Hemispheric Transport of Pollutants: Model Diagnostics and Performance Metrics

- How good are the models?
- What is the consistency of model-derived information? How model dependent are the results?
- How uncertain are the model predictions?
- What do the observations tell us about the quality of the calculation?
- How confident are we in the predictions? Are the important individual processes treated? …“correctly”?……
How do we build upon what is done and move beyond to address the most pressing issues for intercontinental transport of pollutants?

- Informed by model inter-comparison studies.
- Informed by comparisons of predictions with observations.
- Informed by process studies.
Model Intercomparison Studies Provide Valuable Information on Diversity of Model-Derived Information

Does low diversity reflect scientific understanding or consensus?

Textor et al., ACP, Atmos. Chem. Phys. Discuss., 5, 8331–8420, 2005
What do the agreements and disagreements with observations tell us?

Possible Reasons for Discrepancies:
- Emissions
- Meteorology
- Chemical processes
- Inaccuracy of measurements and representativeness

Comparison of observed surface ozone levels (black squares) and model ensemble mean (blue line). The observations are averages over several sites, and the black line represents the standard deviation. The blue shaded area gives the standard deviations of the model ensemble. The green area indicates the variation among the models, the upper line of the green shaded region gives the maxima of the model ensemble, the lower line gives the model ensemble minima.

Ellingsen et al., 2006
Ensemble Estimates are Important Outcomes from Intercomparison Studies

- However, caution is needed as the ensembles are typically not prepared from members that reflect the uncertainty in the system.

Summary of Major Sources of Uncertainty in the Calculations of Aerosol Columns

<table>
<thead>
<tr>
<th>Source</th>
<th>Emissions</th>
<th>Wet removal</th>
<th>Vertical Transport</th>
<th>Chemical Formation</th>
<th>Total Uncertainty</th>
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<tbody>
<tr>
<td>nss SO4</td>
<td>1.3</td>
<td>1.3</td>
<td>1.5</td>
<td>1.3</td>
<td>1.8</td>
</tr>
<tr>
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<td>3</td>
<td>2</td>
<td>1.5</td>
<td>--</td>
<td>3.9</td>
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<tr>
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<td>2</td>
<td>1.5</td>
<td>3</td>
<td>6.4</td>
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<td>5</td>
<td>1.3</td>
<td>1.5</td>
<td>--</td>
<td>5.4</td>
</tr>
</tbody>
</table>

*Bates et al., ACPD, in review, 2006*
Transport Mechanisms Play a Critical Role in Source Receptor Relationships --- so need to analyze them.

- Convection (dry/wet/deep/shallow)
- Warm conveyor belt lifting
- Post-frontal boundary layer transport
- Low level pre-frontal
- Advection in the westerlies
- Cold front subsidence
- Large-scale subsidence
- Mountain wave subsidence
- Boundary layer transport → FT (diff. spatial scales)

Orography / coastal circulation

Deficiencies to be examined:
- Dissipation of pollution plumes in FT in global models
- Scale of mixing issues: re-entrainment/venting

Liang et al., JGR, 2004
Regional Analysis and Transport Above the Boundary Layer Are Important Factors

*Textor et al., ACP, Atmos. Chem. Phys. Discuss., 5, 8331–8420, 2005*
Example: Results from Peace/ITCT2K2

Convection 8% of time accounts for ~35% of outflow flux

Oshima et al., JGR, 2004

What do the models tell us?

Figure 4. Vertical profiles of CO mixing ratio (10-s mean data) measured during the PEACE-B period. The black and gray lines denote CO mixing ratios sampled during flight 10 (14 May 2002) and the other flights, respectively.
What do the observations tell us?

**Model-based**

- Sulfate and Sulfur dioxide
  - Mass loading in the atmosphere: 0.30 Tg-SO₂ (4%)
  - Dry deposition: 1.74 Tg-SO₂ (21%)
  - Wet deposition: 2.72 Tg-SO₂ (32%)
  - Total emission: 8.40 Tg-SO₂
    - Anthropogenic: 6.11 Tg-SO₂
    - Volcanic: 2.29 Tg-SO₂

- Outflow from simulation domain
  - East: 2.27 Tg-SO₂ (27%)
  - West: 0.11 Tg-SO₂ (1%)
  - South: 0.02 Tg-SO₂ (0.2%)
  - North: 1.24 Tg-SO₂ (15%)

**Observation-based**

- ~40% exported

**Both approaches have large uncertainties!!**

Koike et al., JGR, 2003
<table>
<thead>
<tr>
<th></th>
<th>M₁</th>
<th>M₂</th>
<th>M₃</th>
<th>M₄</th>
<th>M₅</th>
<th>M₆</th>
<th>M₇</th>
<th>M₈</th>
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<td>SCAPE 2</td>
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*Sartelet et al., MICS*
<table>
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<th>MNGE (%)</th>
<th>Sulfate</th>
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<th>Nitrate</th>
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<td>Max</td>
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<td>Max</td>
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<td>1708</td>
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<td>--</td>
<td>--</td>
<td>59</td>
<td>147</td>
<td>282</td>
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For sulfate
- Variability is larger for models M₁-M₈ (60%) than for runs R₁-R₇ (27%).
- If R₈ (sensitivity to vertical diffusion) is taken into account, the variability for R₁-R₇ (49%) is almost as high as the variability for M₁-M₈.

For nitrate
- Variability is larger for models M₁-M₈ (1649%) than for runs R₁-R₇ (224%).
- If M₄ is not taken into account, the variability for R₁-R₇ (224%) is as high as the variability for M₁-M₈ (223%).
Source receptor relationships pose additional problems

What are the diagnostic metrics to use to understand the reasons for the differences?

Model Intercomparison Study (MICS) Asia: Source/Receptor Predictions
http://www.adorc.gr.jp/adorc/mics.html
Uncertainty in the Source-Receptor Relationships

Interannual Variability (25-yrs)

Distance between S/R

Journal Global Environmental Engineering, 2002
Transport to Asia

Wild, et al., 2004

viz. Newell and Evans [2000]
Super-imposed on the measurements are the trends in emissions – these are large in Asia
So de-convolution of the signal is challenging!
and Requires good measurements and models!!
Many of the key issues have to do with how the system responds to changes in emissions (e.g., S/R determined by emission perturbation)

O3 Violation-metric $(1 + 8 \text{ hr})$

July 2004

NOx Emissions

Hakami et al., in review 2005

Response of O3 metric wrt to emissions –(adjoint analysis)

Figure 2: Monthly gradients from various species emissions.
Adjoint analysis → Sources that contribute most to ozone violations

Response of O3 metric wrt to emissions – by sector

We need to evaluate model responses!

O3 Violation-metric

NOx Emissions

Hakami et al., 2005

Aggregated regional contributions to national metric
Model Diagnostics and Performance Metrics

How do we build upon what is done and move beyond to address the most pressing issues for intercontinental transport of pollutants?

✓ Informed by model inter-comparison studies.
✓ Informed by comparisons of predictions with observations.
✓ Informed by process studies.

What are the added activities needed to evaluate model performance related to hemispheric transport of pollutants?
Global /Regional Modeling → Impact of boundary conditions
Impact of BC on STEM Predicted CO and O3 During ICARTT

Observed and 60km-simulated CO and O3 mean profiles and standard deviations for all DC-8 flights (upper)