Development and Application of a Lagrangian Process Analysis Tool for Tracking the Chemistry of Plumes within a 3-D Eulerian Photochemical Model

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Yosuke Kimura
David T. Allen
University of Texas at Austin
Outline

- Conventional Process Analysis
- Lagrangian Process Analysis
  - Motivations
  - Design Principles
- Example Cases
  - Process Time Series of Selected Species
  - Selected Reaction Cycles Metrics
  - Comparison of Cycles Metrics using Two EI
- Summary and Potential Applications
What is Process Analysis (PA)?

- A diagnostic tool for photochemical models
  - Assessing the relative impacts of key chemical and physical processes on model predictions
  - Examining whether the underlying reasons for the model behavior are correct and consistent with observations
Lagrangian PA: Motivation and Design
Eulerian Modeling Domain and Houston-Galveston Area
Houston-Galveston Area

Left: NO\textsubscript{x} Emission
Right: VOC Emission

Units: short tons/day
(\sim0.9 metric ton/day)
Houston High O₃ events
9/14/2006

- Wind field shown by wind barbs
- Number shows ground level O₃ in ppb

Source: http://www.tceq.state.tx.us/compliance/monitoring/air/monops/sigevents06.html
Motivation for Lagrangian Process Analysis (LPA)

- Conventional PA has only been applied in an Eulerian framework either on
  - Per grid-by-grid basis
  - Pre-defined “box” within modeled domain, metrics aggregated
- Limitations: cannot track the chemical evolution within plumes that travels
Design of LPA

- Inert tracer is introduced at user-specified time and location. LPA box is defined based on tracer concentration (region where tracer concentration is high)
- Operator splitting of in host Eulerian model allows separation of transport processes from movement of LPA box
- Process metrics are integrated at instantaneous location of the plume
- CAMx 4.20 is used as a host Eulerian model

→ Allows Process Analysis on moving air body
Conceptual View of LPA

- The diagram shows the order operations applied in CAMx
- When advection is calculated in CAMx, instantaneous location of LPA box was redefined to the new location thereby canceling the concentration change due to advection by LPA box movement
Example Application:
8/25/2000, Houston, TX
Tracer (LPA box) location
Released over the Ship Channel @10:00am, 8/25/2000

White mass represents location of PA box (inert tracer)

Color represents ground level $O_3$ concentration

Stagnant until ~13:00, then flows to the west toward downtown
Process Time Series Analyses:

- Nitrogen Species
  - $\text{NO}_x$
  - NO
  - NO$_2$
- VOC Species
  - All VOC
  - Terminal Olefins
- Ozone
NO$_x$ is continually emitted during the day with peak photochemical loss at noon. “Adj.” corresponds to noise in concentration curve (due to box movement).
Emitted NO is rapidly consumed by chemistry especially mid-day.
**Process Time Series: NO₂**

- **Concentration or Concentration Change (ppb or ppb/hr)**

- **Conc.**
- **Chem.**
- **Low Emi.**
- **Elev. Emi.**
- **Horiz. Adv. (Adj.)**
- **Horiz. Diff.**
- **Vert. Adv. (Adj.)**
- **Vert. Diff.**
- **Depo.**

**NO₂** is also net chemical loss except in the morning (NOₓ termination)
Emitted throughout day, relatively faster chemical consumption mid-day
Relative change in concentration is not pronounced
Process Time Series: OLE (CB4)

Almost exclusively emitted before 13:00 when the plume is in the Ship Channel. Monotonically decreases due to rapid chemistry.
Concentration continually builds up until 4:00 pm
Concentration change in the plume is due entirely to chemistry, not physical processes
Budget of radicals and NO\textsubscript{x} characterizes the ozone chemistry. Source strength, overall throughput rate, termination rate, re-use efficiency (chain length), are some of quantitative metrics for the system.
Radical and NO\textsubscript{x} Cycles

Radical throughputs synchronized with light intensity
Radical chain length stays constants throughout the day
Abundant NO in the morning makes NO\textsubscript{x} chain length short
Increased radical availability mid-day makes higher utilization of NO\textsubscript{x}
Second set of EI: Future Year (2007) with Control

Values are for eight counties for greater Houston region
Large NO$_x$ reduction in point source
Selective reduction of high-reactivity VOC from point sources (by >70%)
Source: http://www.tceq.state.tx.us/implementation/air/sip/dec2004hgb_mcr.html
2007 case has 1) Decreased radical and NO\textsubscript{x} throughput and 2) Higher NO\textsubscript{x} efficiency
Summary

- Lagrangian Process Analysis (LPA) tools allow application of conventional Process Analysis (PA) approach to moving air mass.
- The results show that LPA is particularly suitable for studying the role of chemistry in the air, as the effect of transport on species concentration tends to be cancelled out.
Potential Applications

- Model Verification: TexAQS II study gives ambient concentration including photochemical intermediates. Match/mismatch of those species between model/obs can be evaluated using LPA with focus on evolution of chemistry.
- Industrial Upsets Simulation: What is the consequence of additional emissions to the downwind atmosphere? How chemistry is affected?
- Others? → mailto:yosuke@ccwf.cc.utexas.edu
This page requires inputs from Dr. Allen
yosuke kimura, 11/17/2006
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Backup slides follow:
Process Time Series: HNO₃
Process Time Series: NO$_2$
Process Time Series: Ethene
Process Time Series: HCHO
Process Time Series: Isoprene
Process Time Series: ALD2 (CB4)

![Graph showing the process time series for ALD2 (CB4)]
Summary Case Study: 8/25/2000 Houston

- Air is rich with olefins in the Ship Channel.
- Plume is continually receiving NO emissions while it travels through the Ship Channel and Houston downtown.
- NO\textsubscript{x} is continually oxidized during the day forming, e.g., HNO\textsubscript{3}.
- Ozone levels continue to increase until 4:00 pm.