Current Status of SAPRC Mechanism Development

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Outline

• Mechanism development objectives
• Evaluating predictive capability
• SAPRC mechanisms: description, recent updates, plans
• Recommendations
Mechanism Development Objectives

• **Predictive capability**
  - First priority for mechanisms for regulatory models.
  - Requires evaluation of predictions against measurement data representing environments to be modeled

• **Consistency with accepted laboratory data and theories**
  - Necessary for scientific credibility. First priority for many research mechanisms
  - Reduces chance of compensating errors
  - *Sometimes consistency with accepted data is in conflict with predictive capability*

• **Appropriate condensation for the modeling application**
  - Too much condensation limits utility and accuracy
  - Too much detail wastes resources and may not increase accuracy
Evaluating Predictive Capability

- Conditions used to derive the evaluation data must be less uncertain than the mechanism being evaluated.
- Environmental chamber data provide the most practical test of mechanisms without emissions and meteorological uncertainties:
  - Has uncertainties and disadvantages: uncertain chamber effects, artificial conditions, etc.
  - Important uncertain parameters in many current mechanisms have to be adjusted to fit chamber data.
  - SAPRC mechanism development has always been closely linked to conducting and using chamber experiments.
- Ambient measurements provide an important and necessary test to predictive capability:
  - But uncertainties in ambient conditions limit utility for mechanism development and adjustment.
Problems with Evaluating Condensed Mechanisms Against Experimental Data

- Lumped model species (e.g., OLE1, PAR) do not really exist, so we cannot conduct experiments with them.
- Fits to data with representative compounds do not test how well the lumped model fits data for ambient mixtures.
- Experiments with mixtures can evaluate condensed mechanisms. But such evaluations have problems:
  - Cause of problems unclear if the fits are poor.
  - Good fits may be due to compensating errors or low sensitivity to errors for components.
  - May not be relevant when ambient mixtures are different.
- Evaluations against experimental data do not separately test for effects of condensation and errors in the chemistry.
Effects of VOC Lumping on Simulations of Ozone Formation Rates in Propene – NO\textsubscript{x} Chamber Experiments

\[ \Delta ([O_3] - [NO]) \text{ Model Error} \]

Initial Propene (ppm)

<table>
<thead>
<tr>
<th>Mole %</th>
<th>Compound</th>
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<tbody>
<tr>
<td>29%</td>
<td>Propene</td>
</tr>
<tr>
<td>24%</td>
<td>1-Hexene</td>
</tr>
<tr>
<td>12%</td>
<td>1-Butene</td>
</tr>
<tr>
<td>11%</td>
<td>1-Pentene</td>
</tr>
<tr>
<td>11%</td>
<td>1-Heptene</td>
</tr>
<tr>
<td>10%</td>
<td>C_9-C_{12} 1-alkenes</td>
</tr>
<tr>
<td>3%</td>
<td>3-Methyl-1-Butene</td>
</tr>
</tbody>
</table>

From ambient mixture used to derive reactivity scales
What is SAPRC?

• The SAPRC mechanisms are a series of gas-phase atmospheric chemical mechanisms developed primarily by W.P.L. Carter

• SAPRC stands for (California) Statewide Air Pollution Research Center, a research center at UCR where the mechanism was first developed in the 1980’s

• Research center name changed to APRC in 1990’s. Now SAPRC is just a name, and doesn’t mean anything else (like “NARSTO”)

# History of the SAPRC Mechanisms

<table>
<thead>
<tr>
<th>Year</th>
<th>Event</th>
</tr>
</thead>
<tbody>
<tr>
<td>1979-1980</td>
<td>First papers by Carter et al. on mechanisms</td>
</tr>
<tr>
<td>1985</td>
<td>Paper on mechanism generation for alkanes published</td>
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<tr>
<td>1987</td>
<td>Reports to EPA, USAF and CARB on multi-VOC mechanisms that served as basis for subsequent detailed SAPRC</td>
</tr>
<tr>
<td>1990</td>
<td>SAPRC-90 detailed mechanism developed and published</td>
</tr>
<tr>
<td>1991</td>
<td>Condensed SAPRC-90 for airshed models developed</td>
</tr>
<tr>
<td>1994</td>
<td>Paper on MIR and other reactivity scales using SAPRC-90</td>
</tr>
<tr>
<td>1999-2000</td>
<td>Reports on SAPRC-99 mechanisms. Current SAPRC mechanism generation system first developed</td>
</tr>
<tr>
<td>2008-2010</td>
<td>Reports and papers on SAPRC-07 detailed and condensed mechanisms. Mechanism generation system updated</td>
</tr>
<tr>
<td>2011-2012</td>
<td>SAPRC-11 for aromatics and aromatic SOA developed</td>
</tr>
<tr>
<td>2013-2014</td>
<td>Updates to gas-phase SAPRC planned. SOA uncertain</td>
</tr>
<tr>
<td>2015</td>
<td>Carter plans to be <em>really</em> retired. Future of SAPRC uncertain</td>
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</tbody>
</table>
Versions of the SAPRC Mechanisms: Mechanism Generation System

- Mechanism type: semi-explicit
  - Mechanism generation software used
  - Uses measured rate constants and branching where available, estimation methods where not
  - Reaction pathways <1% for single steps are ignored
  - Because of limitations, not currently used to generate complete mechanisms for models (but could in principle)

- Major limitations:
  - Not used for aromatics and cannot estimate reactions with radicals whose heats of formation cannot be estimated
  - Does not understand steric factors
  - Currently limited to generating mechanisms in presence of NO_x (peroxy + peroxy mechanisms not generated)
Versions of the SAPRC Mechanisms: Mechanism Generation System (cont’d)

- Utility
  - Full capability: alkane and alkene hydrocarbons, compounds with -O-, -OH, -CO-, -CHO, & -ONO₂ groups, simple amines
  - Partial capability: cyclic compounds, dialkenes, alkynes, compounds with -Cl and -F groups
  - Generates reactions with: OH, O₃, NO₃, hν (carbonyls), Cl (limited capability for alkenes)
- Used to derive SAPRC-07 mechanisms for >600 VOCs
  - Derives overall process for reactions in presence of NOₓ, eliminating most intermediate organic radicals
  - “Lumping Rules” used to derive lumped model species for each predicted products
- Documentation at http://www.cert.ucr.edu/~carter/SAPRC
- Now available online at http://mechgen.cert.ucr.edu
From Generated Mechanism to SAPRC-07: Lump Reactions, but Keep Chemical Detail

90% $\text{CH}_3\text{CH}_2\text{OH} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}(\cdot)\text{OH}$
5% $\text{CH}_3\text{CH}_2\text{OH} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}_2\text{O}$
5% $\text{CH}_3\text{CH}_2\text{OH} + \text{OH} \rightarrow \text{H}_2\text{O} + .\text{CH}_2\text{CH}_2\text{OH}$

90% $\text{CH}_3\text{CH}(\cdot)\text{OH} + \text{O}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2\cdot$

5% $\text{CH}_3\text{CH}_2\text{O}$ + $\text{O}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2\cdot$

5% $\cdot\text{CH}_2\text{CH}_2\text{OH} + \text{O}_2 \rightarrow \cdot\text{OOCH}_2\text{CH}_2\text{OH}$
5% $\cdot\text{OOCH}_2\text{CH}_2\text{OH} + \text{NO} \rightarrow \text{NO}_2 + .\text{OCH}_2\text{CH}_2\text{OH}$
1% $\cdot\text{OCH}_2\text{CH}_2\text{OH} + \text{O}_2 \rightarrow \text{HOCH}_2\text{CHO} + \text{HO}_2\cdot$
4% $\cdot\text{OCH}_2\text{CH}_2\text{OH} \rightarrow \text{HCHO} + .\text{CH}_2\text{OH}$
4% $\cdot\text{CH}_2\text{OH} + \text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2\cdot$

$\text{CH}_3\text{CH}_2\text{OH} + \text{OH} \rightarrow 0.95 \{\text{HO}_2 + \text{CH}_3\text{CHO}\} + 0.08 x\text{HCHO} + 0.01 x\text{HOCH}_2\text{CHO}$
$+ 0.05 \{x\text{HO}_2 + \text{RO}_2\text{C} + y\text{ROOH}\}$
Versions of the SAPRC Mechanisms: Adjusted Product “Detailed” Mechanisms

- Mechanism type: detailed VOC, semi-explicit + lumped products
  - Mechanisms for reactive product lumped model species derived based on mechanisms for products they represent
  - Used for VOCs whose primary and reactive product mechanisms could be derived by mechanism generation
  - Lower reactivity or lower yield (<5%) products represented using lumped product model species
  - Used for reactivity scale calculations if this method changed the SAPRC-99 “averaged conditions” MIR by >8% (134 VOCs)
  - Not currently used for other purposes, but could potentially be the basis for deriving an explicit product version of SAPRC (comparable in size or larger than MCM)
Versions of the SAPRC Mechanisms: Lumped Product “Detailed” Mechanism

- Mechanism type: explicit VOC, lumped products
  - Used in reactivity calculations (in conjunction with a lumped VOC version that represents the base ROG mixture)
  - Mechanisms for >600 VOCs from mechanism generation
  - Mechanisms for ~130 others estimated using other means
  - 31 model species used to represent organic products
- Ozone predictions extensively evaluated against chamber data
  - >2500 experiments, 11 chambers, 4 laboratories
  - $\Delta([O_3]-[NO])$ generally simulated within $\pm$ 30%
- Used to calculate MIR and other VOC reactivity scales
  - 774 calculated explicitly, 407 others based on explicit VOCs
  - “Adjusted product” version used for 134 VOCs (next slide)
- **Used to derive the lumped VOC versions of SAPRC-07**
Differences Between Adjusted Product and Lumped Product Ozone Reactivity Values

- SAPRC-07 Results should be similar
- Differences may be greater for multi-day scenarios
Versions of the SAPRC Mechanisms: SAPRC-07 Lumped VOC Mechanisms

- Mechanism type: lumped VOC
  - Developed for use in airshed models.
  - Same inorganic and lumped product mechanisms as detailed
  - 10 Lumped VOC species: ALK1-5, OLE1-2, ARO1-2, TERP
  - Currently two versions:
    - Standard version: methane, ethene, benzene, isoprene, acetylene explicit (total of 15 VOC species)
    - “Toxics” version: these + 11 other selected VOCs explicit
- Derived from explicit VOC, lumped product mechanisms, with lumped VOC reactions based on the compounds they represent
  - Weighting factors from base ROG mixture used in reactivity scales. (But ambient mixture needs updating)
  - Used to represent base case when calculating reactivity scales
Versions of the SAPRC Mechanisms: CSAPRC-07 Condensed Mechanisms

- Mechanism type: lumped VOC
  - Developed for giving almost same O₃ in airshed calculations as standard lumped SAPRC-07 with fewer model species.
  - Number of organic product model species reduced from 30 to 13, VOCs species reduced from 15 to 10.
- Derived from standard lumped SAPRC-07
  - Test calculations used to examine incrementally increasing lumping effects on O₃, NOₓ, H₂O₂, OH and total PANs.
    - Static, dynamic, multi-day ambient simulations
    - Static simulations with individual types of VOCs
  - Most extensive condensations that did not significantly affect O₃ results were adopted for CSAPRC07
Ozone Changes Caused by Condensations

Average of absolute change in $O_3$ for scenarios at various ROG and NO$_x$ levels, relative to uncondensed SAPRC-07

Condensation Levels

<table>
<thead>
<tr>
<th>Condensation Levels</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>SAPRC-99 Peroxy lumping</td>
</tr>
<tr>
<td>1</td>
<td>(A) + Low reactivity product compounds lumped</td>
</tr>
<tr>
<td>2</td>
<td>(1) + Higher PANs lumped with PAN2</td>
</tr>
<tr>
<td>3</td>
<td>(2) + 1-Product isoprene mechanism</td>
</tr>
<tr>
<td>4</td>
<td>(3) + Aromatics mechanism simplified</td>
</tr>
<tr>
<td>6</td>
<td>(4) + Fewer lumped species for alkanes (CSAPRC-07)</td>
</tr>
<tr>
<td>7</td>
<td>(6) PAN lumped with PAN2 (Change too great, not used)</td>
</tr>
<tr>
<td>8</td>
<td>(7) + Acetaldehyde lumped with RCHO (Not used)</td>
</tr>
</tbody>
</table>
Effects of Lumping on SAPRC-07 Ozone Predictions for a Multi-Day Scenario

- 5-Day simulations with Continuous emissions
- Same ambient mixture as used to derive the lumped mechanism
Relationships Between Current Versions of the SAPRC-07 Mechanisms

Mechanism Generation System (~620 VOCs) → Adjusted product Detailed VOC Mechanisms → VOC Reactivity Scales


Assigned Lumped Product Mechanisms for ~45 Other VOCs → Base Mechanism (Inorganics and Organic Products) → Standard Ambient VOC Mixture

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Updates to SAPRC-07:
SAPRC-11 Gas-Phase Aromatics Mechanism

- Mechanism type: Explicit VOC, lumped products
- Same base mechanism as SAPRC-07, with minor corrections
- Aromatic mechanisms revised, but same general approach
  - Much better fits to results of many new aromatic – NOx experiments, especially at lower concentrations
  - Rate constants, known product yields updated
  - Data and mechanisms for additional compounds
  - Much more reactive mechanisms for phenols
- Most inconsistencies and problems with SAPRC-07 remain
  - Chamber data for benzene and toluene have greater dependence on NO$_x$ than indicated by product studies
  - OH radical levels are still significantly underpredicted
- Lumped versions for airshed models not yet developed
Features of SAPRC-11 Aromatic Reactions

These reactions are necessary to fit O₃ data for high NOₓ benzene and toluene chamber experiments.

Photolysis Quantum yields adjusted to fit chamber data.
Problem with NO\textsubscript{x} Dependences on Benzene and Toluene Model Fits

- Benzene and toluene models adjusted for runs with NO\textsubscript{x}<100 ppb overpredict O\textsubscript{3} formation rates at higher NO\textsubscript{x}.
- Data can be fit if a reaction of the OH-aromatic adduct with NO\textsubscript{2}, forming lower reactivity products, is added, and k(O\textsubscript{2}) / k(NO\textsubscript{2}) is adjusted to fit the chamber data.
- *The NO\textsubscript{2} levels where the rates of the NO\textsubscript{2} and O\textsubscript{2} reactions are equal are not consistent with laboratory product yield data.*

<table>
<thead>
<tr>
<th>Compound(s)</th>
<th>Fits Chamber Data</th>
<th>Derived from Lab Studies</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene</td>
<td>~ 10 ppb NO\textsubscript{2}</td>
<td>~ 1 ppm NO\textsubscript{2}</td>
</tr>
<tr>
<td>Toluene</td>
<td>~ 200 ppb NO\textsubscript{2}</td>
<td>~ 3 ppm NO\textsubscript{2}</td>
</tr>
<tr>
<td>Most others</td>
<td>(Reaction not needed)</td>
<td>Higher NO\textsubscript{2}</td>
</tr>
</tbody>
</table>

- *This is a case where apparent predictive capability and accepted laboratory data disagree.*
### Photoreactive Dicarbonyls: Total Yields and Adjusted Quantum Yields

<table>
<thead>
<tr>
<th>Compound</th>
<th>Total Yields</th>
<th>Radical Quantum Yields</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene</td>
<td></td>
<td>(based on $\alpha$-dicarbonyl co-product yields)</td>
</tr>
<tr>
<td>Toluene</td>
<td></td>
<td>(adjusted to fit low NO$_x$ chamber data)</td>
</tr>
<tr>
<td>Ethyl benzene</td>
<td></td>
<td></td>
</tr>
<tr>
<td>n-Propyl benzene</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Isopropyl benzene</td>
<td></td>
<td></td>
</tr>
<tr>
<td>o-Xylene</td>
<td></td>
<td></td>
</tr>
<tr>
<td>o-Ethyl toluene</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m-Xylene</td>
<td></td>
<td></td>
</tr>
<tr>
<td>m-Ethyl toluene</td>
<td></td>
<td></td>
</tr>
<tr>
<td>p-Xylene</td>
<td></td>
<td></td>
</tr>
<tr>
<td>p-Ethyl toluene</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,2,3-Trimethylbenzene</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,3,5-Trimethylbenzene</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- **Compound**
- **Total Yields**
- **Radical Quantum Yields**

*W. P. L. Carter  12/18/2012  Status of Mechanism Development*
Average Model Biases for Compounds

\[\Delta([O_3]-[NO])\] Formation Rate ([NO\textsubscript{x}] < 90 ppb)

Integrated OH Levels

Large improvement in fits for phenols

SAPRC-11
SAPRC-07


Average Model Bias

-90%  -60%  -30%  0%  30%
Plots of $\Delta ([O_3] - [NO])$ Model Errors against VOC / NO$_x$ for the Surrogate – NO$_x$ Experiments

Initial Surrogate / NO$_x$ Ratio (ppmC / ppm)
SAPRC-11 Aromatic SOA Mechanism

- Results of 164 aromatic – NO\textsubscript{x} and 126 aromatic – H\textsubscript{2}O\textsubscript{2} experiments in UCR-EPA chamber used to develop predictive SOA model for 14 aromatic hydrocarbons and 3 phenols
  - Experiments described in presentation by David Cocker
  - Characterized for both gas-phase and PM evaluations
- SAPRC-11 gas-phase mechanism used as the starting point. No changes made that affect gas-phase predictions
- Lumped SOA precursor model species added to mechanism as needed to predict how SOA affected by reaction conditions
  - No more species added than needed. No attempt to identify specific SOA species. Insufficient information for more detail.
  - Yields and partitioning coefficients adjusted to fit data
- Results documented in report to CARB and will be described in a presentation at the CARB on Friday, December 14.
Aromatic SOA Processes Used

Aromatic Hydrocarbons
- OH
- O₂
- NO
  Abstraction products (all volatile)
  - OH-aromatic adducts
  - OH-aromatic-\(O₂\) adducts

Phenols
- OH
- \(\text{NO}_3\)
- OH
- \(\text{NO}_3\)
  Condensable Phenolic ROOH's
  - \(\text{OH} + \text{volatile products}\)
  - \(\text{OH}, \text{O}_2, \text{NO}\)
  Other Condensables
  - \(\alpha\)-Dicarboxyls and other photoreactive products (all volatile)

Catechols
- OH
- \(\text{NO}_3\)
  Volatile Products

Other Phenolic Condensables
- OH
- \(\text{NO}_3\)
  Volatile Products

Condensable ROOH's
+ Volatile ROOH's

Bicyclic peroxo radicals

Volatile products

\(\text{HO}_2\)
Model Fits for All Experiments used to Derive Aromatic SOA Parameters

Aromatic – NO$_x$ Runs

Aromatic – H$_2$O$_2$ Runs

-200%
-100%
0%
100%
200%

1 10 100 1000

Phenol
o-Cresol
2,4-Xylenol

Aromatic Hydrocarbon
 Added CO or VOC
Distribution of Error Ranges in PM Volume Predictions for all Experiments Modeled

Model Bias Range

-150% - 150%

Fraction of Runs

0% 10% 20% 30% 40%

SOA Fits - All Runs
Used for SOA optimizations
Not used for optimizations

Ozone Fits shown on same scale for comparison

OH adjusted to fit amounts of VOC Reacting

Fit to O3 formation rates
Fit to amounts of O3 formed
No OH Adjustments

SOA Fits - All Runs
Used for SOA optimizations
Not used for optimizations

Fit to O3 formation rates
Fit to amounts of O3 formed
No OH Adjustments
Relative Contributions of Phenolic Products to SOA from Aromatic Hydrocarbons

Averages calculated for aromatic - NO\textsubscript{x} and Aromatic - H\textsubscript{2}O\textsubscript{2} runs

Predicted using parameters adjusted to fit SOA chamber data
Optimized Hydrocarbon SOA Yield Parameters

<table>
<thead>
<tr>
<th>Aromatic Hydrocarbon</th>
<th>SOA Precursor ROOH</th>
<th>Gas-Phase RAOOH</th>
<th>Other SOA Precursors</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene</td>
<td></td>
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</table>

Model Species Yield (molar)
Discussion of Aromatic SOA Mechanism

• Aromatics mechanisms remain highly uncertain and SOA formation even more complex and uncertain
  • Insufficient knowledge to derive useful explicit mechanisms
• Adjusted lumped product mechanisms can simulate available SOA as well as $O_3$ chamber data with relatively low biases
  • Generally reasonable representation of overall processes, but effects of molecular structure on parameters are unclear
• Parameters from fits to yield curve using equilibrium partitioning models do not fit to the same data using kinetic mechanisms
  • May be due to using finite condensation rates in simulations
• Simulations of SOA in chamber experiments have much more scatter and higher model errors than simulations of ozone
  • Suitable adjustments can give low systematic biases, but model errors remain high. The scatter can hide biases.
  • Cause of scatter is unknown, but is probably experimental
Recommended Next Steps for SOA Mechanism Development

• SOA mechanism development is limited by data availability
  • *Projects without a strong experimental component will yield little progress towards a predictive modeling capability*

• Additional experiments needed to expand scope and evaluation of current SOA mechanism. Need *new, well characterized* data on:
  • Effects of temperature, humidity and PM from other sources
  • Evaluation data for other types of important SOA precursors
  • Improved characterization and inter-laboratory comparisons
  • Available chamber data from different laboratories should be compiled, characterized, compared, and used if adequate

• Use the data obtained to update and expand the scope of the detailed mechanism to other VOCs and conditions

• Use the evaluated detailed mechanism to develop and evaluate condensed SOA mechanisms for regulatory modeling
SAPRC Update Projects Currently Underway

- Documentation of SAPRC modeling software and data files
  - Software used for SAPRC mechanism development, evaluation, and use is finally being documented
  - Data files and spreadsheets implementing SAPRC will also be documented and made available for future developers
- Mechanism generation system updates and documentation
  - Estimation methods and assignment database to be updated
  - Publication documenting updated system being prepared
  - Web access being improved (see mechgen.cert.ucr.edu)
- General mechanism updates (detailed and lumped VOC)
  - Complete update of base mechanism
  - Incorporate aromatic and mechanism generation updates
  - Evaluate changes in peroxy and VOC product lumping approaches (implementation mostly for the follow-on project)
SAPRC Update Project Currently Planned

- Develop improved VOC product lumping approach
  - Separate representation of unsaturated PANs and nitrates needed to improve predictions of NO$_x$ recycling
  - Separate representation of higher molecular weight products needed to support process-based SOA modeling
  - Objective is to improve detail for predictive capability, but not more than needed or can be supported by theories and data
- Continue attempting to improve aromatic mechanisms
  - Improve mechanism generation support for aromatics
  - Objectives are to improve
    - Level of detail that is supported by data and theories
    - Consistency with both laboratory and chamber data
- Work on on gas-phase improvements to eventually aid future SOA models being developed by other groups
Proposed SAPRC Updates
Not Currently Funded

• Continue steps needed to develop SAPRC SOA mechanism
  • Requires new well-characterized chamber experiments
  • Use results to develop explicit VOC, lumped product mechanisms with enough detail to represent major processes
  • Use the detailed and experimentally evaluated mechanism to develop condensed mechanisms for regulatory models
• Develop near-explicit SAPRC mechanisms that are chemically consistent with existing condensed SAPRC mechanisms
  • Mechanism generation system can be adapted to produce models with any level of detail based on current estimates
  • Allows comprehensive studies of condensation effects
  • Update or alternative to MCM for similar research needs
  • Potential framework for detailed SOA modeling when basic understanding improves
General Recommendations for Mechanism Development

• *Investment in chamber experiments* with high characterization standards is critical to developing predictive mechanisms
  • We would not have reliable models for ozone without the well characterized chamber database developed since the 1970’s
  • SOA is more complicated, requires more data, and the availability of suitable data is limited. *This is the main factor limiting predictive SOA model development*

• Start by developing and evaluating the *most chemically detailed mechanism possible* given the available state of knowledge
  • Developing more scientifically valid condensed mechanisms, based on a more detailed understanding, can follow

• *Mechanism generation* is the “wave of the future”
  • Provides a framework to organize theory and data
  • Research in improving estimation methods (including thermochemical) needs to be given higher priority
Acknowledgements

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