

Multiphase Tropospheric Chemistry in Modal-CAM with MECCA/KPP's Rosenbrock Solvers

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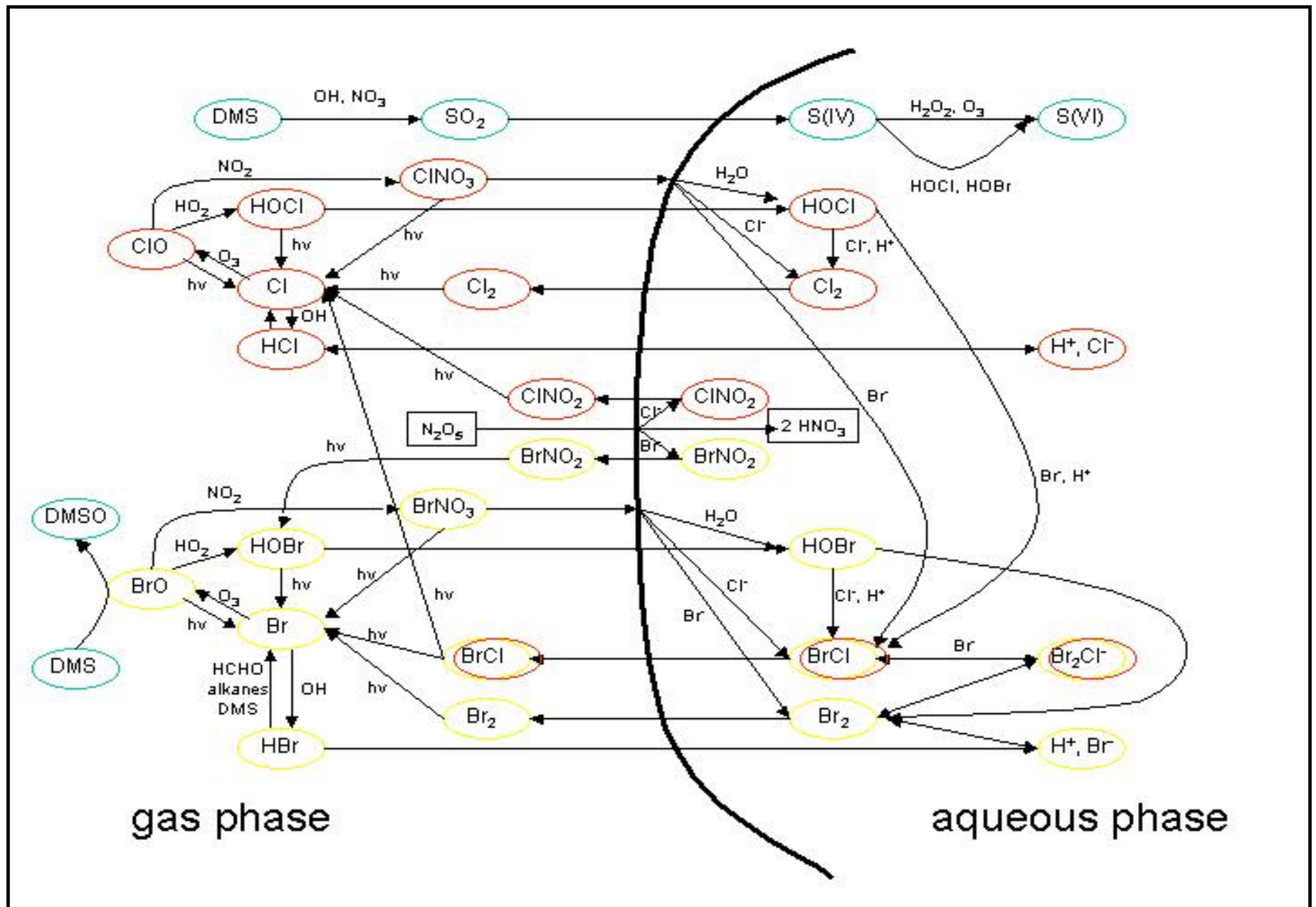
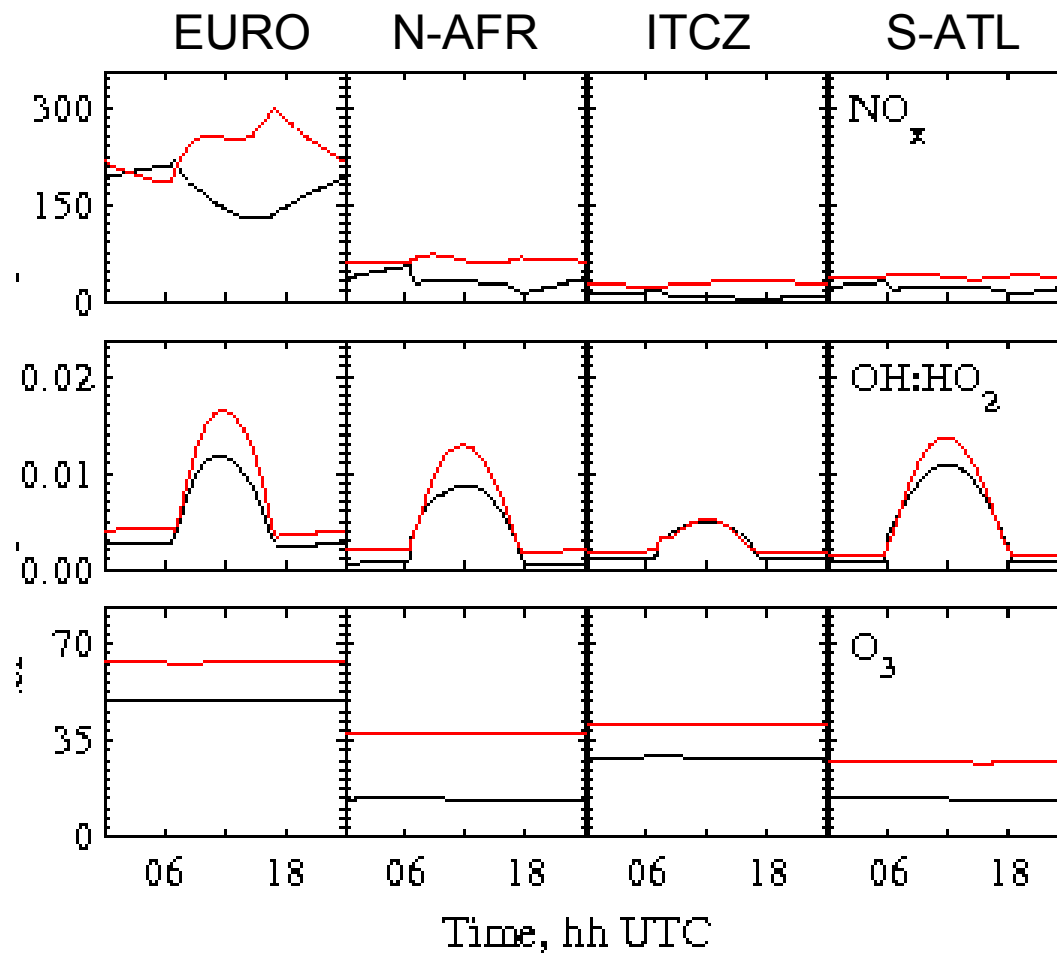
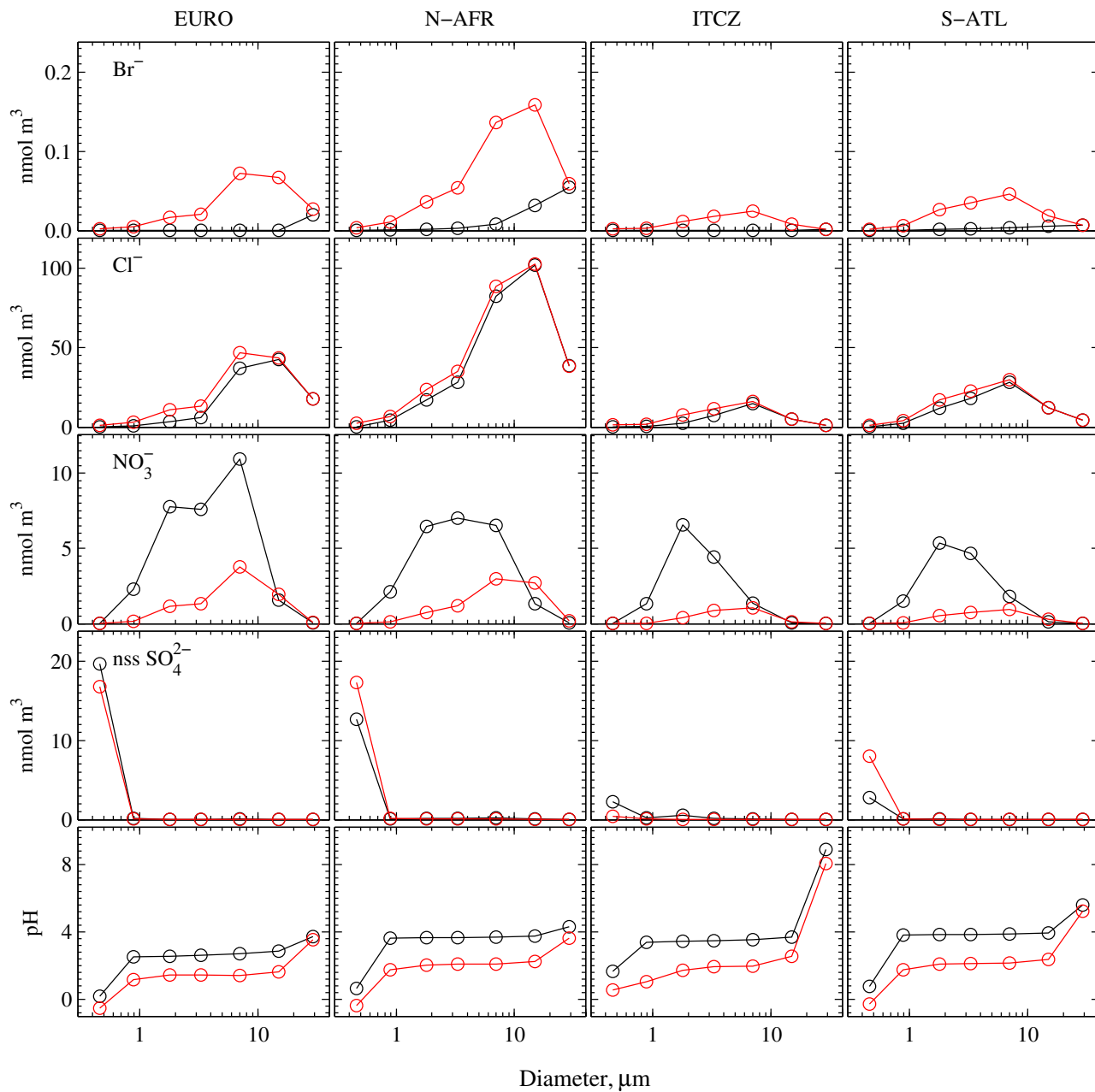


Image courtesy R. Sander



— w/ Marine Aerosol Chemistry
 — w/o Marine Aerosol Chemistry



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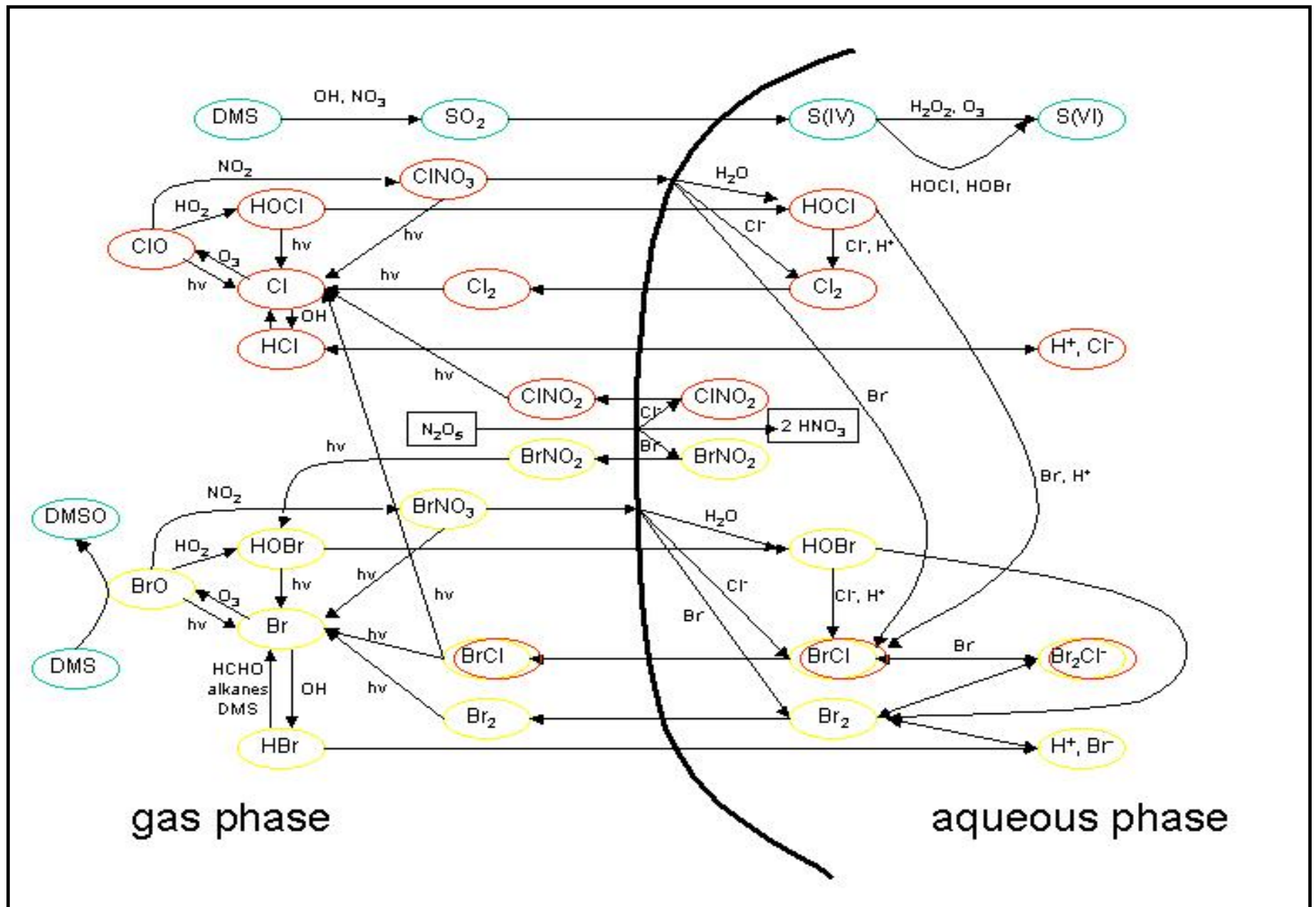
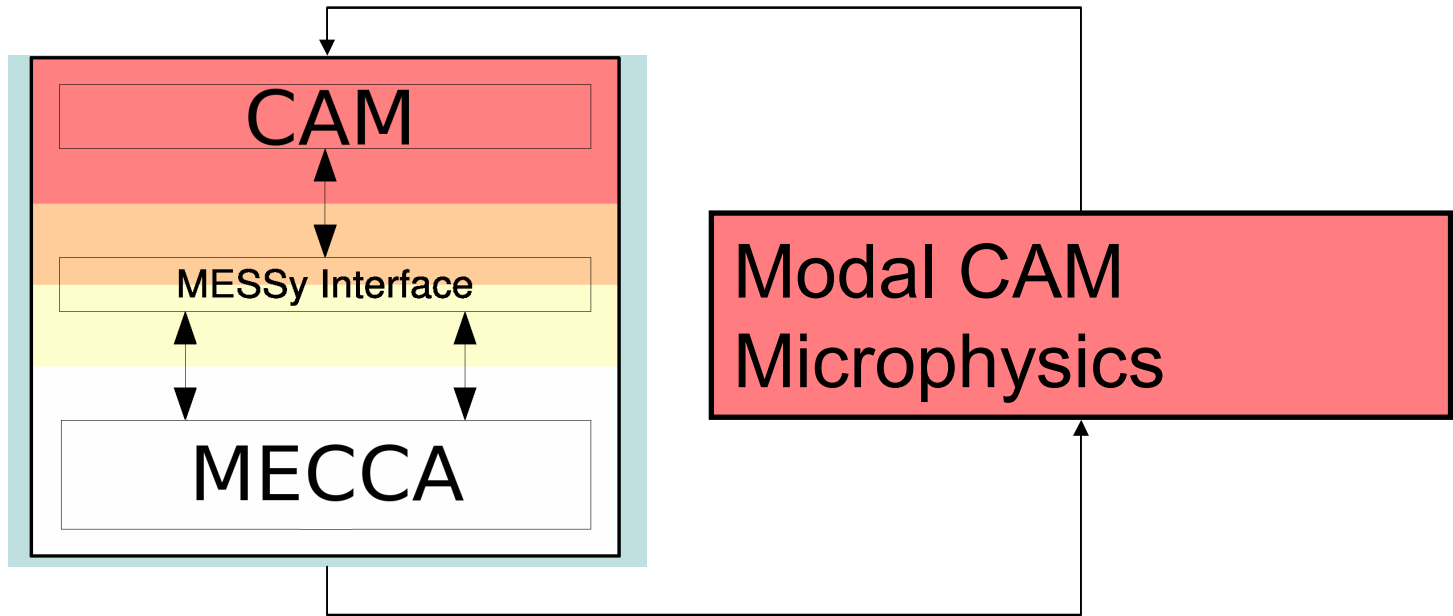


Image courtesy R. Sander

CAM Coupling



Great Big ODE

- Photolysis
- Gas-phase
- Aqueous-phase
- Mass Transfer

- Particle Formation
- Coagulation
- Condensation
- Nucleation
- Particle Deposition

- Dynamics
- Cloud Processing*

Kinetics PreProcessor (KPP)

Damian et al., 1995; Sandu & Sander, 2006

Available Numerical Solvers

- *Rosenbrock: Ros1-4, Rodas3-4*
- *Radau5, SDIRK, SEULEX*
- *LSODE/LSODES, VODE, ODESSA*

Multi-stage Rosenbrock Solvers

Adjustable Timestep / Positive Definite

- Ros2: L-stable, 2 stages, order 2
- Ros3: L-stable, 3 stages, order 3 **
- Ros4: L-stable, 4 stages, order 4
- Rodas-3: “stiffly-stable”, 4 stages, order 3
- Rodas-4: “stiffly-stable”, 6 stages, order 4

A. Sandu recommends Radau5 for reference run

3-mode ModalCAM with “Full” Chemistry

- Modal-CAM v3 6 33 (10x15 resolution)
- FV Dynamics
- 156 active tracers (aq. & gas) / 360 Reactions

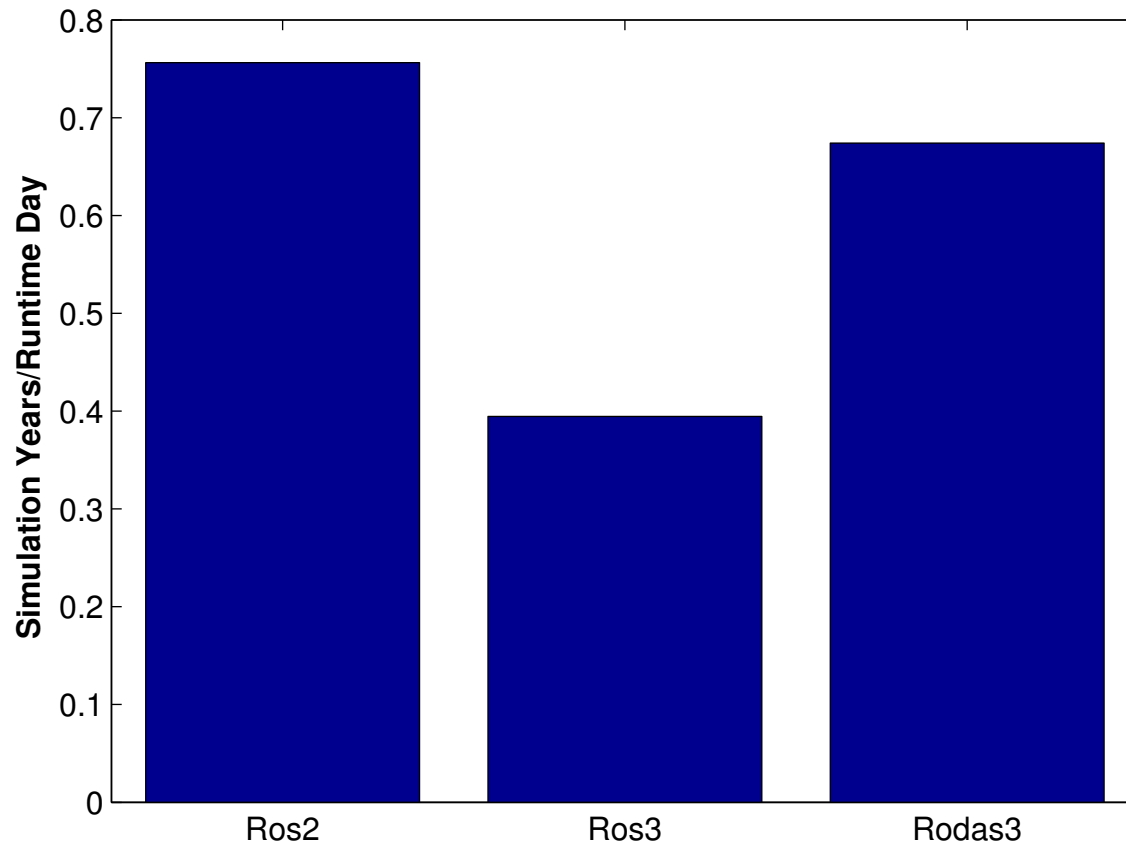
- Spun-up^{***} from zero concentration vector
- 10-minute timestep

- with 1° Emissions
- 1-month run

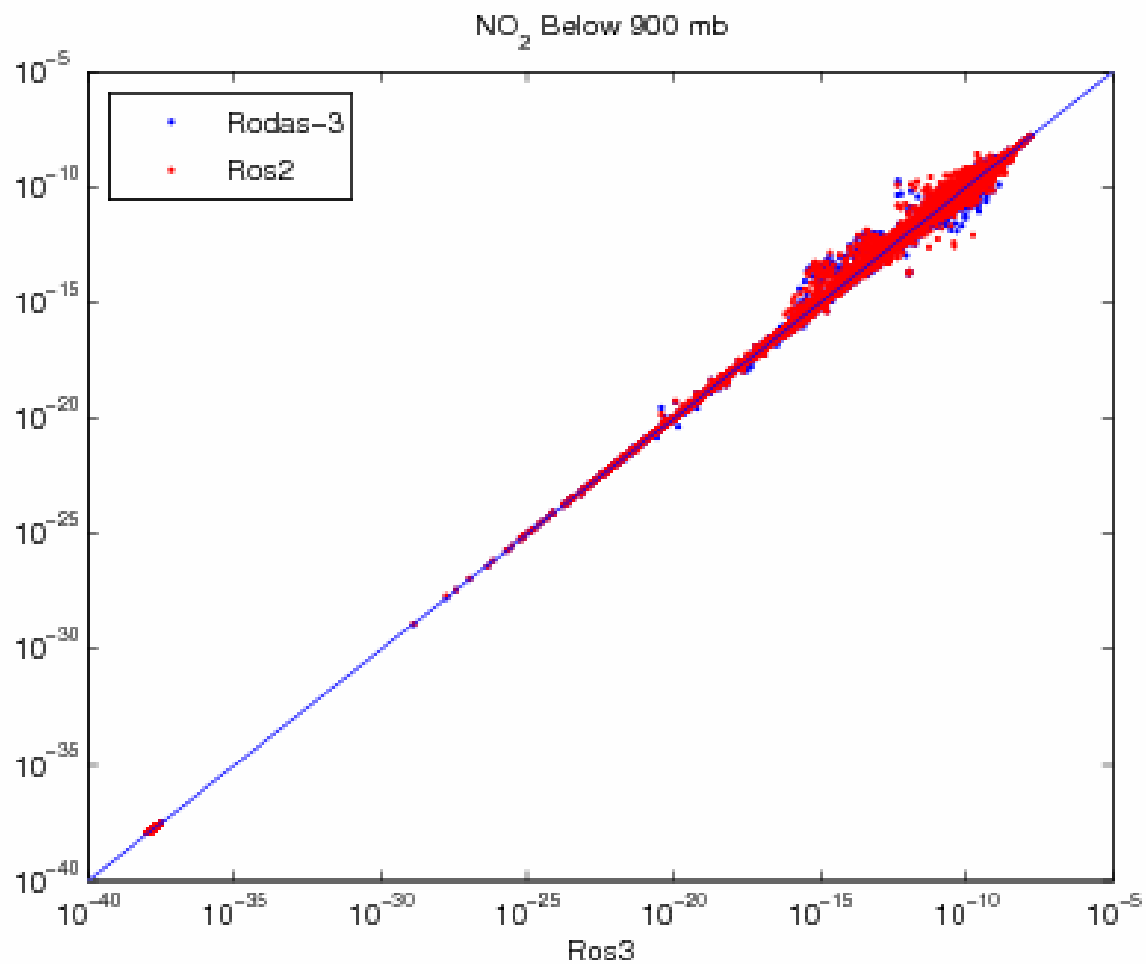
3-mode ModalCAM with “Full” Chemistry

- Basic Gas/Aqueous Chem.
- Complete Inorganic Br & Cl, CH₄ (no NMHC or organic chem.)

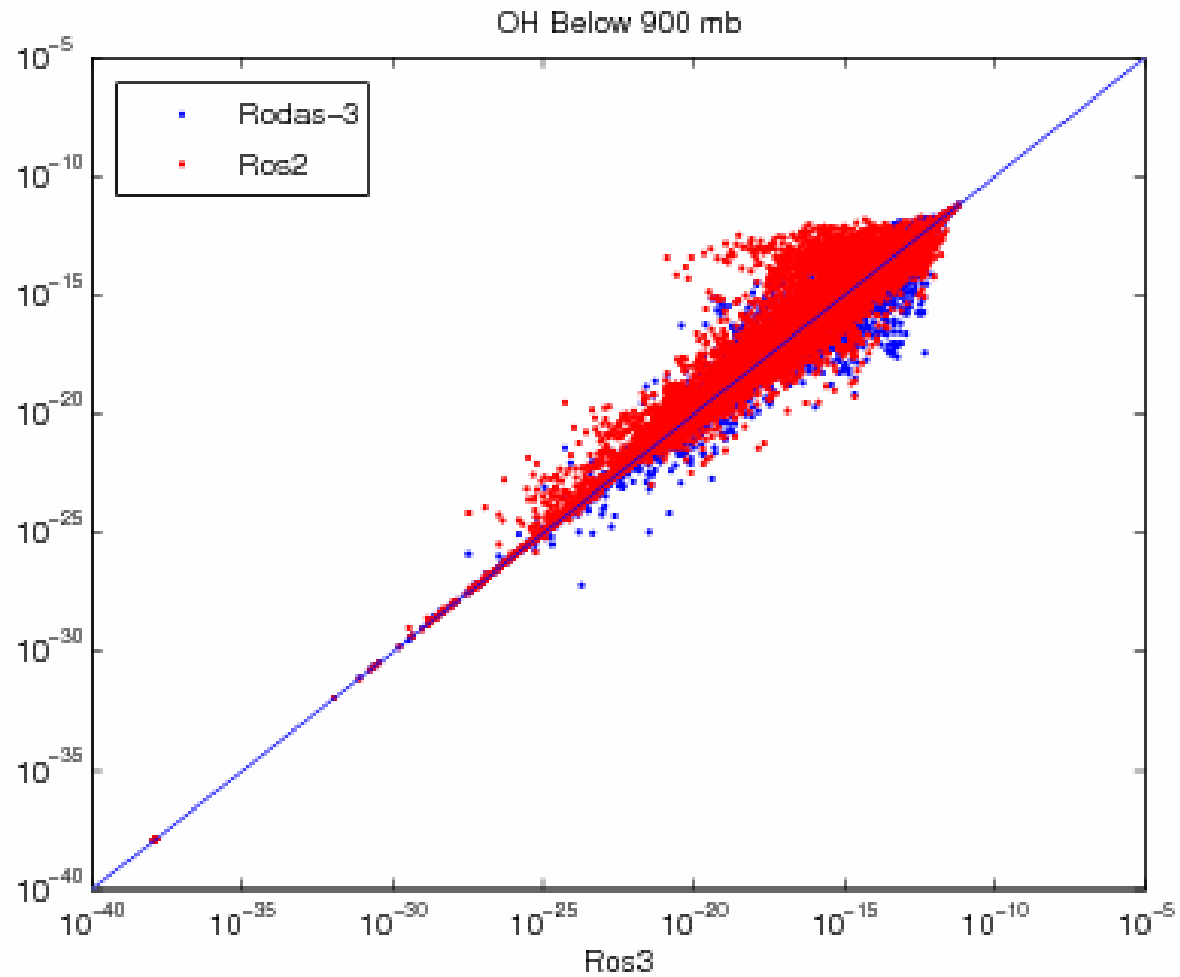
- No Optimizations
(no short-lived species; no high-performance mods, strict tolerances)



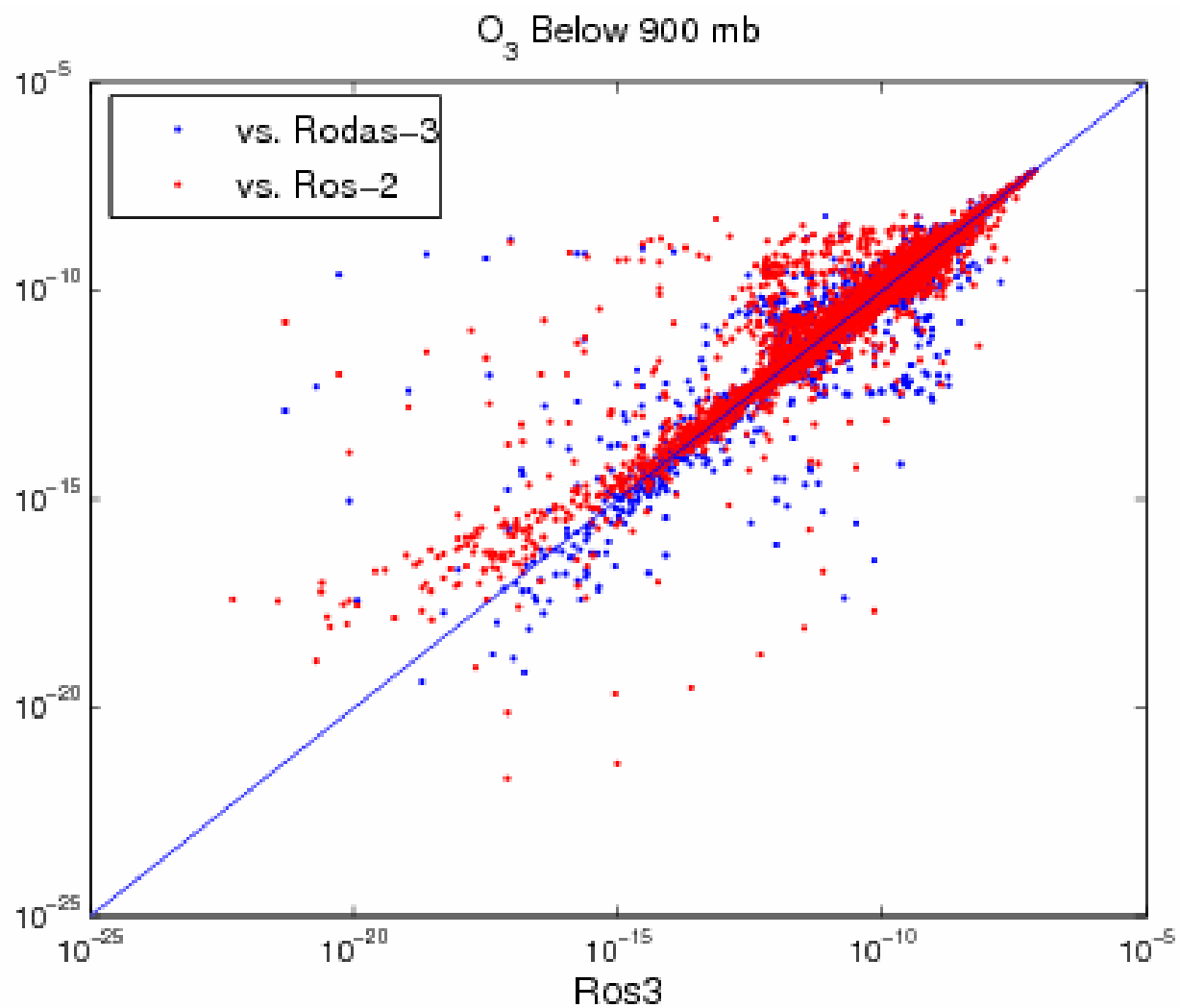
Preliminary Results: Intercomparison



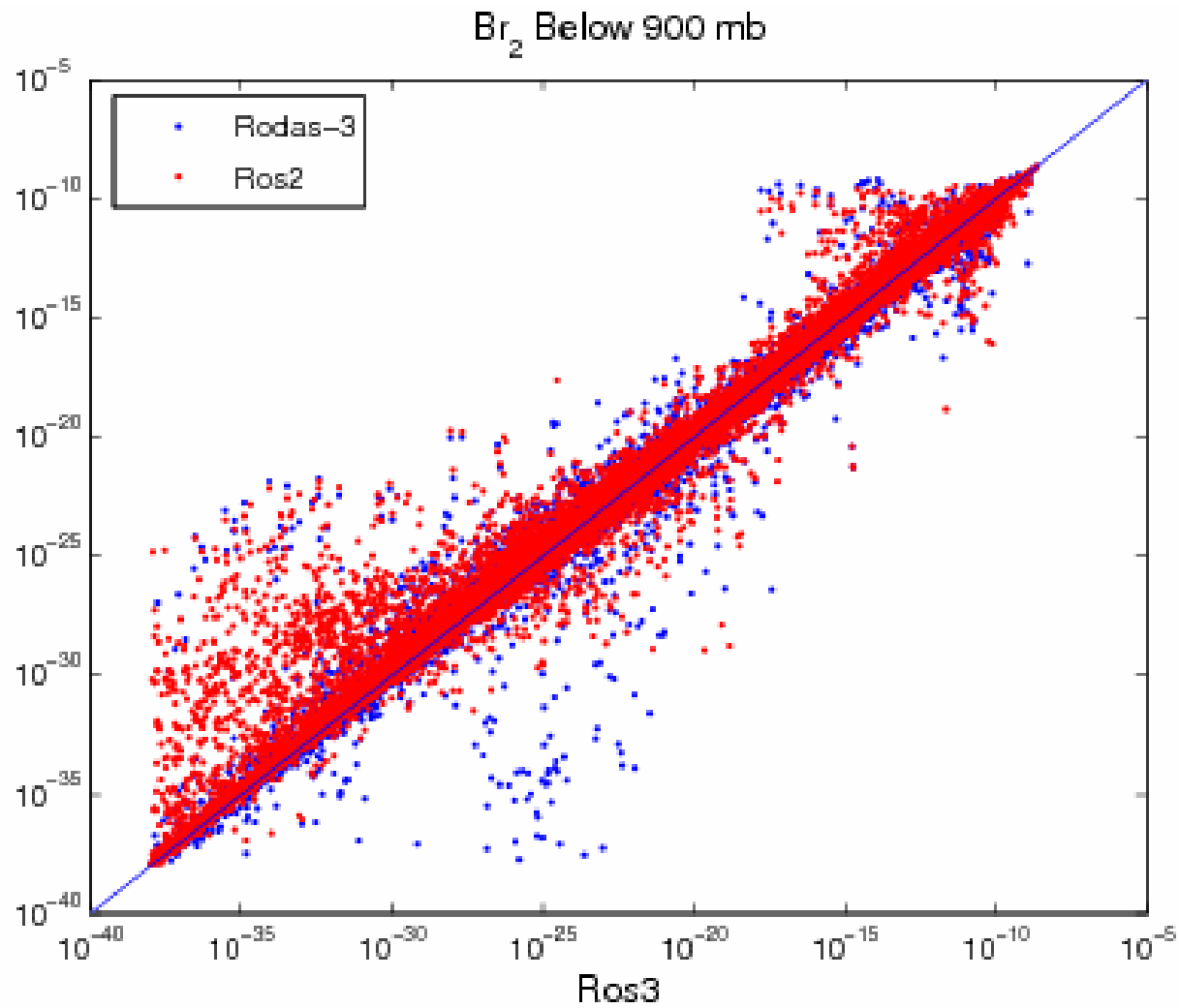
Preliminary Results: Intercomparison



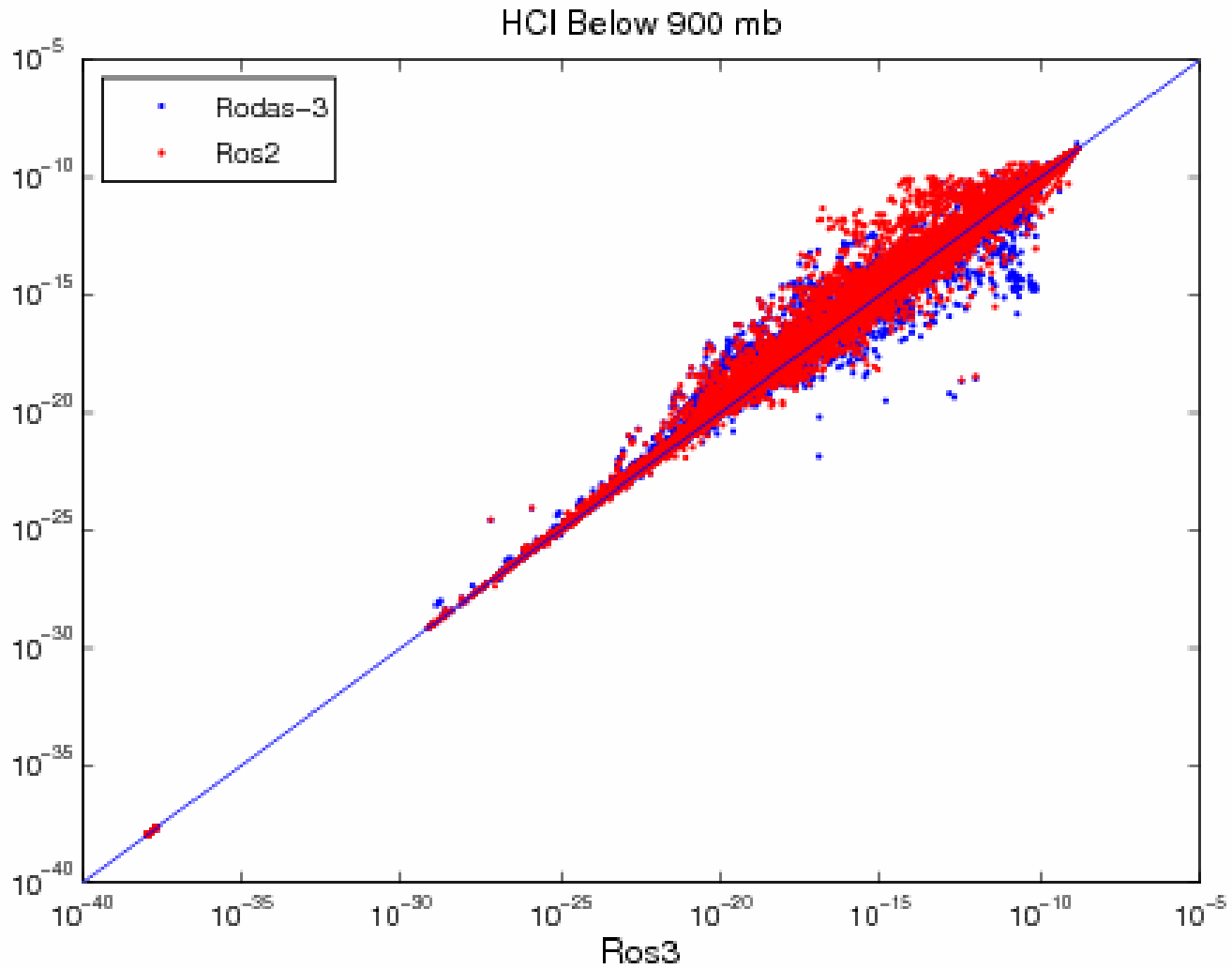
Preliminary Results: Intercomparison



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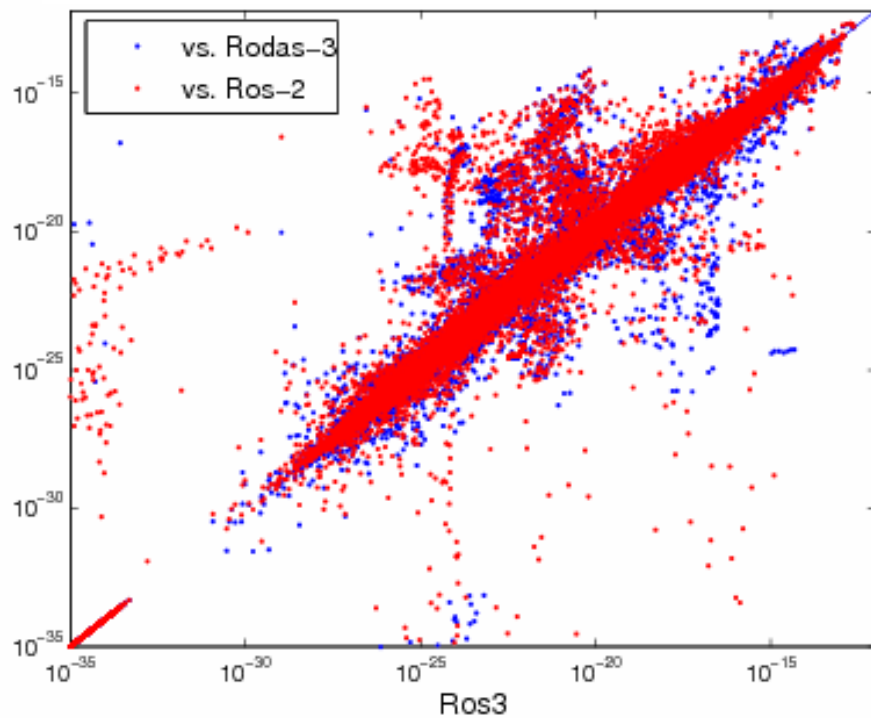


Preliminary Results: Intercomparison

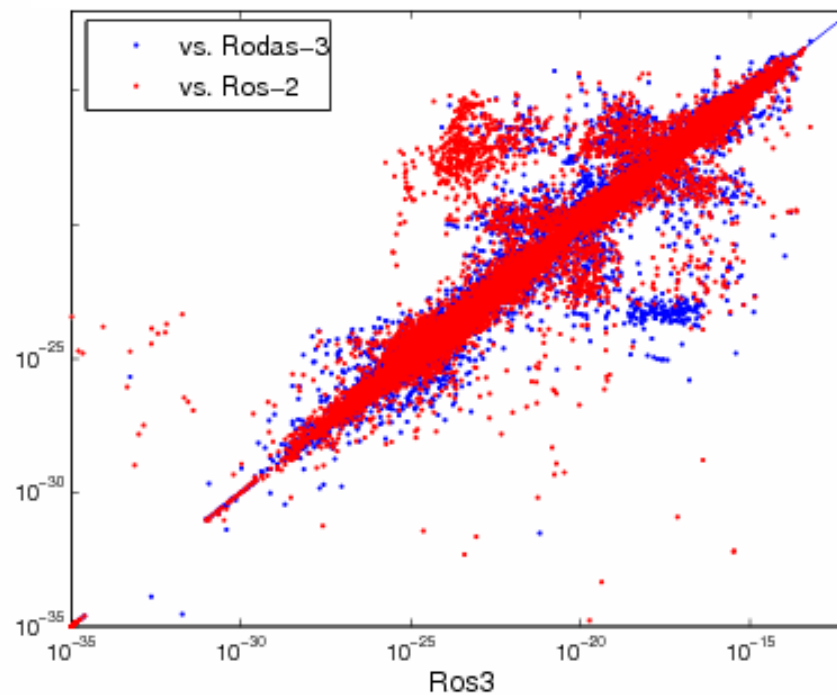


Preliminary Results: Intercomparison

H⁺ (aq.) Mode-1 Aerosol below 900 mb



H⁺ (aq.) Mode-3 Aerosol below 900 mb



Looking Forward: Short-term

- Can KPP be parallelized within CAM?
 - Abandon Sparse Algebra for Full → ScaLAPACK
 - Pseudo-operator splitting
- Remove short-lived species from dynamics
- Tune (loosen) the solver's tolerances
- 7-mode Modal-CAM (short-short-term)... ironically