Inventory of NOAA Atmospheric Chemistry Models

Summary of Local Scale Models

Model	Laboratory	Principal NOAA Contacts
Cloud Parcel	ESRL	Barbara Ervens Graham Feingold
RAMS/LES	ESRL	Graham Feingold Hongli Jiang
MCM	ESRL	Roberto Sommariva
MAIA	ESRL	Jan Kazil Ned Lovejoy

NOAA Atmospheric Chemical Modeling Workshop
October 10-11, 2007
NOAA ESRL, Boulder, CO

Cloud Parcel

Model description

- Adiabatic air parcel (constant updraft) <u>or</u> driven by trajectories (prescribed RH, temperature, height, etc) from LES model
- Growth of population of aerosol particles (internal mixtures) in a rising parcel of air
- Particle growth solved on moving mass grid

  ⇨ retain full information on aerosol composition within droplets
- Detailed gas and aqueous phase chemistry (~300 reactions).
- Description of sulfate and organic mass information in cloud droplets

Some science questions

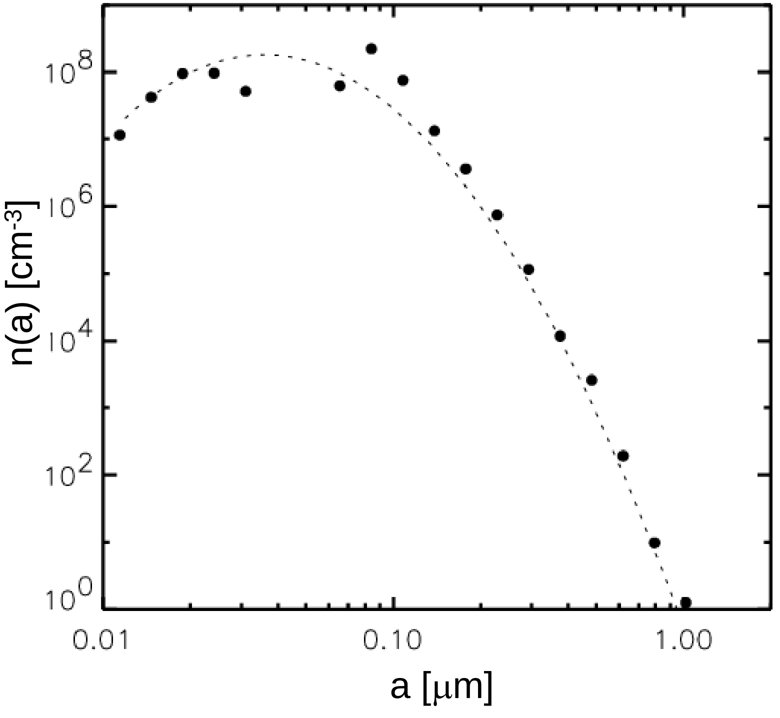
- How does aqueous chemistry (sulfate) modify aerosol size distributions and in so doing affect the aerosol-cloud system?
- To what extent do chemical processes in cloud droplets contribute to secondary organic aerosol (SOA) burden (e.g., oxalate)?

Cloud Parcel

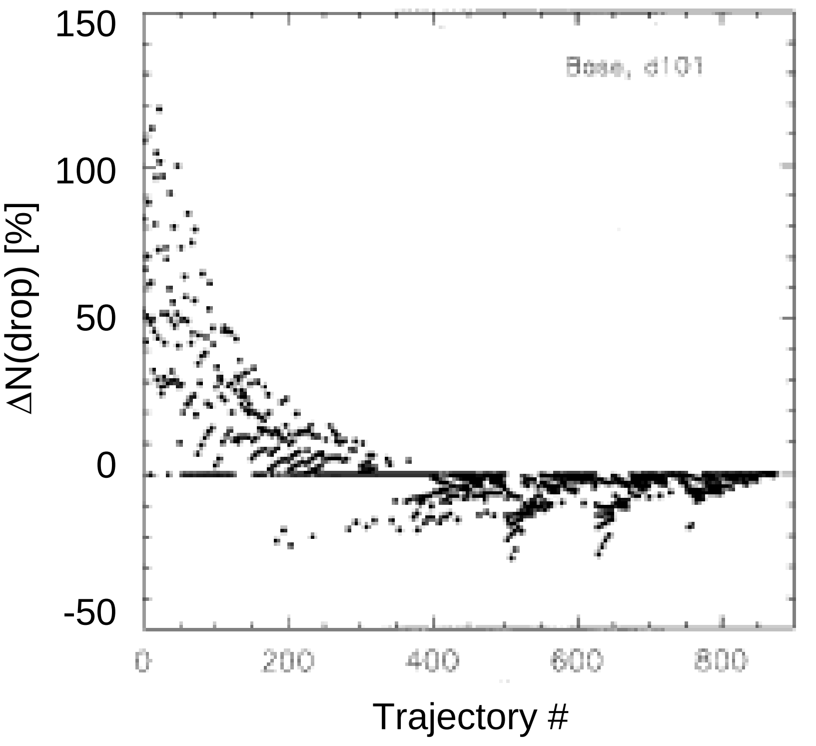
Does cloud processing of aerosol enhance droplet concentrations?

- 500 trajectories (stratocumuli) from LES model
- Sulfate formation in cloud droplets

Bimodal distribution after cloud-processing



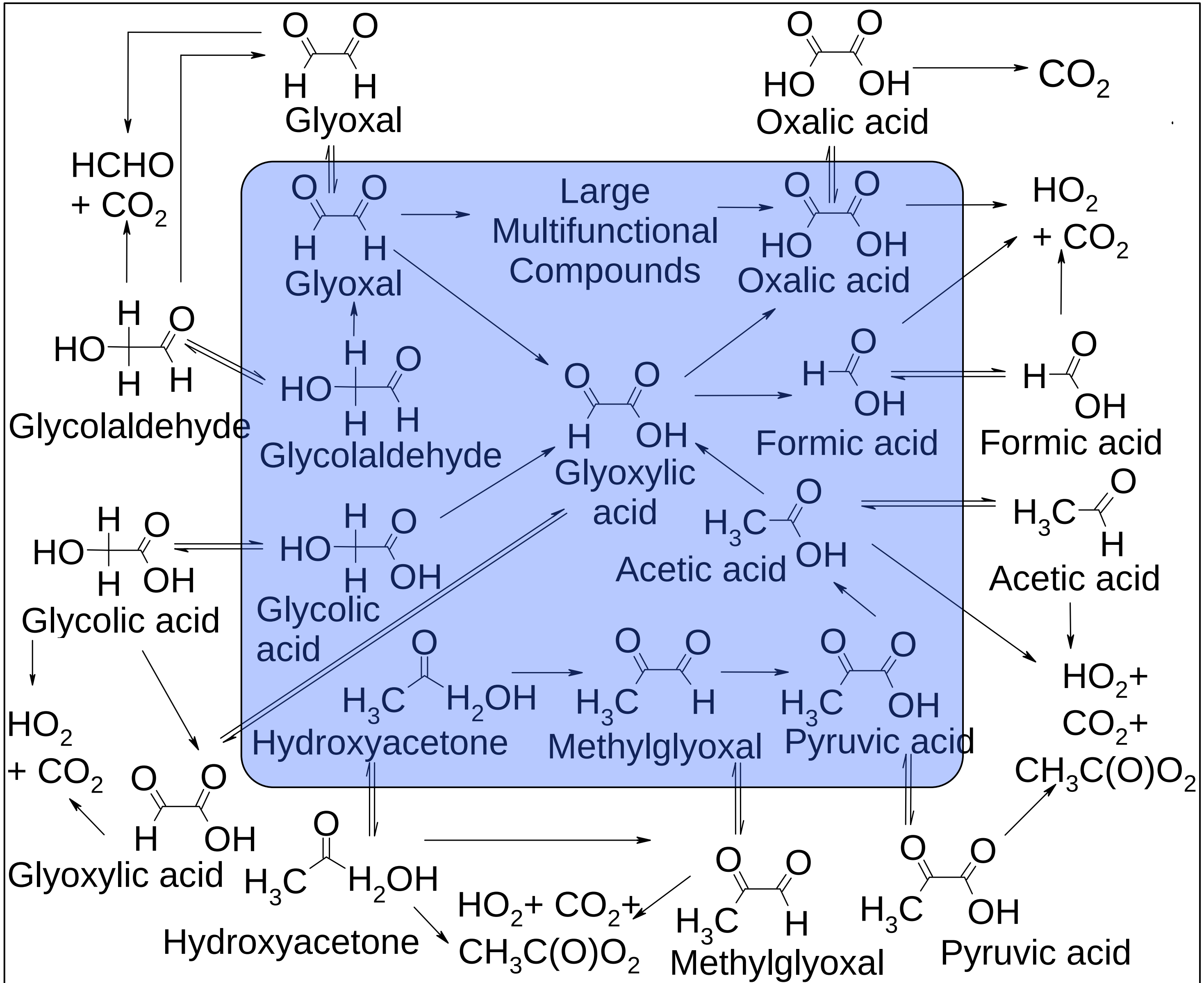
Change in cloud drop number concentration with/out sulfate formation



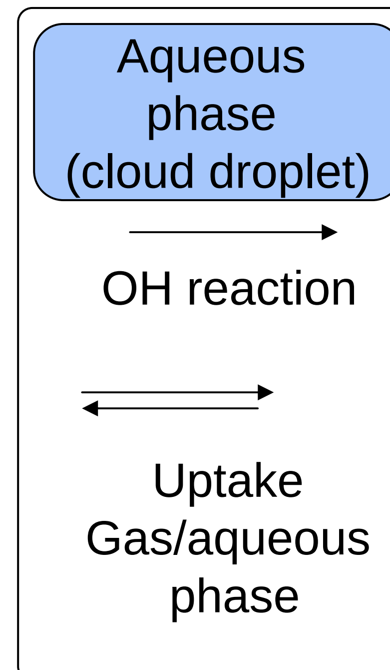
Feingold and Kreidenweis, 2000

Cloud Parcel

SOA formation in cloud droplets



Mechanism development based on lab studies



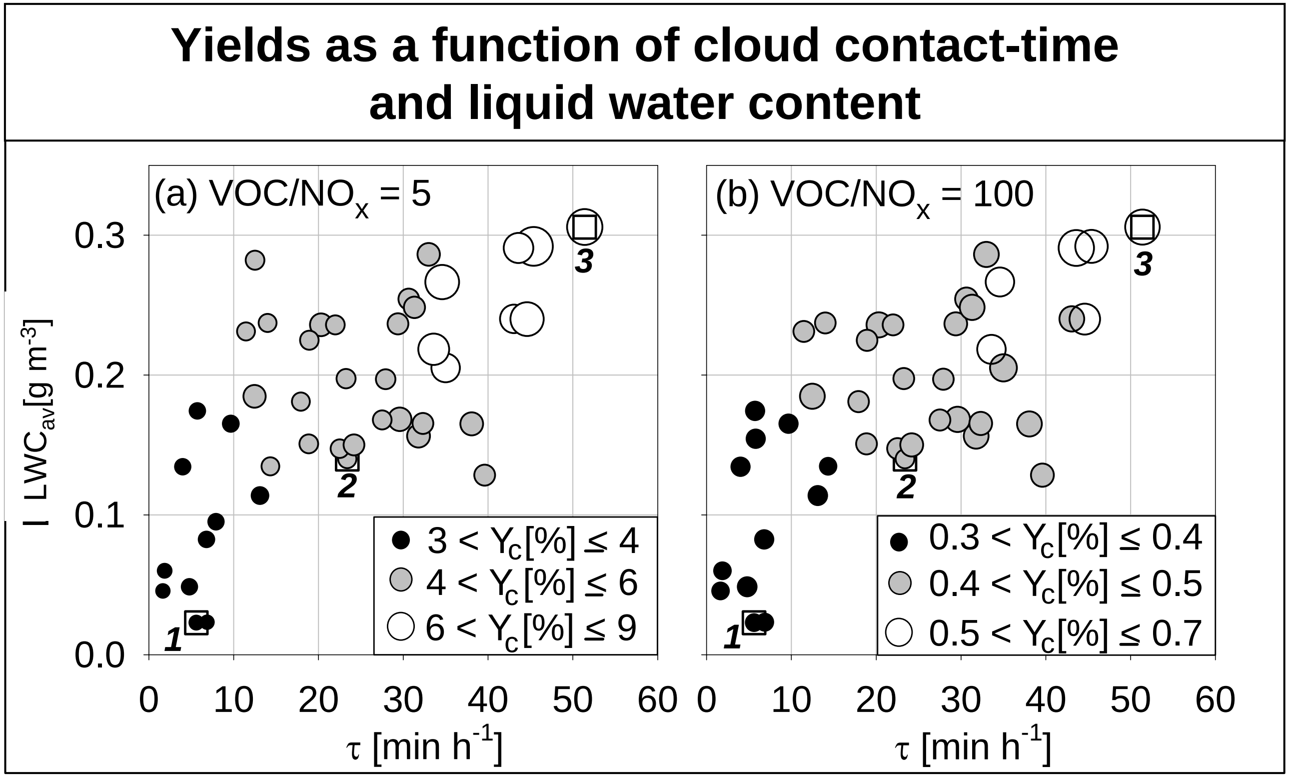
Cloud Parcel

SOA yields from cloud-processing of isoprene oxidation products

How much SOA mass is formed in cloud droplets and remains in the particles after cloud evaporation?

$$Y_c = \frac{SOA_{mass}}{\text{Initial isoprene mass}}$$

- SOA can be efficiently formed in clouds
- Yields are comparable to those on particles



Parameterization for use in large scale models:

$$Y_c = a_0 + a_1 \cdot \tau + a_2 \cdot LWC_{av}$$

a_0, a_1, a_2 = f(VOC/NO_x)

Ervens et al., 2007 (in review)

RAMS/LES

***R**egional **A**tmospheric **M**odeling **S**ystem in **L**arge **E**ddy **S**imulation mode*

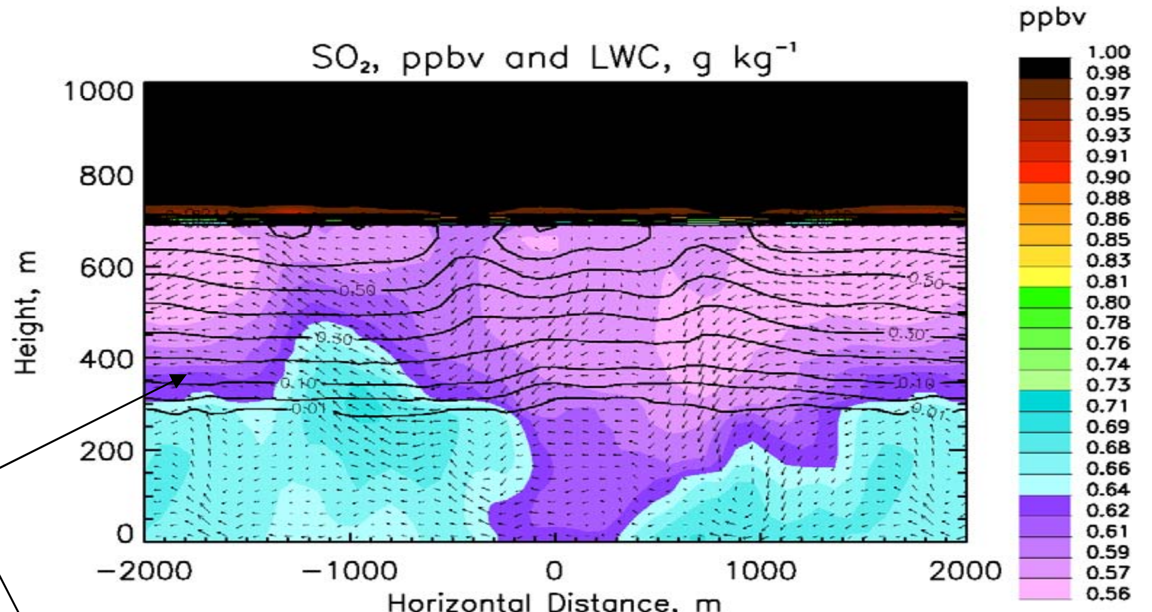
Model Description

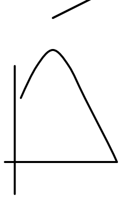
- Coupled dynamics, microphysics, aerosol, aqueous chemistry, radiation, & land surface model
    - Size resolved bin microphysics (warm processes)
    - Size-resolved aerosol
    - Solute tracking
    - Aqueous chemistry (sulfate)
    - Radiation (coupled to aerosol and cloud optical properties)
    - Land surface model (soil and vegetation)
    - Scalable from large eddy simulations to regional/global modeling
    - Nested grids (two-way)

Some Science Questions

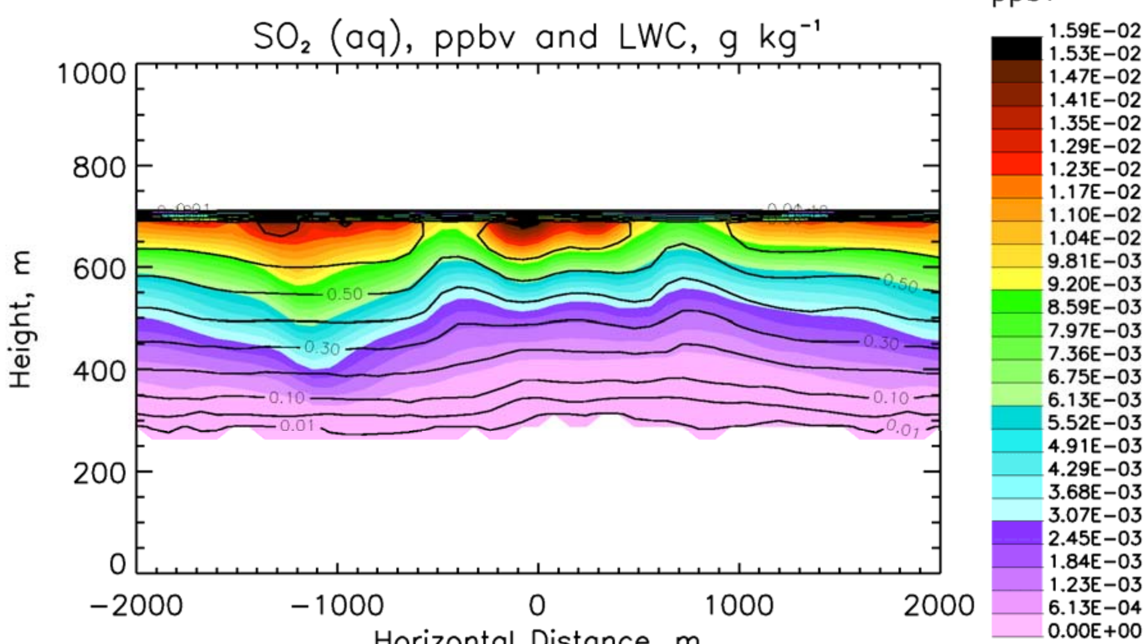
- How does aerosol influence clouds in a tightly coupled system that includes feedbacks?
    - How does aqueous chemistry (sulfate) modify aerosol size distributions and in so doing affect the aerosol-cloud system?
- How well does the model reproduce observed cloud fields?
    - Radiative forcing
    - Precipitation formation

RAMS/LES





Solid contours: cloud water

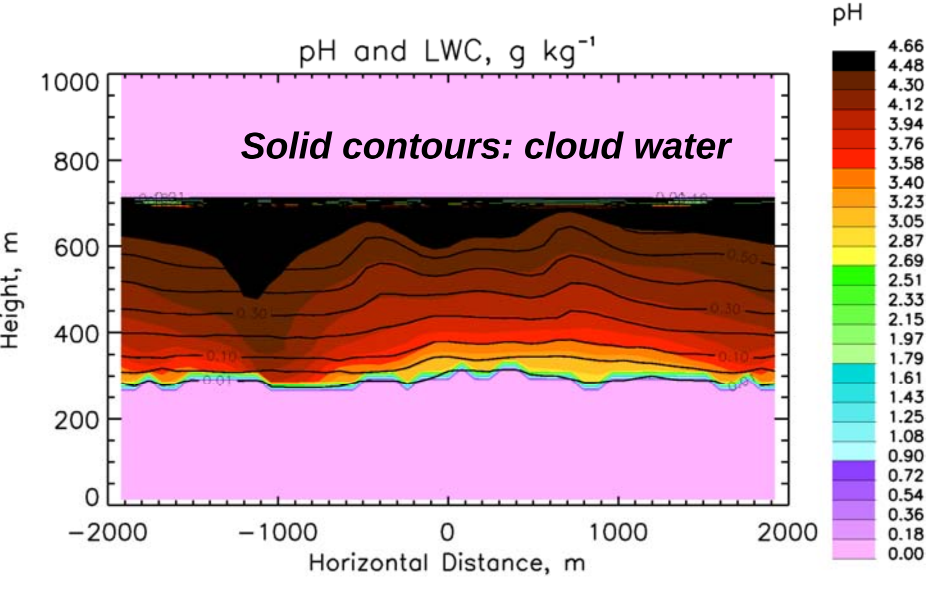


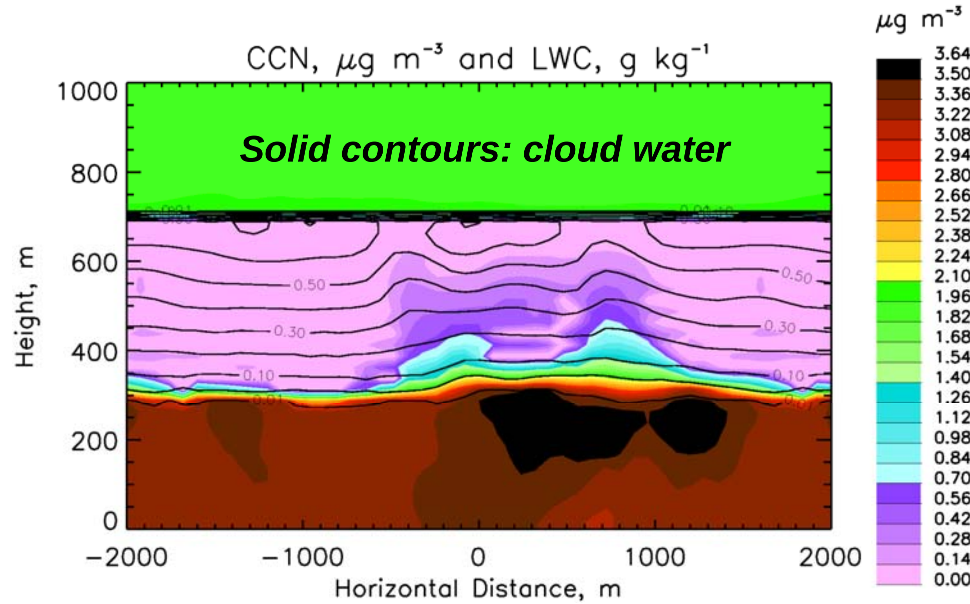
LES of stratocumulus clouds with aqueous chemistry

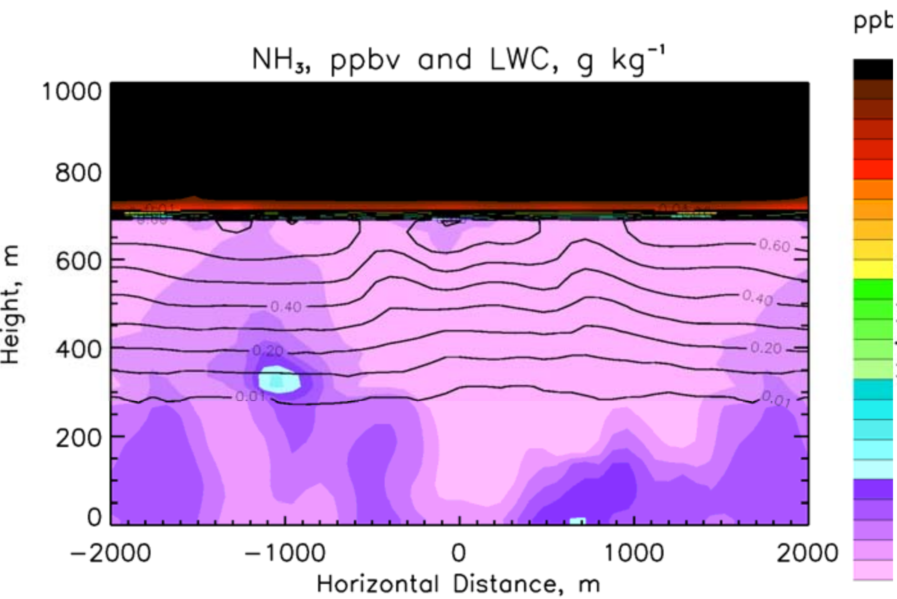
Gas	[ ], ppbv
SO_2	1
O_3	40
H_2O_2	0.75
NH_3	0.1
HNO_3	0.1

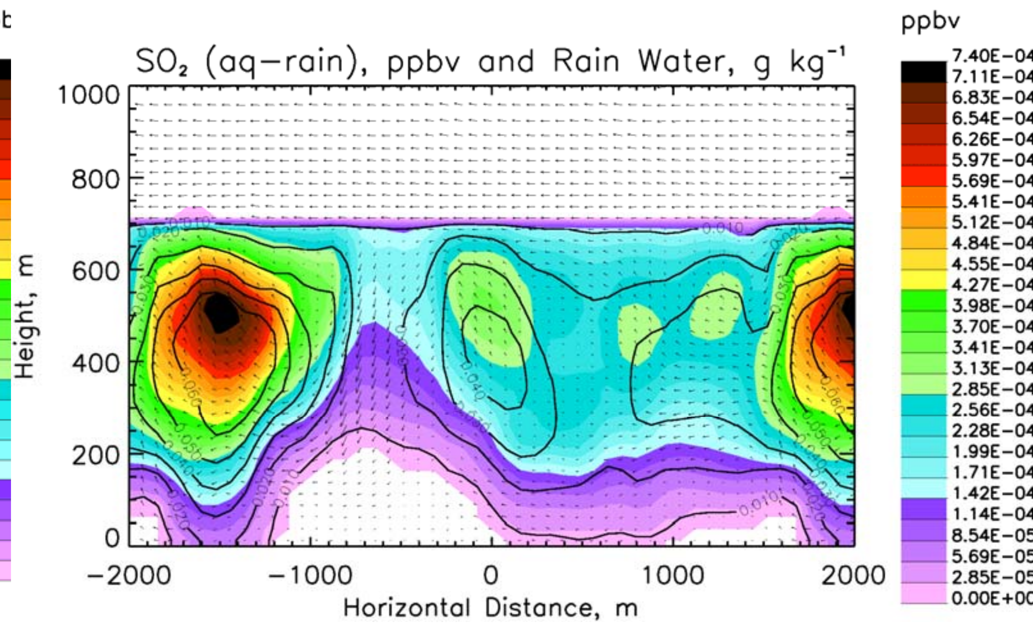
Feingold et al. 2002

RAMS/LES









Solid contours: cloud water

Solid contours: rain water

MCM

***M**aster **C**hemical **M**echanism*

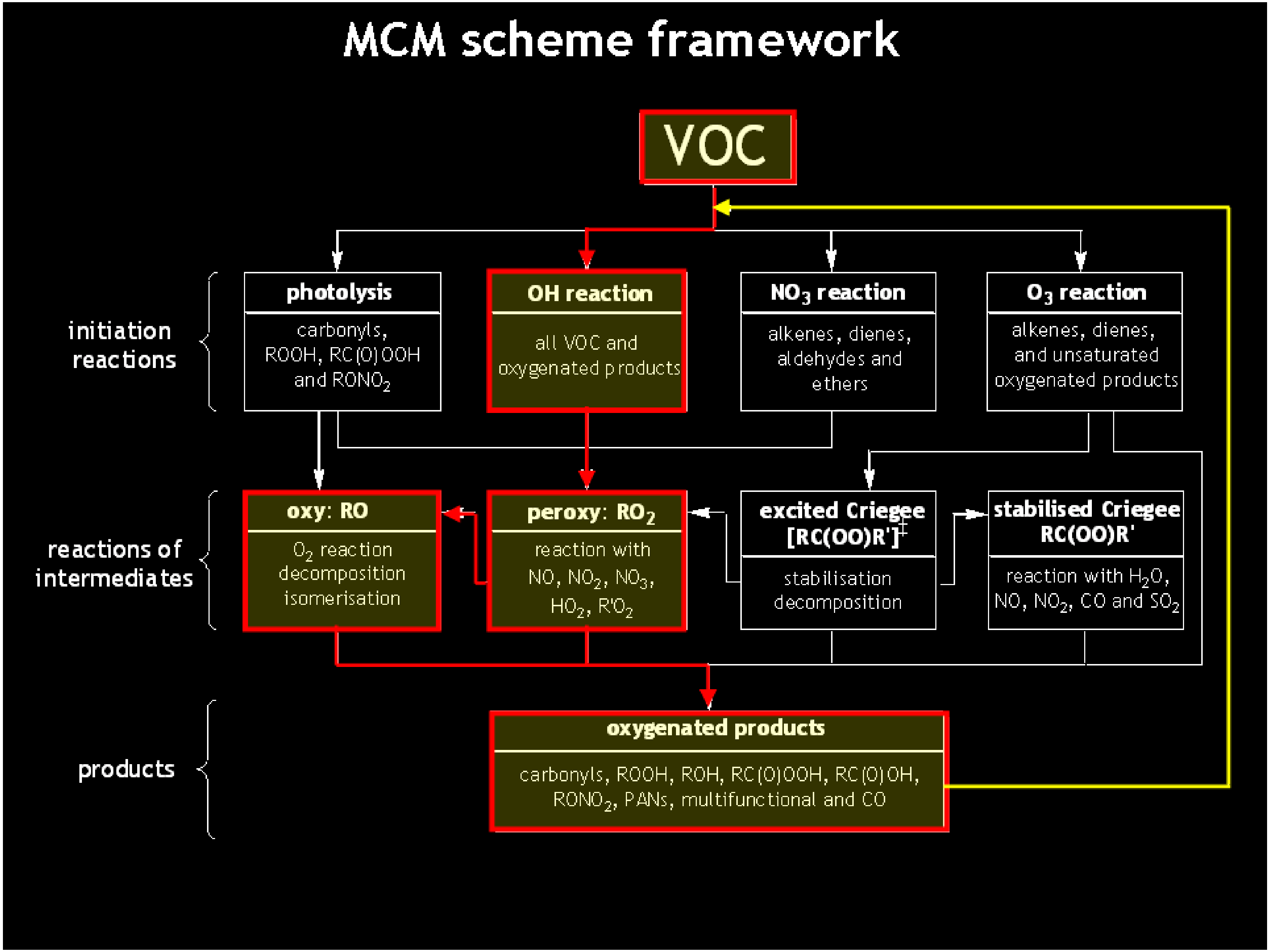
Model Description

- Explicit representation of VOC degradation mechanisms built from information on kinetics and products of elementary reactions
    - Apply measured and evaluated parameters (e.g. rate coefficients, branching ratios) from the literature where possible.
    - Use analogy and 'structure-reactivity correlations' to define the other reactions and parameters.
    - Parameterization of peroxy-peroxy reactions to reduce number of reactions.
    - **MCM protocol:** Jenkin et al., *Atmospheric Environment*, 1997. Updated in Saunders et al. and Jenkin et al., *ACP*, 2003.
- Current version (3.1) contains 135 VOCs with 4602 species and 13496 reactions (http://mcm.leeds.ac.uk).
- Synched with IUPAC evaluation database.

Applications

- The MCM is 'just' a chemical mechanism. It can be used to build models, by adding other relevant processes (aerosol, deposition, etc…)
- 0-D box models: constrained to field measurements, e.g. for modelling radicals (OH, HO_2, RO_2, NO_3).
- 1-D box models: simulation of the chemical evolution of long-lived species, e.g. in urban plumes (HNO_3, PANs, $RONO_2$, O_3).
- Reduction techniques can be applied to use it in larger scale models.

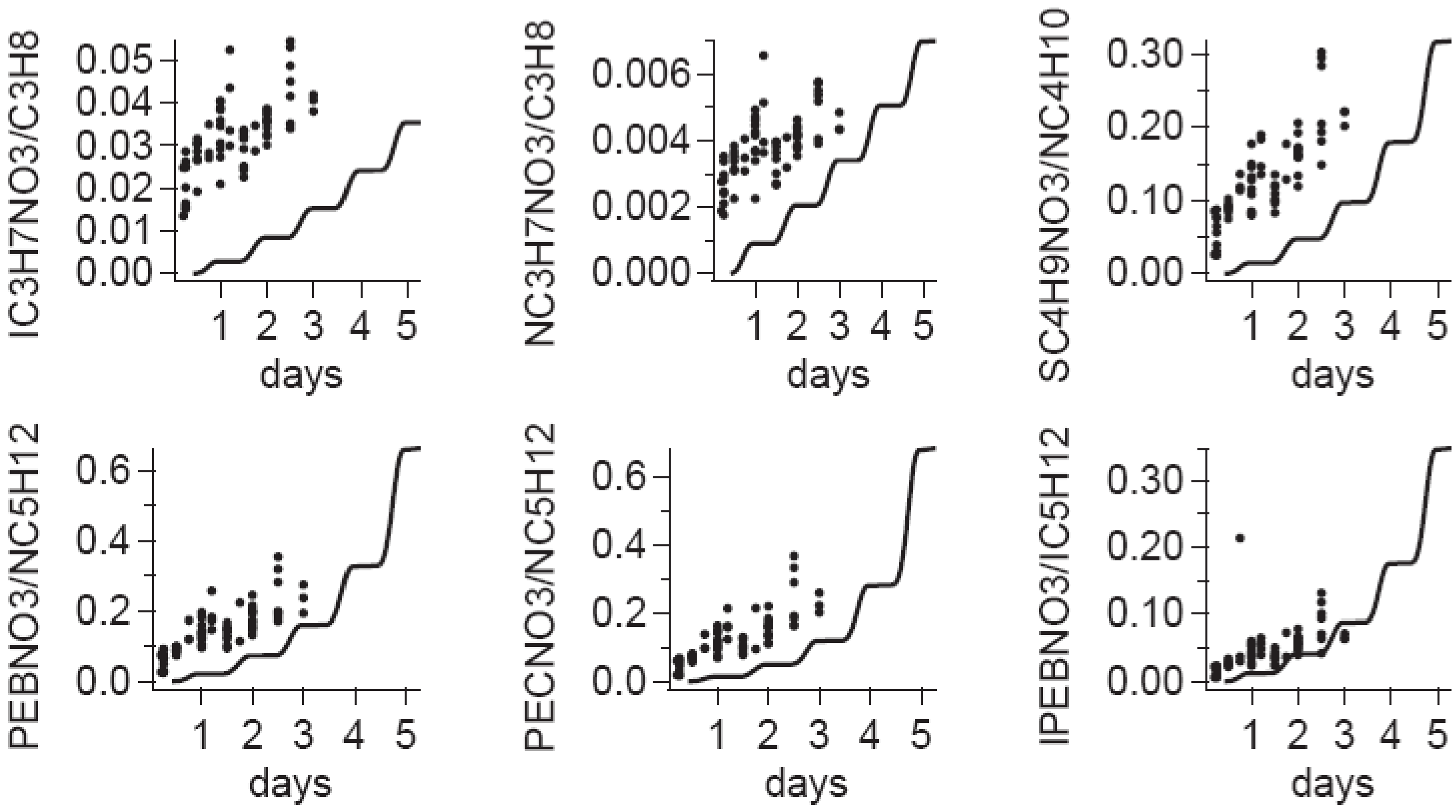
MCM


MCM scheme framework
VOC
initiation reactions
photolysis
carbonyls, ROOH, RC(O)OOH and $RONO_2$
OH reaction
all VOC and oxygenated products
NO_3 reaction
alkenes, dienes, aldehydes and ethers
O_3 reaction
alkenes, dienes, and unsaturated oxygenated products
reactions of intermediates
oxy: RO
O_2 reaction decomposition isomerisation
peroxy: RO_2
reaction with NO, NO_2, NO_3, HO_2, $R'O_2$
excited Criegee $[RC(OO)R']^{‡}$
stabilisation decomposition
stabilised Criegee RC(OO)R'
reaction with H_2O, NO, NO_2, CO and SO_2
products
oxygenated products
carbonyls, ROOH, ROH, RC(O)OOH, RC(O)OH, $RONO_2$, PANs, multifunctional and CO

MCM

Example of MCM use in box model

- Measurements of alkylnitrates taken during the NEAQS 2004 campaign on the WP-3D.
- Explicit chemistry of the MCM => the chemical formation processes of these species can be explored in high detail.



MAIA

***M**odel of **A**erosols and **I**ons in the **A**tmosphere*

Model Description

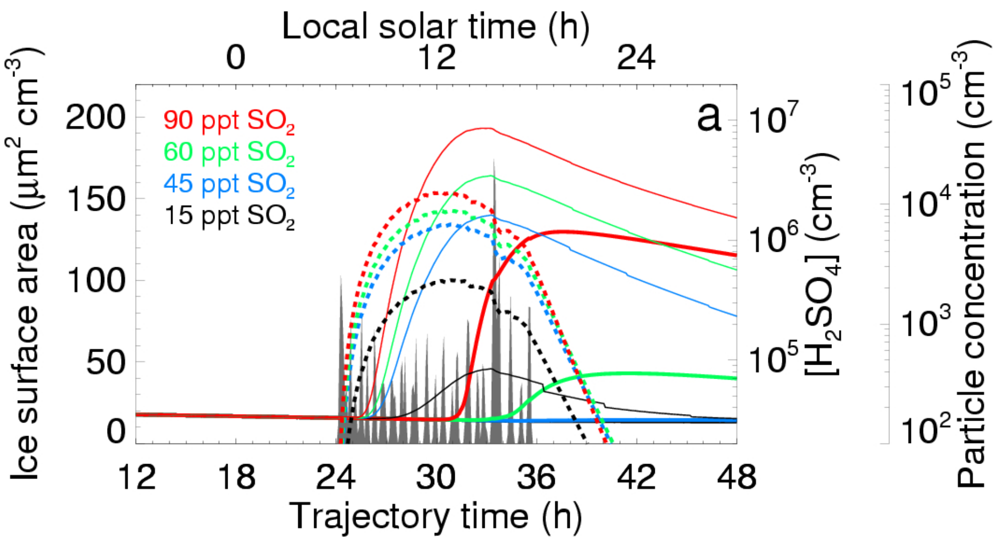
- Models neutral & negative sulfate aerosol particles, starting from small H_2SO_4-H_2O clusters formed from the gas phase up to their larger (CCN) sizes
  - Small H_2SO_4-H_2O clusters treated with molecular size resolution
  - Larger aerosol particles described by geometric size sections
  - 1st order scheme resolving the aerosol size distribution within these sections efficiently suppresses numerical diffusion
  - Laboratory thermodynamic data for H_2SO_4 uptake and loss by small neutral and charged clusters => reliable at very low temperatures of upper troposphere and lower stratosphere
  - Global box model version
  - Lagrangian version, run on trajectories inside and outside of clouds

Applications

- Ion-induced aerosol nucleation in the H_2SO_4-H_2O system in the middle and upper troposphere
- Aerosol nucleation in convective clouds over tropical oceans occurs in upper troposphere via ion-induced processes, role of cosmic rays
- Aerosol nucleation from the gas phase inside cirrus clouds

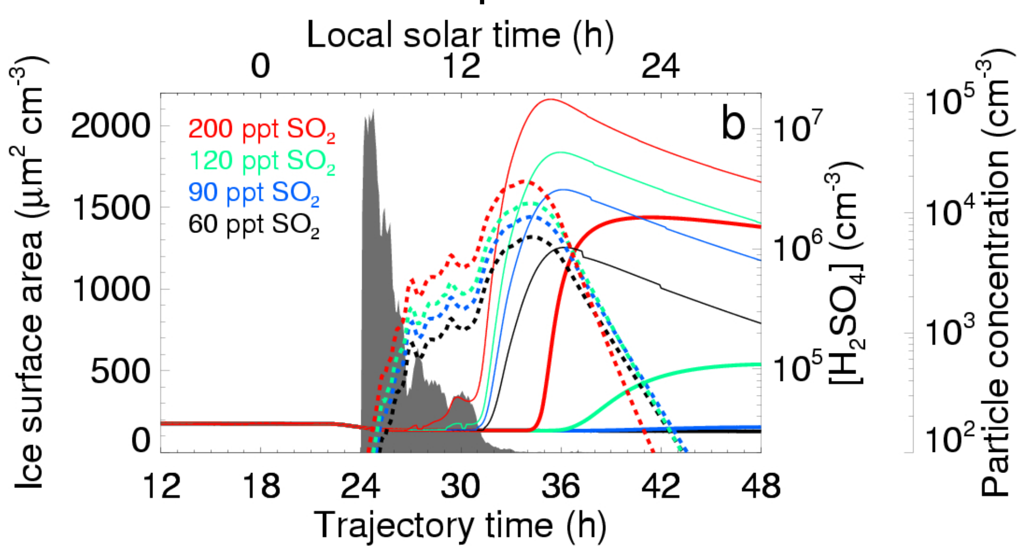
MAIA

Slow updraft cirrus



MAIA calculations on trajectories from an offline 1-D cirrus cloud model with ice crystal nucleation, growth, advection, & sedimentation

Fast updraft cirrus



Gray areas: cirrus ice surface area

Broken lines: $[H_2SO_4]$

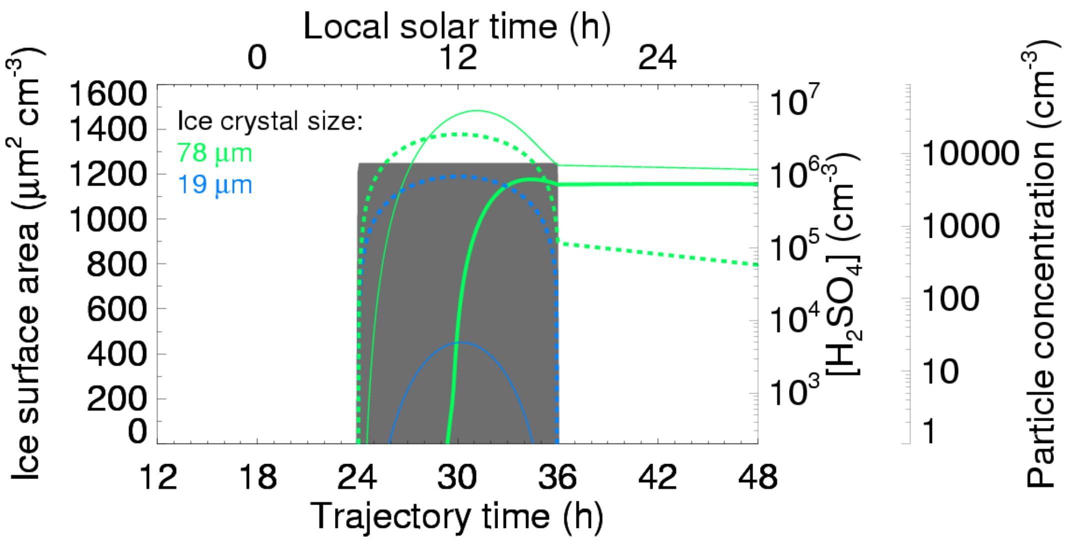
Thin solid lines: [supercritical aerosols]

Thick solid lines: [aerosols > 3 μm]

Kazil et al., ACP, 2007

MAIA

Aerosol formation in 2 idealized cirrus clouds with small and large ice crystals



Gray areas: cirrus ice surface area

Broken lines: $[H_2SO_4]$

Thin solid lines: [supercritical aerosols]

Thick solid lines: [aerosols > 3 µm]

Findings

- Aerosol nucleation inside cirrus clouds possible even at very high ice surface area concentrations if ice crystals are sufficiently large
- Observations of ultrafine particles inside cirrus clouds can be due to aerosol nucleation inside the cloud, and not just result of ice crystal shattering on measurement platform

Kazil et al., ACP, 2007