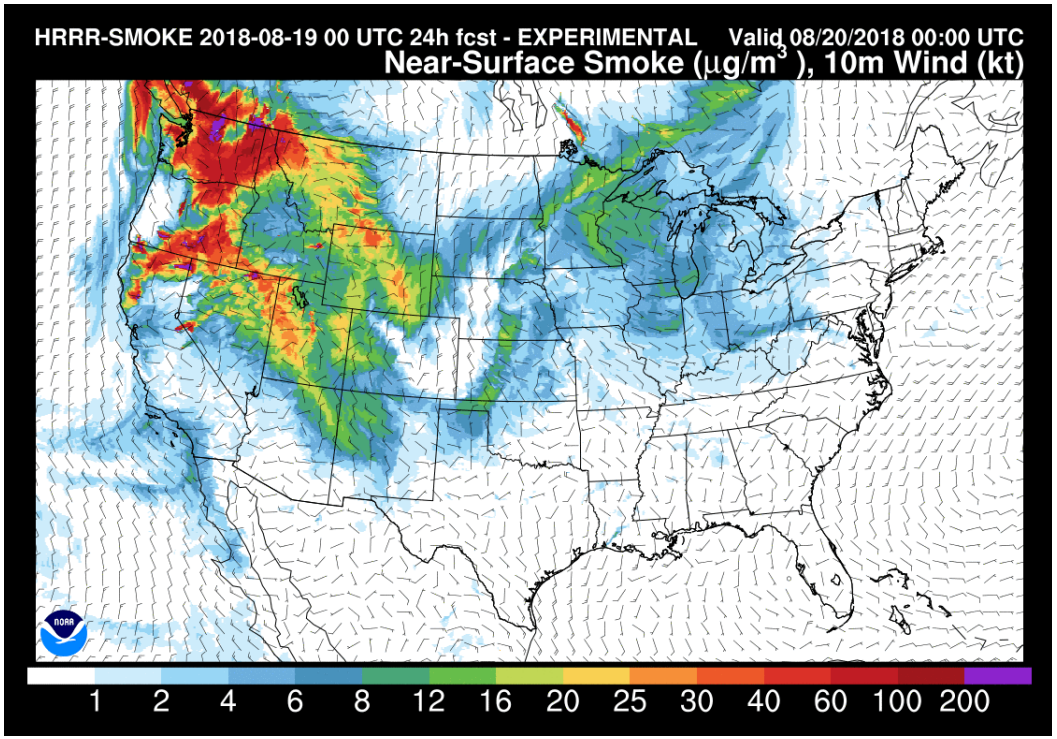
WRF-Chem applications

some examples

Smoke forecasting using Rapid Refresh and High Resolution Rapid Refresh models (based on WRF-Chem)



RAP-Smoke (13.5 km resolution)



HRRR-Smoke (3 km resolution)

https://rapidrefresh.noaa.gov/RAPsmoke/
https://rapidrefresh.noaa.gov/hrrr/HRRRsmoke/

Dust modeling for Middle East by WRF-Chem

JGR Atmospheres

RESEARCH ARTICLE
10.1029/2019JD030248

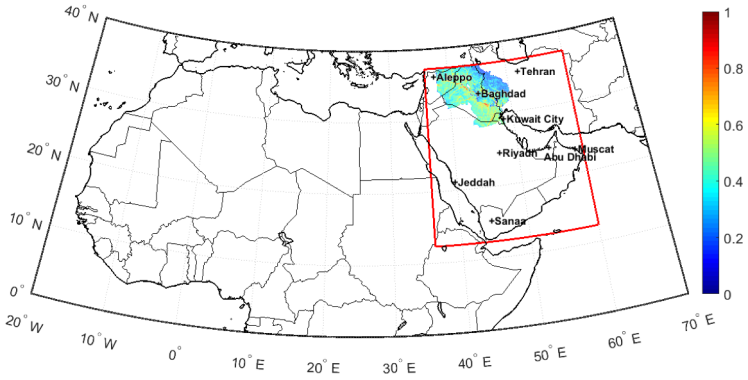
Key Points:

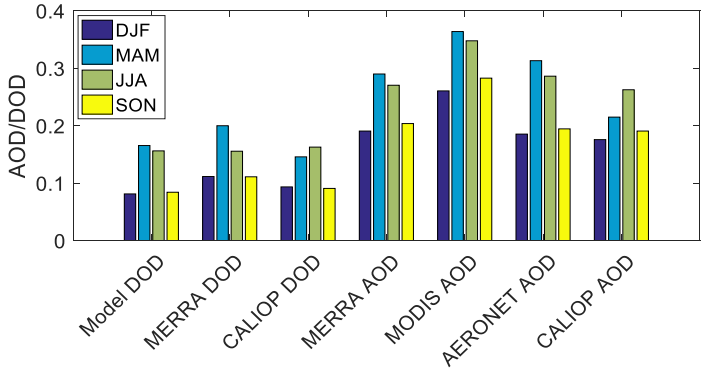
- A new high-resolution dust source function is used in WRF-Chem to simulate dust emissions over Middle East and North Africa (MENA)
- Contribution of Tigris-Euphrates dust sources on total dust distribution over the Arabian Peninsula is quantified

Dust Emission Modeling Using a New High-Resolution Dust Source Function in WRF-Chem With Implications for Air Quality

Sagar P. Parajuli[1], Georgiy L. Stenchikov[1], Alexander Ukhov[1], and Hyunglok Kim[2]

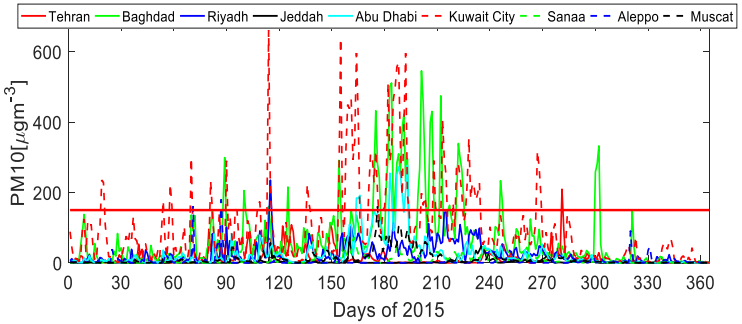
[1]Division of Physical Sciences and Engineering, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia, [2]Department of Engineering Systems and Environment, University of South Virginia, Charlottesville, VA, USA





- WRF-Chem simulated DOD is consistent with several other datasets.
- Atmospheric dust originating from the Tigris-Euphrates basin alone exceeds the PM10 standards in several downwind cities.

- Application of WRF-Chem in air quality modeling.
- A high-resolution (~500m) dust source function is used to simulate dust emission and transport from Tigris-Euphrates region across the Arabian Peninsula.
- ECMWF operational analysis (~15km) used as boundary conditions.



https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2019JD030248

Applications

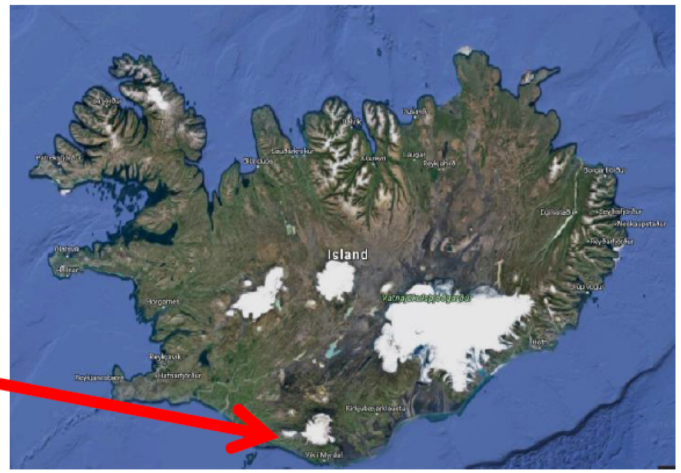
WRF-Chem

Marcus Hirtl

Volcanic eruptions

On 14 April 2010 the character of the eruption at the Eyjafjallajökull volcano changed from basaltic lava fountaining to explosive emissions of high levels of ash. According to Gudmundsson et al (2012) the eruption could be divided in 3 phases. An explosive period from 14th to 18th April 2010 followed by a low discharge effusive period from 18th of April until 4th of May and then a second explosive period from 5th to 17th of May.

Impacts:
Air traffic was closed for many days
Air Quality where plume hit ground
Meteorology

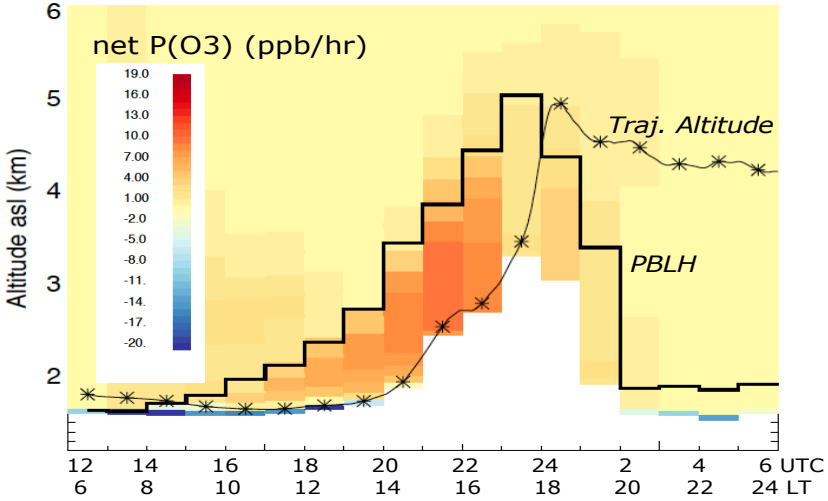


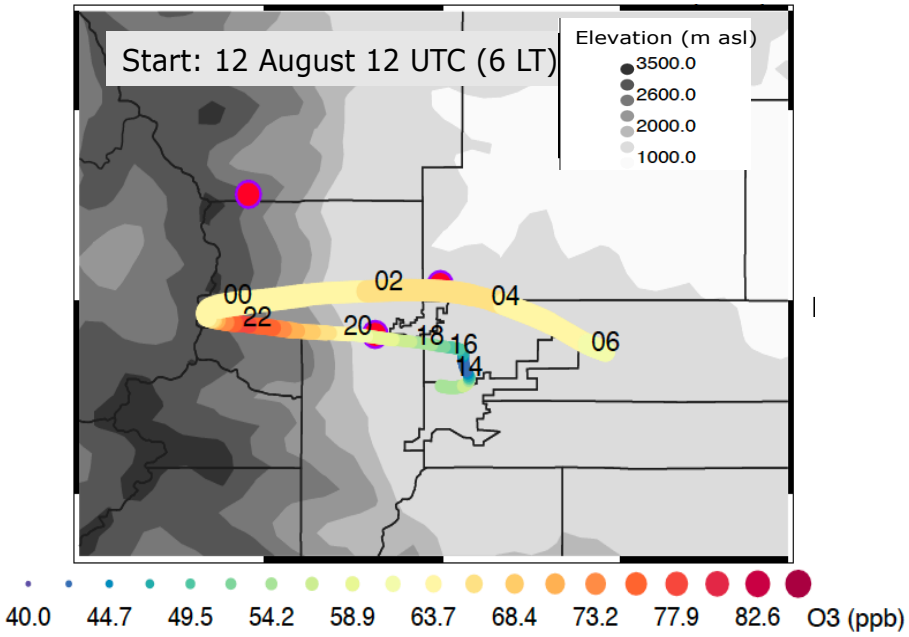
ZAMG
Zentralanstalt für Meteorologie und Geodynamik

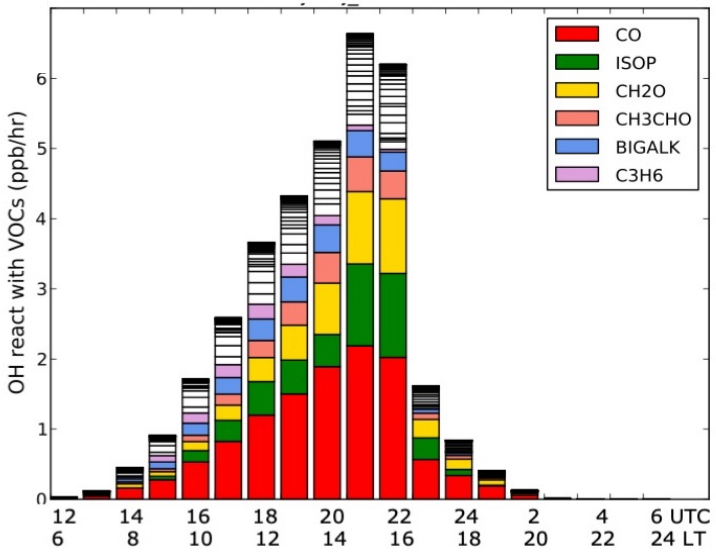
New diagnostic schemes/options in WRF-Chem (NCAR/ACOM)

Using WRF-Chem to study the role of different VOCs in Ozone Production

- **Integrated Reaction Rate Analysis (IRR)**: 3D output of individual gas phase reaction rates
- **Chemical Tendencies**: difference in concentrations before and after certain processes are called in model
- **Online Trajectories**: Model output along online forward trajectories released at user defined location and time



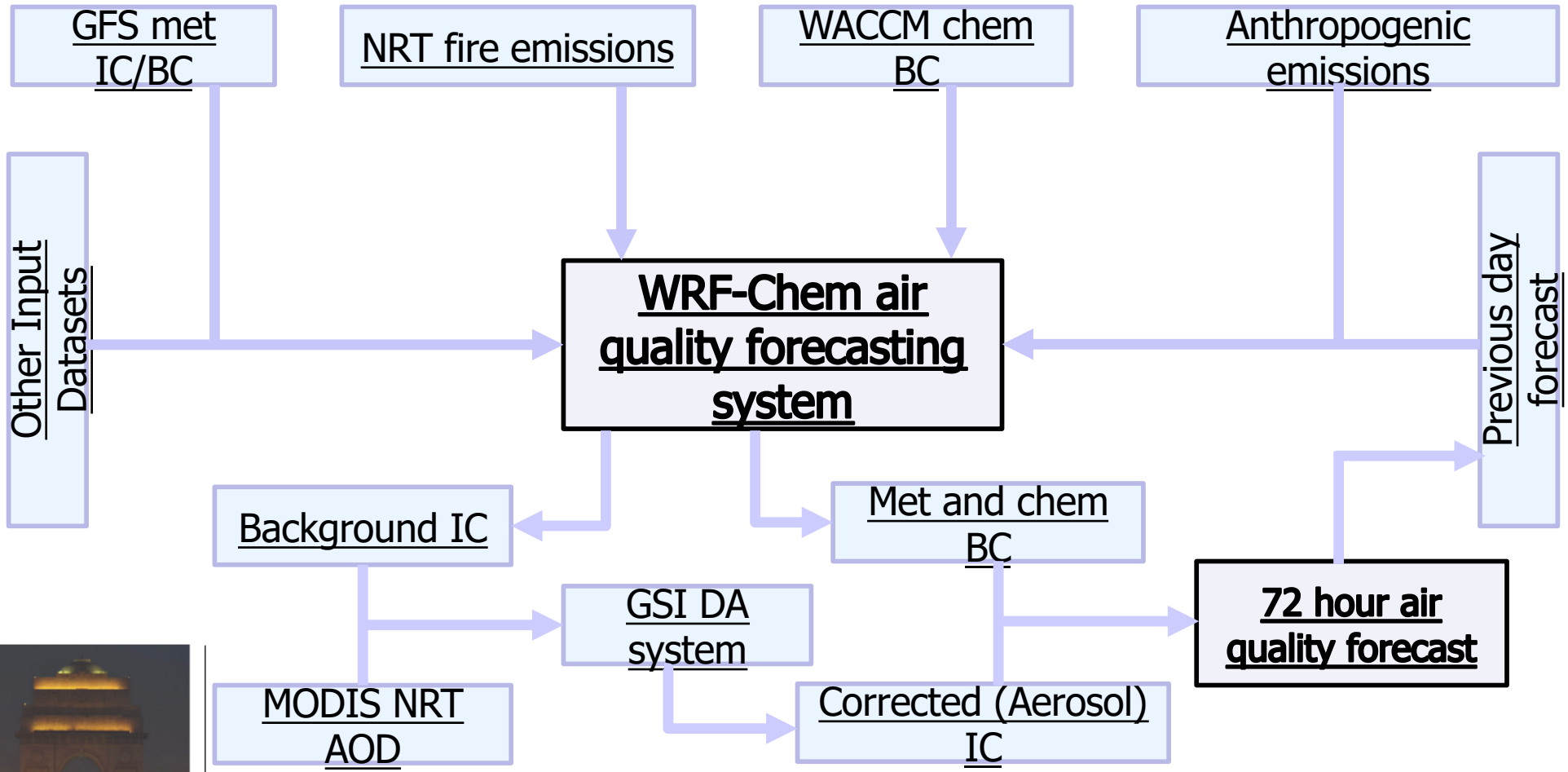


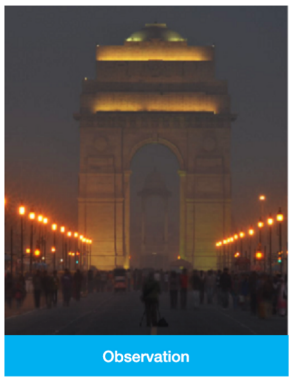


Pfister et al., Chemical Characteristics and Ozone Production in the Colorado Front Range, 2019

Fully coupled meteorology-chemistry forecasting system based on WRF-Chem

Delhi Air Quality Forecasting System

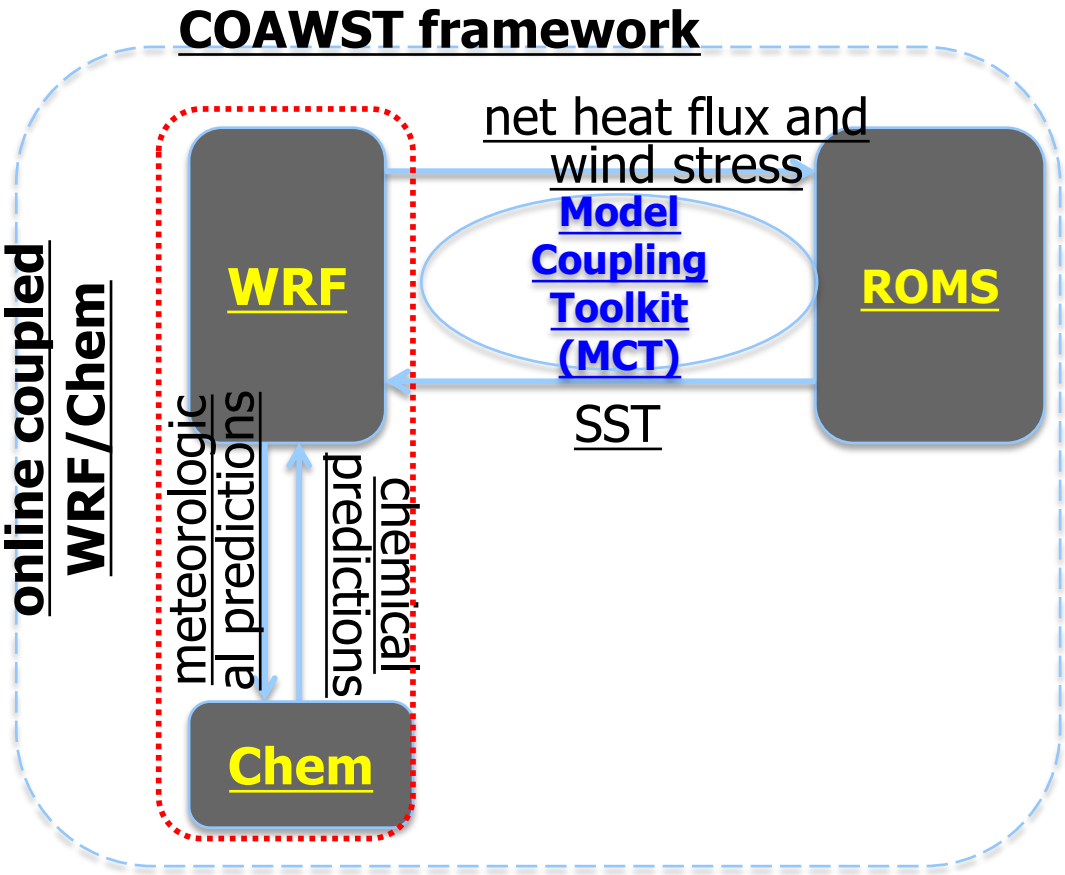




https://ews.tropmet.res.in/)

Kumar et al. (NCAR)

WRF-Chem coupling with the ocean model (ROMS) (He et al., 2018)

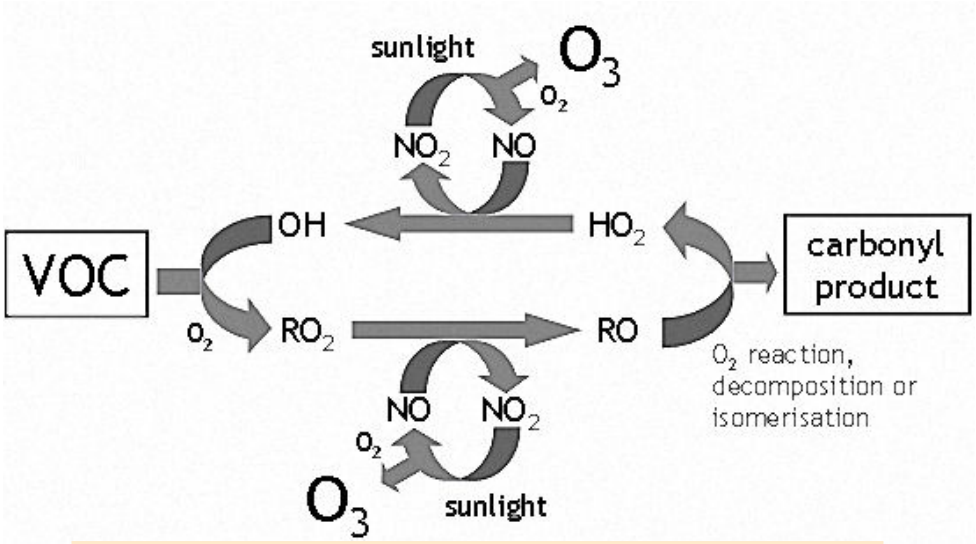


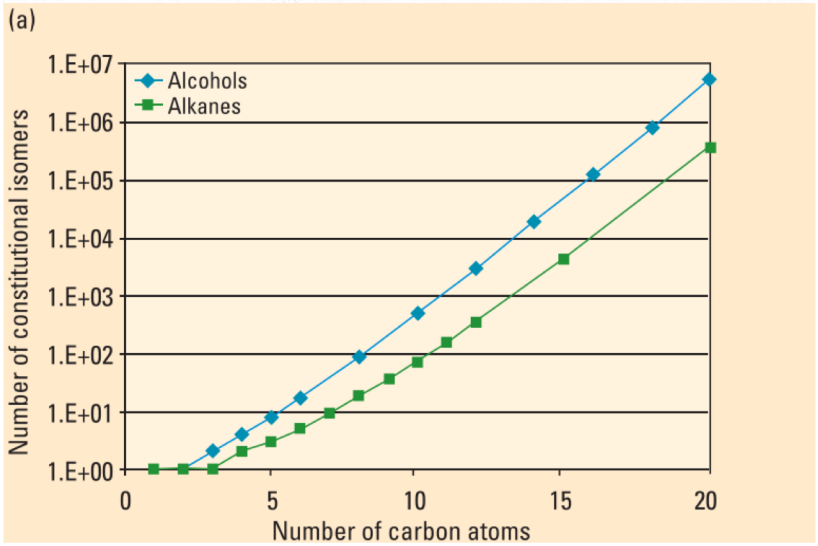
Coupled-Ocean-Atmosphere-Wave-Sediment Transport Modeling System (COAWST) (Warner et al., 2010) developed by US Woods Hole Coastal and Marine Science Center

Regional Ocean Model System (ROMS) v3.7 (as of COAWST v3.1) (Shchepetkin et al., 2005)

Ozone chemistry schemes in WRF-Chem

- VOC and NOx photochemistry drives Ozone formation (and other processes) in troposphere.
- Many 1000's of VOCs identified in the atmosphere.
- Near-explicit schemes too complex e.g. Master Chemical Mechanism, MCMv3.1: 4361 species, 12,775 reactions.
- Need to parameterise tropospheric chemistry in 3D models. But how can we be confident the necessary simplifications preserve key processes?





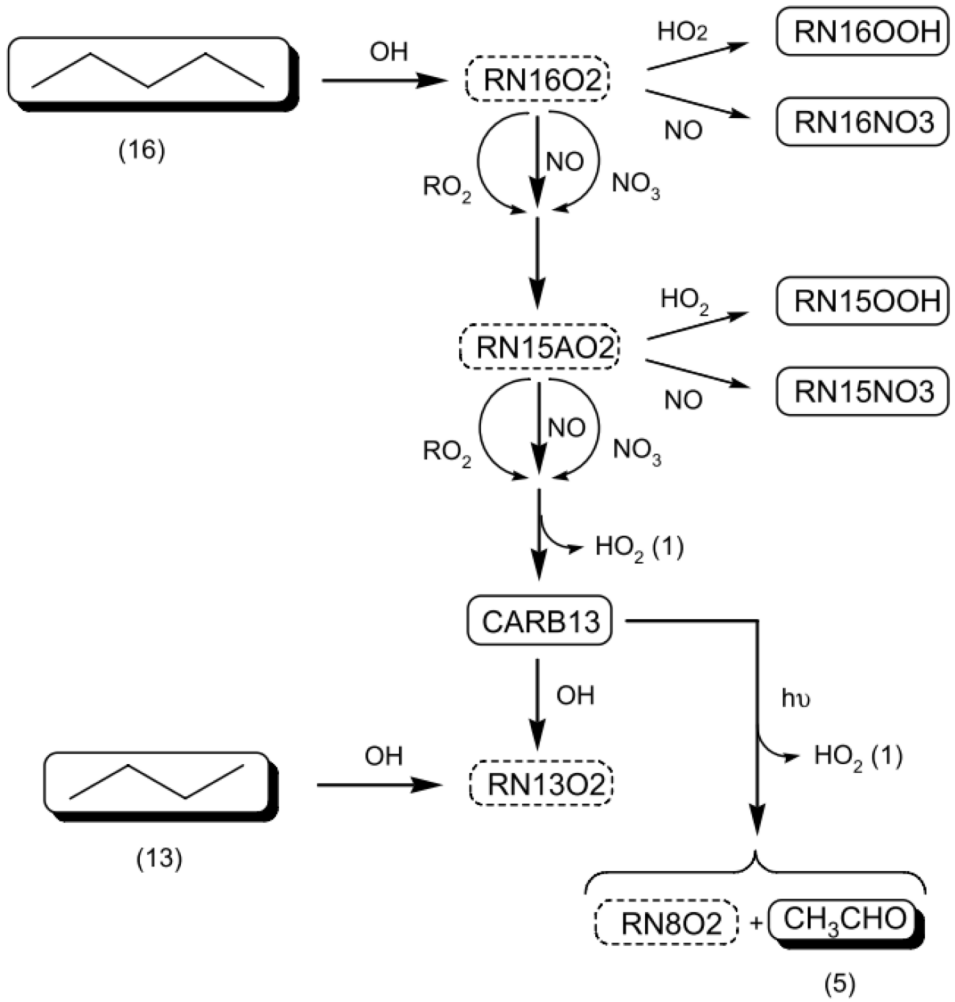
Goldstein et al., 2007

Website: http://mcm.leeds.ac.uk/MCM/

Bloss, C., et al (2005). *ACP*, *doi:* 10.5194/acp-5-641-2005

Common Representative Intermediates (CRI) Mechanism

the most complex gas chemistry scheme in WRF-Chem



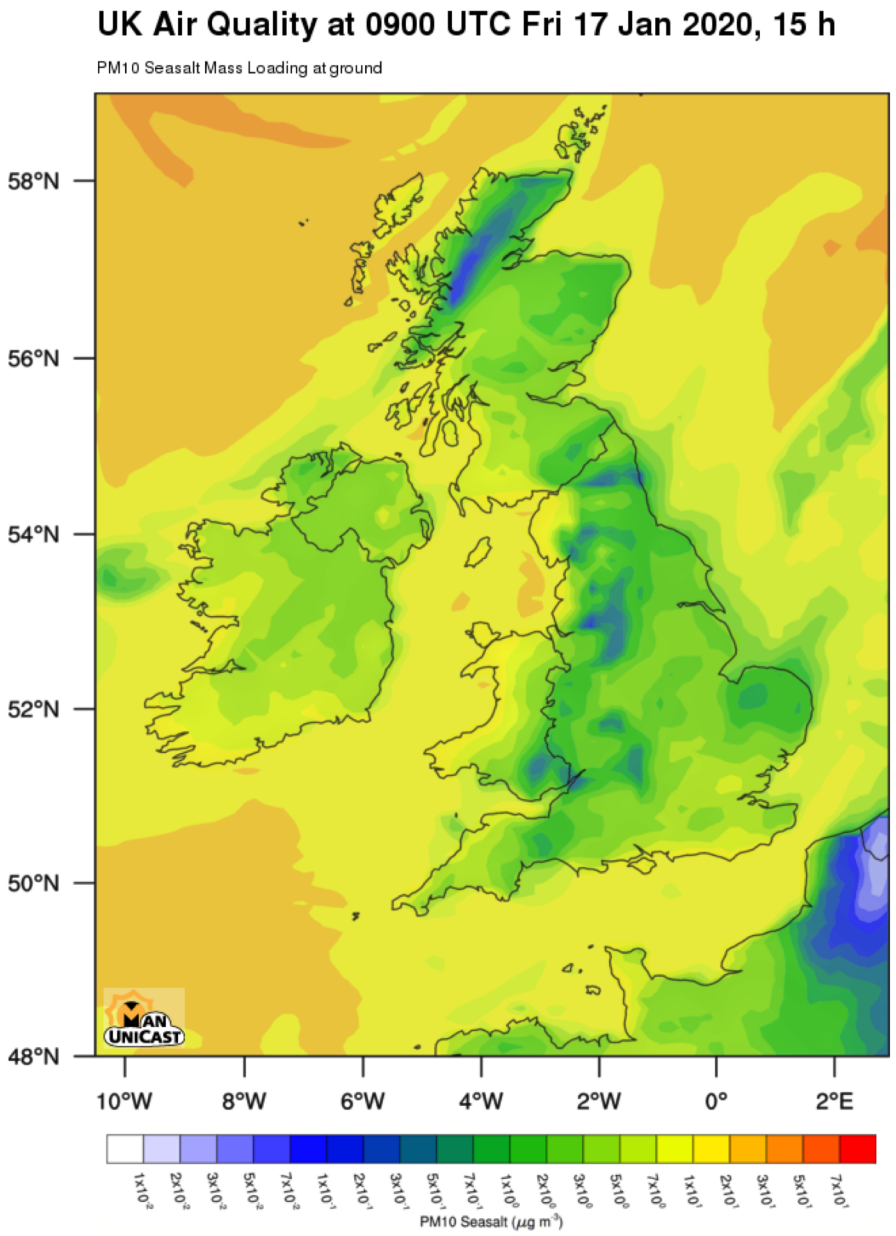
- "Intermediate complexity" scheme, conserving ozone forming potential from MCM v3.1.
- Oxidation products lumped based on 'CRI index': number of C-C and C-H bonds in each molecule.
  - CRIv2 = 434 species, 1183 reactions; (Jenkin et al., 2008).
- Further reductions in complexity achieved by lumping emitted VOCs (Watson et al., 2008):
  - CRIv2-R5 in WRF-Chem:

    196 species, 555 reactions.

Website: http://mcm.leeds.ac.uk/CRI/

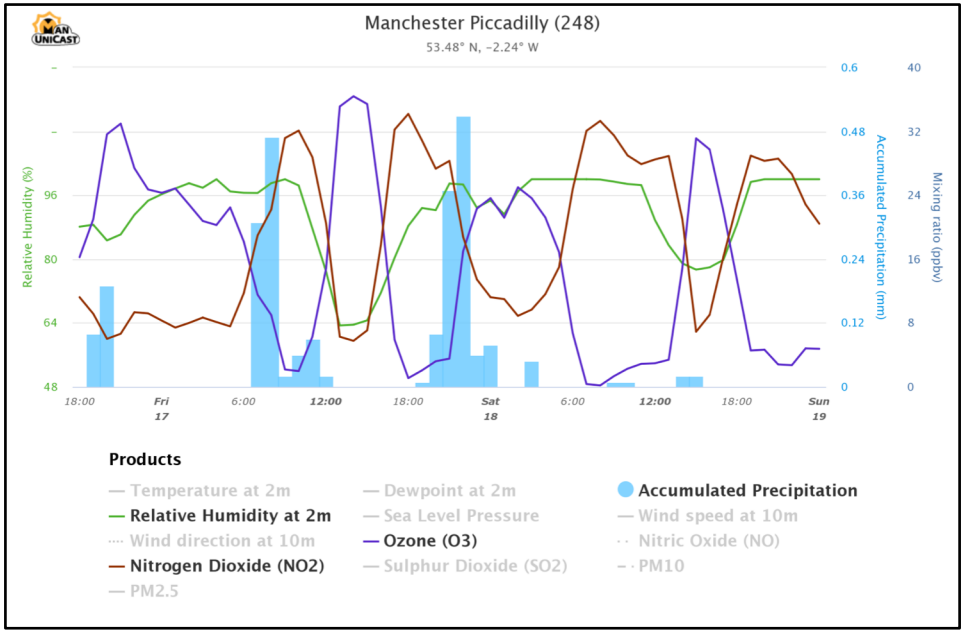
Bloss, C., et al (2005). *ACP*, *doi:* 10.5194/acp-5-641-2005

Air Quality Forecasting for UK: ManUniCast

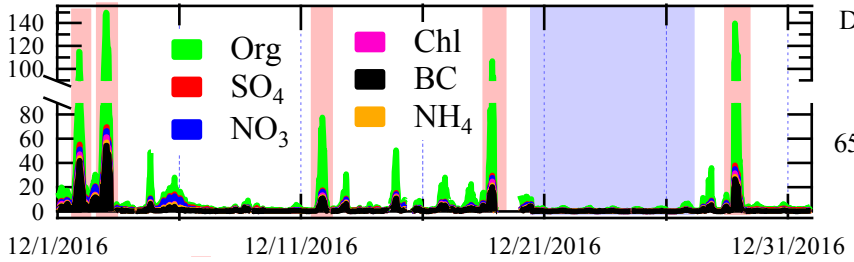


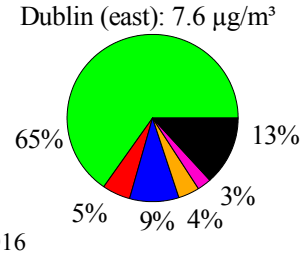
http://manunicast.seaes.manchester.ac.uk

- Meteorology & AQ teaching tool
  - Daily forecasts
  - CRIv2-R5 & 8-bin MOSAIC
  - 12 x 12 km resolution
  - Maps & Meteograms
  - Chemical Outputs:
  - 13 gas-phase components
  - Speciated PM10, PM2.5, PM1 aerosol

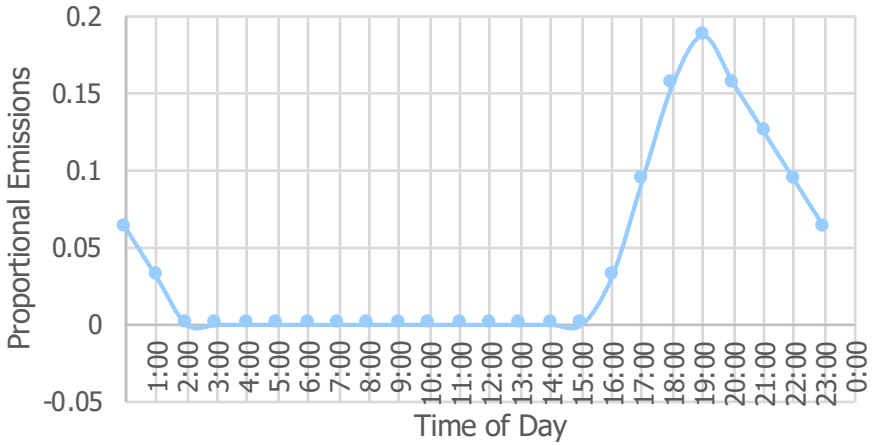


Dublin Pollution Events: Solid Fuel





Emission Profile

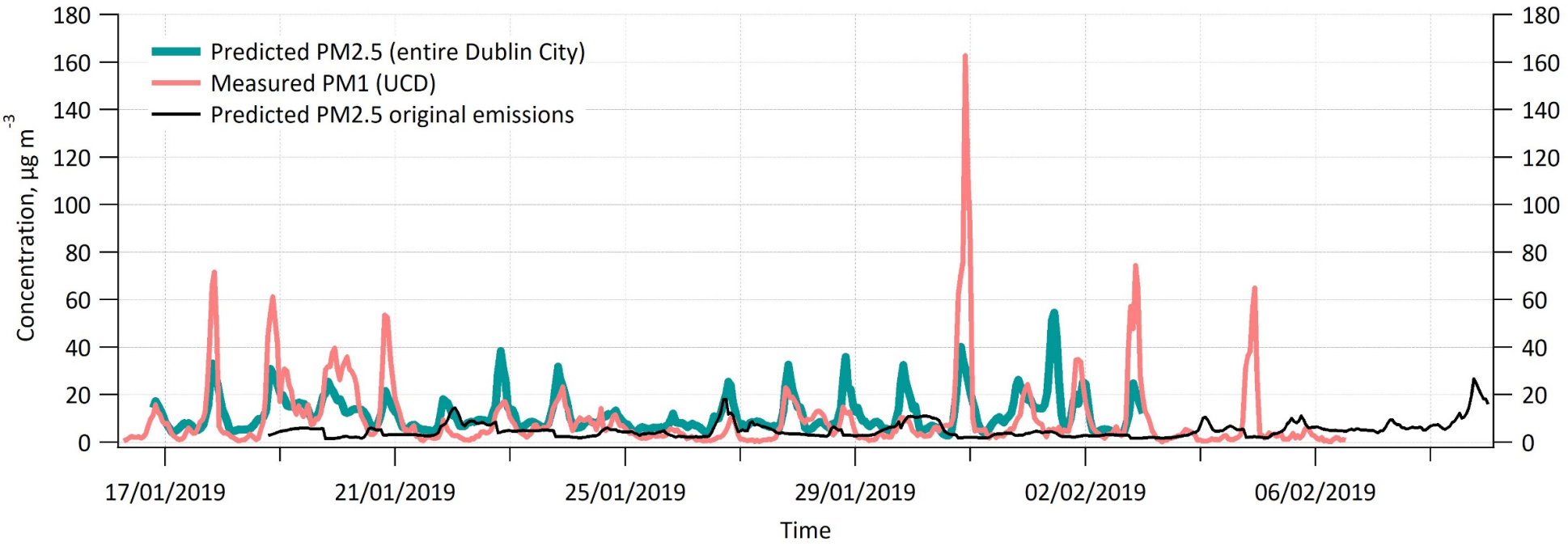


Emission Factors (kg PM2.5/TJ) & Calorific Values (MJ/kg) => PM released per kg fuel consumed

Houses/m^2 (CSO) => PM released/m^2

Assume houses burn 10kg fuel per night. Temperature dependent enhancement factor

Adjustment of the anthropogenic emissions for Dublin by WRF-Chem according to air temperature

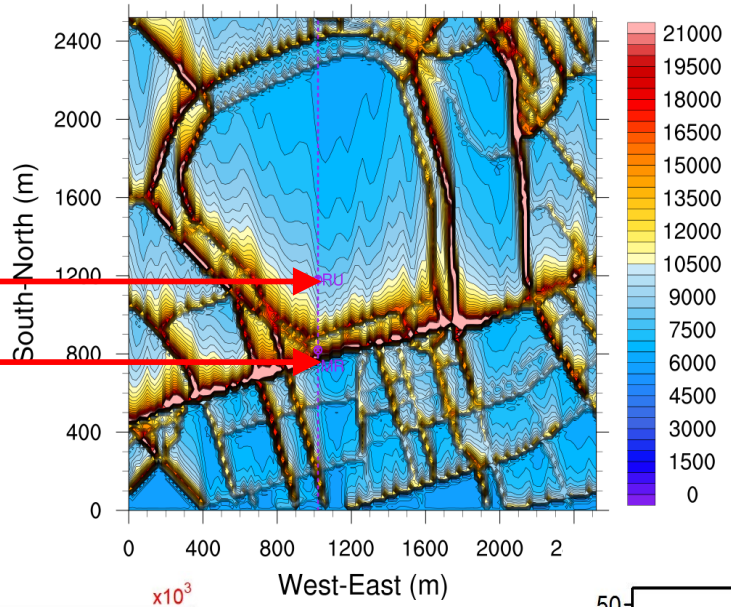


Small-scale dispersion of ultrafine particles from traffic in London (WRF-Chem) by University of Birmingham

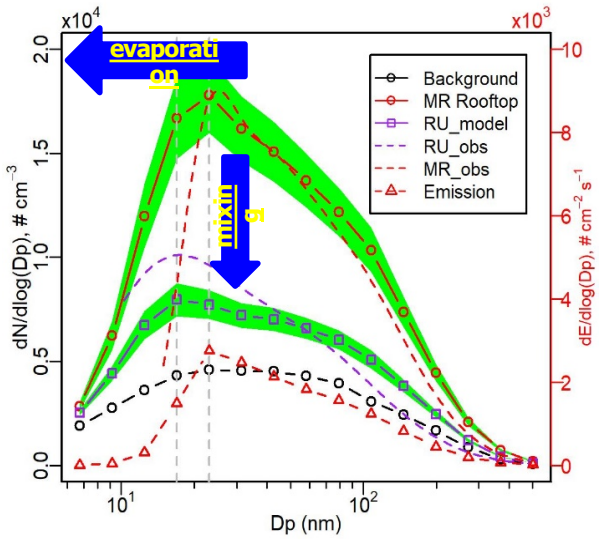
20m resolution

(RU) site

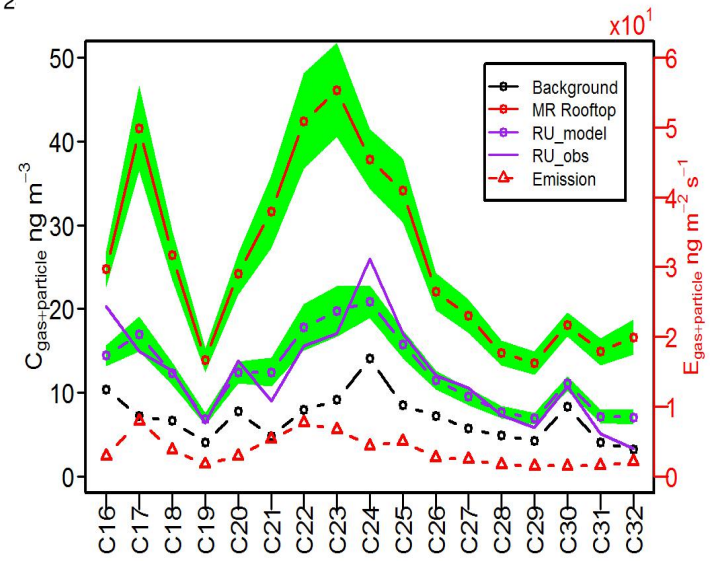
(MR) Marylebone



(a) Total UFP number concentration (# cm^{-3})



(b) UFP number-size distribution dN/dlog(Dp) (# cm^{-3})



(c) Total (gas + particle) SVOCs concentrations at roof top level.

New Anthropogenic Global Emission Inventory

(For use with prep_chem_sources package)

Community Emissions Data System (CEDS)

Rachael Hoesly, Steve Smith et al., 2017, GMDD.

U. Maryland/PNNL's Joint Global Change Research Institute

Based on HTAP-2010

Basis for CMIP modeling projects

Current configuration:

0.5 X 0.5 degree horizontal resolution

Global monthly emissions from 1750 to 2014

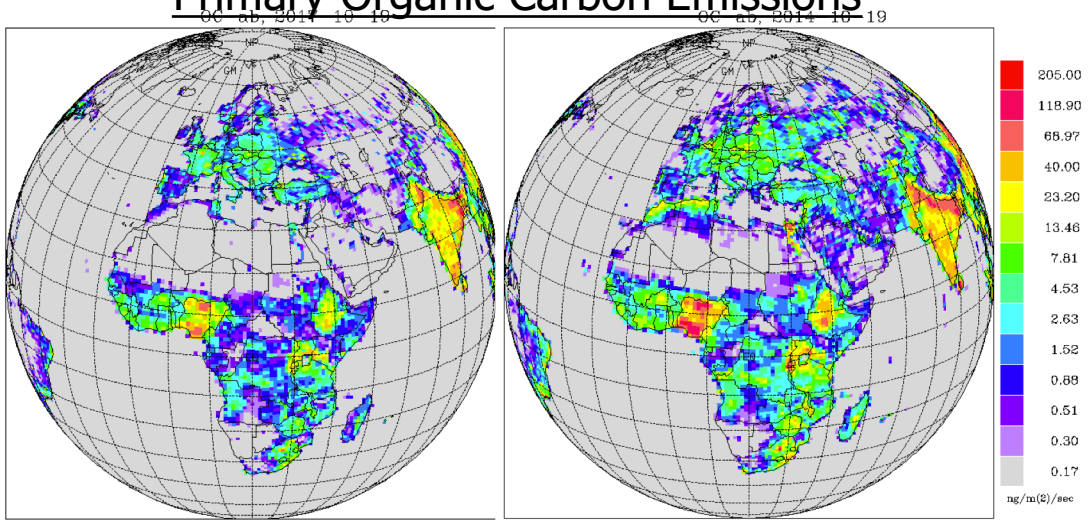
Anthropogenic BC, OC, and other Aerosol

26 VOC species

NOx, SO2, CO, NH3, CO2, CH4

Nine Energy/Use Categories

Primary Organic Carbon Emissions



HTAP-2010 CEDS-2014

Available for WRF-Chem

- GOCART aerosol (currently)
- CEDS (2014) datasets
- Modified prep_chem_sources
- Contact: Stu McKeen

Concluding remarks

- Check out WRF-Chem references to know who is working on what, what should be cited, and maybe where to get additional help if needed.
- We recommend all the users signing up to the WRF-Chem discussions email group (forum).
- Also, please send us info on your peer reviewed WRF-Chem publications.
- For more details about WRF-Chem check the user's guides and tutorial presentations: https://ruc.noaa.gov/wrf/wrf-chem/tutorial2017.htm

WRF-Chem info on the WEB:

- WRF-Chem web-page: https://ruc.noaa.gov/wrf/wrf-chem/
- WRF and WRF-Chem user forums: http://forum.mmm.ucar.edu/phpBB3/index.php
- WRF-Chem discussions: https://list.woc.noaa.gov/cgi-bin/mailman/listinfo/wrf-chem-discussions/
- Publications: https://ruc.noaa.gov/wrf/wrf-chem/References/WRF-Chem.references.htm

For questions contact us at **wrfchemhelp.gsd@noaa.gov**

A list of recent global inventories

Author	Acronym	Reference or Website	Years	Resolution
Lamarque et al.	ACCMIP	eccad.sedoo.fr	1900-2000	0.5x0.5
Riahi et al.	RCPs	eccad.sedoo.fr	2000-2100	0.5x0.5
Granier et al.	MACCity	eccad.sedoo.fr	2000-2015	0.5x0.5
Maenhout et al.	EDGAR4.2	edgar.jrc.ec.europa.eu	1970-2008	0.1x0.1
Crippa et al.	EDGAR4.3	edgar.jrc.ec.europa.eu	1970, 2010	0.1x0.1
Maenhout et al.	HTAPv2	edgar.jrc.ec.europa.eu	2008, 2010	0.1x0.1
Klimont et al.	ECLIPSE v4, v5	iiasa.ac.at	1990-2030	0.5x0.5
Schultz et al.	RETRO	juelich ftp	1960-2000	0.5x0.5
Bond et al.	Bond	Hiwater.org	1850-2000	country
Junker&Liousse	J&L	eccad.sedoo.fr	1860-2003	1x1
Huang Y. et al.	PKU	inventory.pku.edu.cn	1960-2009	0.1x0.1
Smith et al.	PNNL	sedac.ciesin.columbia.edu	1850-2005	1x1

Blue: inventories providing just a few species

All the data are publicly available. Most available at: eccad.sedoo.fr, the database of the **Global Emissions InitiAtive (GEIA)**