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

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Image courtesy R. Sander
Image courtesy R. Sander
CAM Coupling

- CAM
  - MESSy Interface
  - MECCA

- Modal CAM Microphysics

Great Big ODE
- Photolysis
- Gas-phase
- Aqueous-phase
- Mass Transfer

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

- Dynamics
- Cloud Processing*

*Note: Cloud Processing is indicated with an asterisk.
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*
<table>
<thead>
<tr>
<th>3-mode ModalCAM with “Full” Chemistry</th>
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</thead>
<tbody>
<tr>
<td>• Modal-CAM v3_6_33 (10x15 resolution)</td>
</tr>
<tr>
<td>• FV Dynamics</td>
</tr>
<tr>
<td>• 156 active tracers (aq. &amp; gas) / 360 Reactions</td>
</tr>
<tr>
<td>• Spun-up*** from zero concentration vector</td>
</tr>
<tr>
<td>• 10-minute timestep</td>
</tr>
<tr>
<td>• with 1° Emissions</td>
</tr>
<tr>
<td>• 1-month run</td>
</tr>
</tbody>
</table>
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)

![Bar Chart]

<table>
<thead>
<tr>
<th></th>
<th>Simulation Years/Runtime Day</th>
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<tbody>
<tr>
<td>Ros2</td>
<td>0.8</td>
</tr>
<tr>
<td>Ros3</td>
<td>0.3</td>
</tr>
<tr>
<td>Rodas3</td>
<td>0.6</td>
</tr>
</tbody>
</table>

Simulation Years/Runtime Day
Preliminary Results: Intercomparison
Preliminary Results: Intercomparison
Preliminary Results: Intercomparison

![Graph showing O3 Below 900 mb](image)
Preliminary Results: Intercomparison

Br$_2$ Below 900 mb

- Rodas-3
- Ros2
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 \(\rightarrow\) ScaLAPACK
  - Pseudo-operator splitting

- Remove short-lived species from dynamics

- Tune (loosen) the solver’s tolerances

- 7-mode Modal-CAM (short-short-term)... ironically