Stochastic Modeling of Ambient Ozone Formation with Emission Variability

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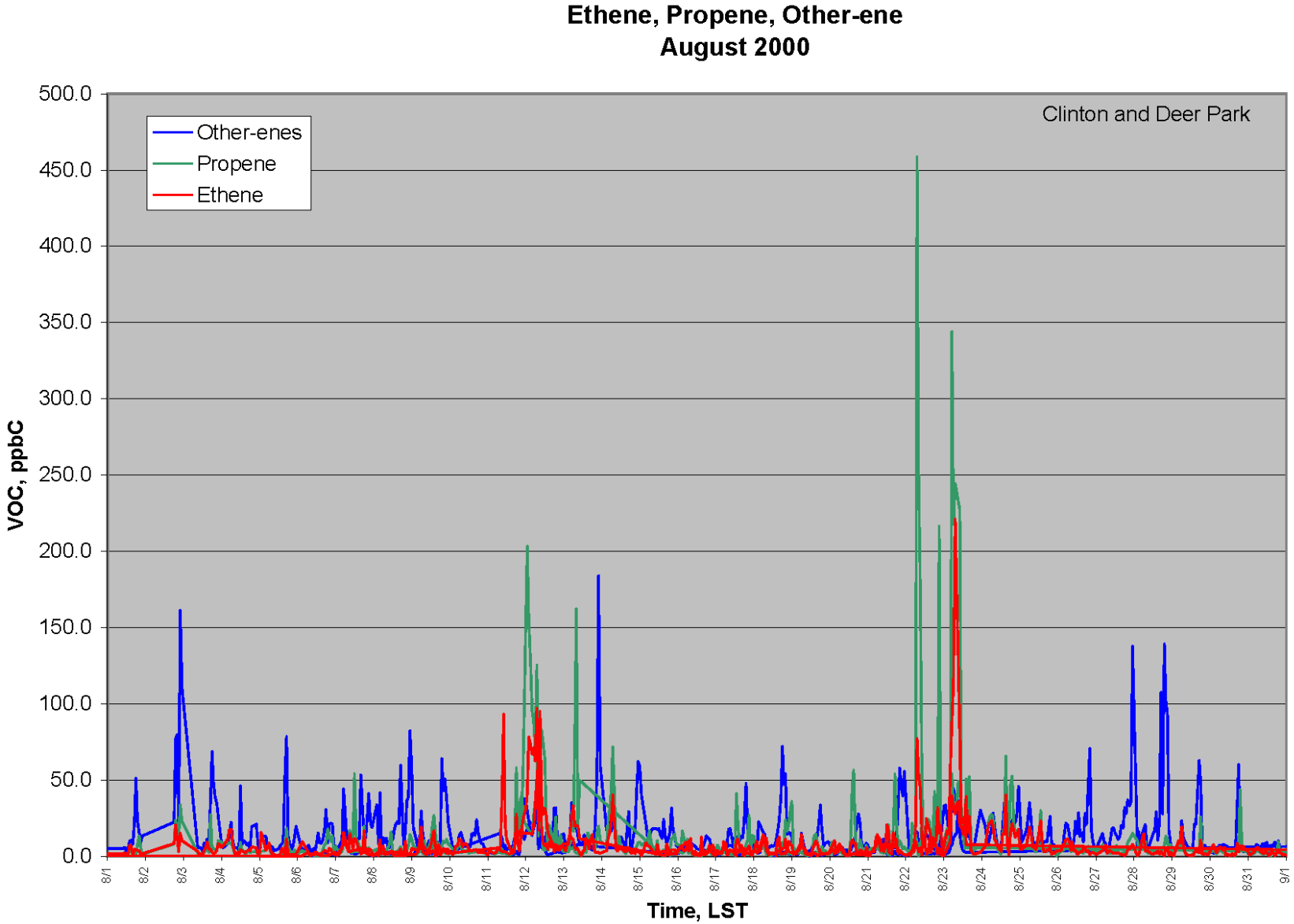
Stochastic nature of EI

- Point source emissions have typically been assumed to be constant
- However, recent studies suggest that emission of reactive VOCs from industrial area may vary greatly (100s to 1000s times) on an hourly basis
- Industrial process operation records support that such variability can occur

Auto-GC (Industrial Area)

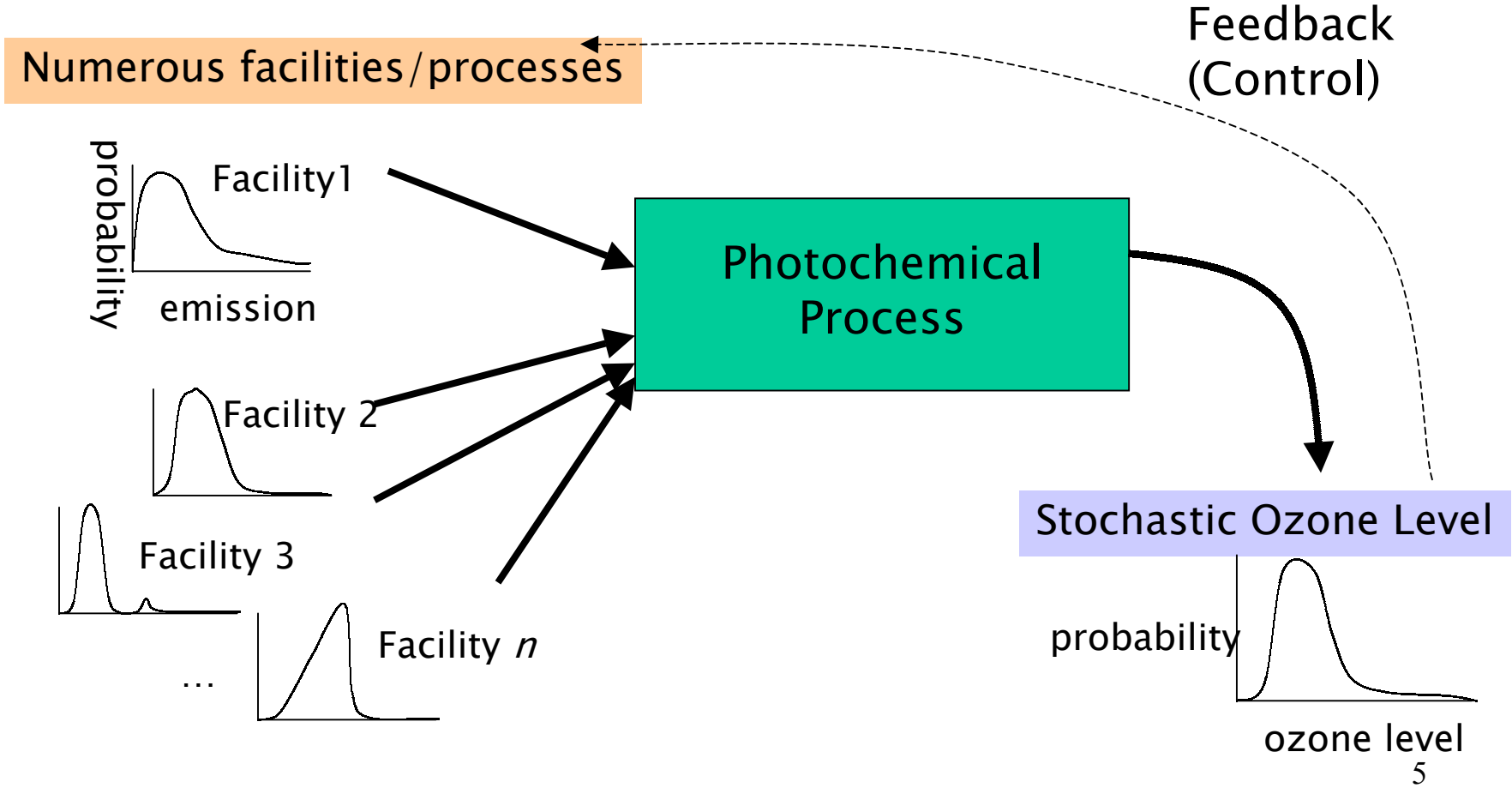


Sexton, Jeffries, 2001

Implication for Ozone Formation/Modeling

- Variability in emissions leads to variability in ozone formation
- Stochastic simulation, e.g. Monte Carlo simulation, is needed in order to characterize the variability in ozone formation

Implication for Ozone Formation/Modeling



Outline of Approach

1. Develop a stochastic EI
2. Develop a scheme modeling ozone formation for large numbers of emission scenarios
3. Stochastic simulation by applying (1) to (2) to examine variability of ozone formation
4. Analyze relationships between emission and ozone formation

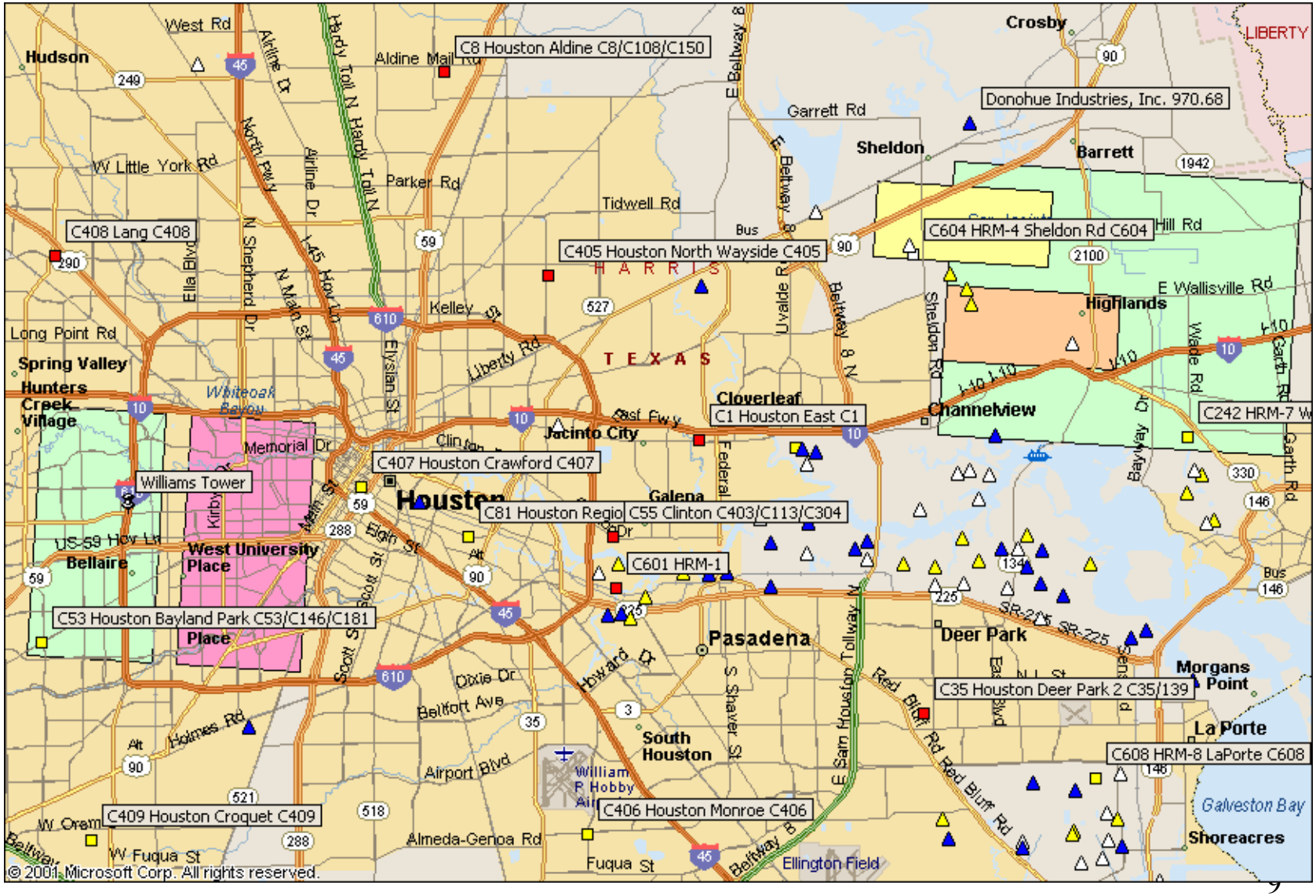
What AQ Modeling Tool Do We Use?

- **Eulerian grid models** – Most accurate among available tools, but computationally too expensive for stochastic simulation
- **Sub-domain model** – Coupled closely with a grid model in terms of photochemical property and other characteristics, sub-domain model becomes suitable tool for stochastic simulation
- **Process Analysis Tools** are used to match box model with a grid model

Develop a Coupled Box Model

- Historic episode is created using measurements in a field study (TexAQS2000) and stochastic EI
- Industrial source regions are selected and photochemistry in the region is evaluated with Process Analysis
- Box model episode is developed for the above region
  1. Boundary conditions for the region are extracted from the gridded model to run the box model
  2. Process analysis confirms that the nature of photochemistry is reasonably close between grid model and box model

Selection of the Region



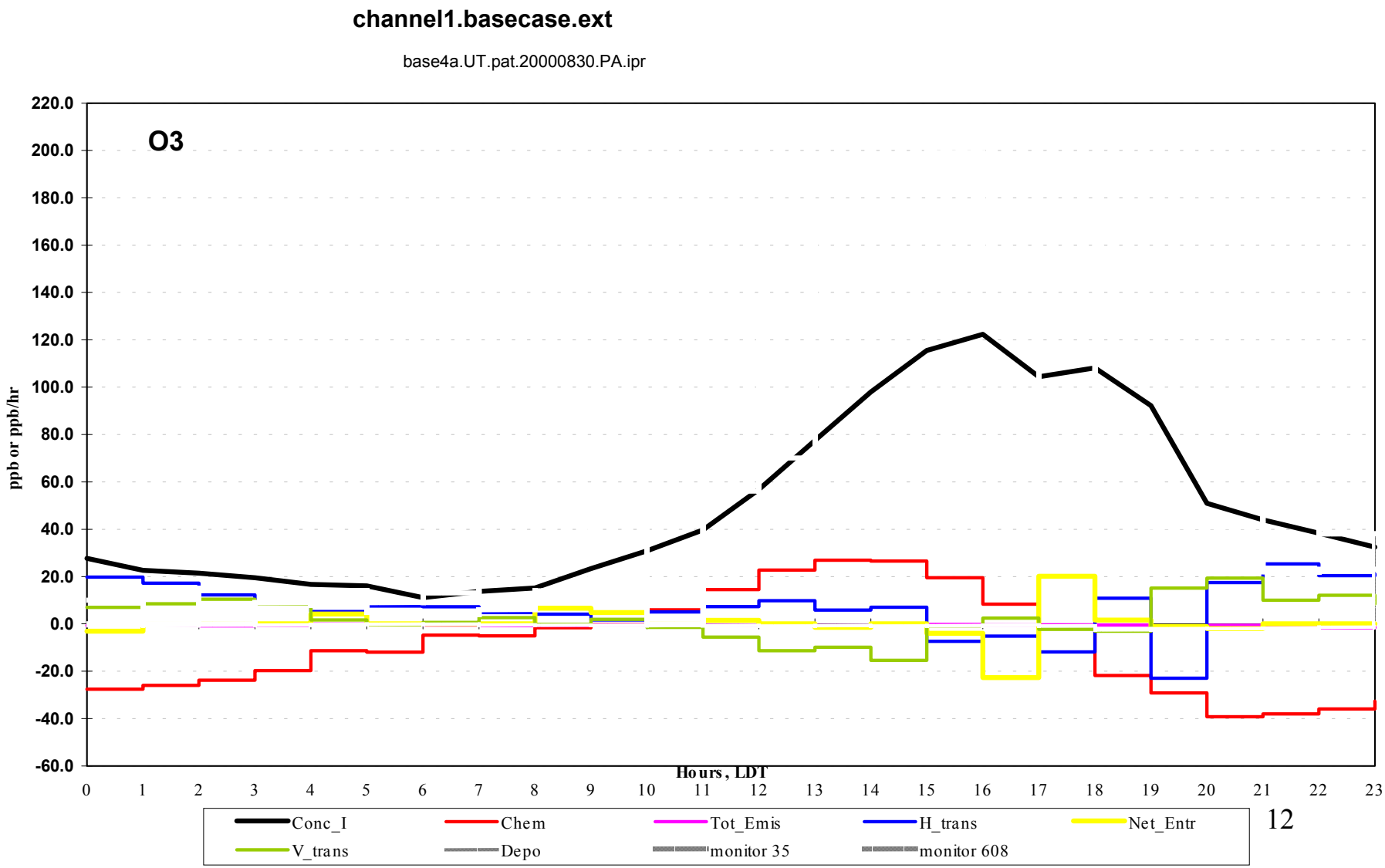
Parameters Extraction

- Following parameters are extracted from grid model to drive the box model
  - Initial concentration
  - Mixing height
  - Aloft concentration
  - Horizontal exchange rate
  - Upwind concentration
  - Emission rate
  - Deposition velocity
  - Photolysis rate
  - Temperature/Pressure/Humidity

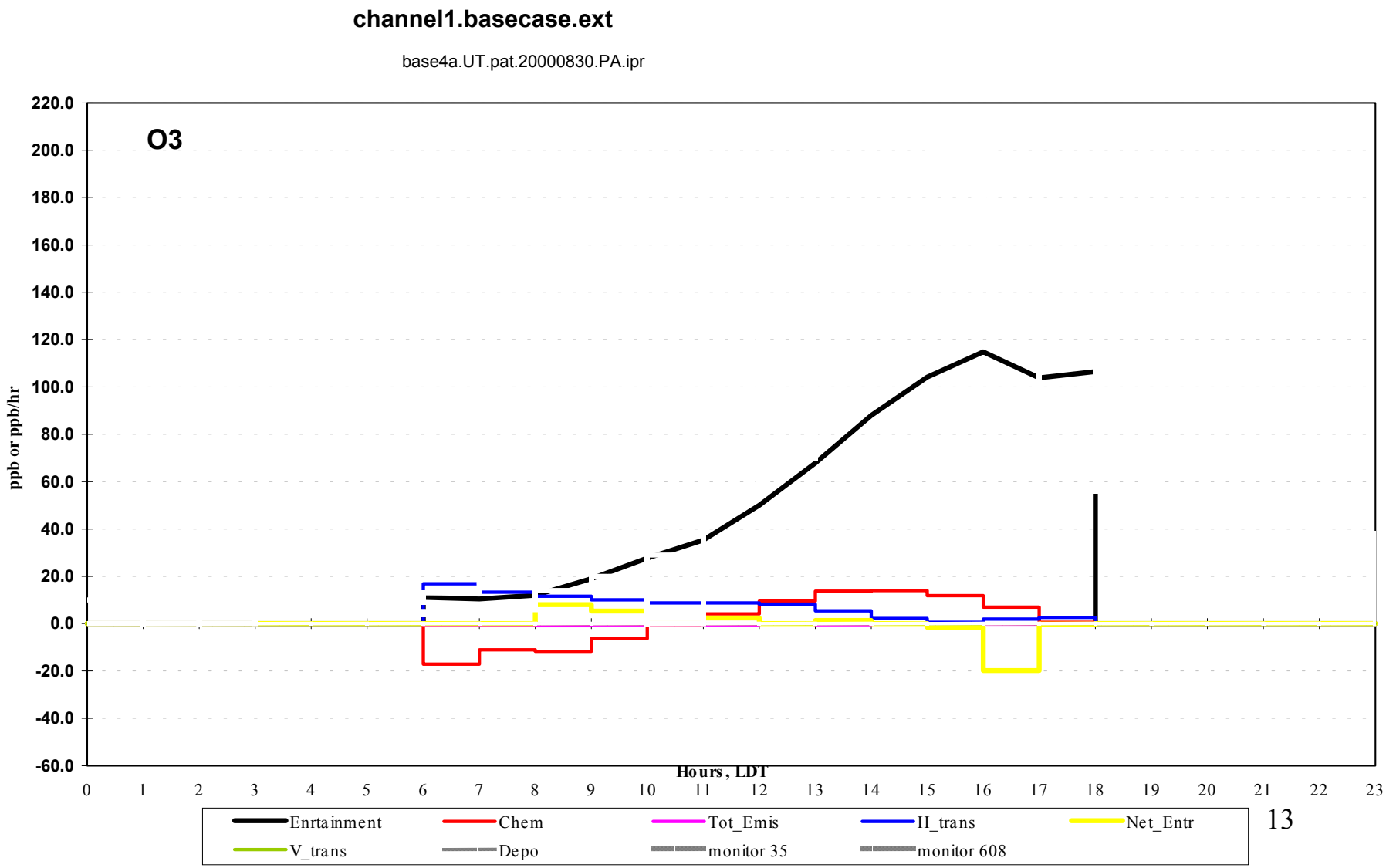
Process Analysis

- Process Analysis tools allows comparison of photochemistry of grid model and box model can be compared
- Example of parameters to be compared are:
  - Contribution of key processes (e.g. emission, chemistry, transport) to key species' (e.g. O_3, NO_x) concentration
  - Key chemical properties, e.g. cycle and fate of nitrogen species and radicals

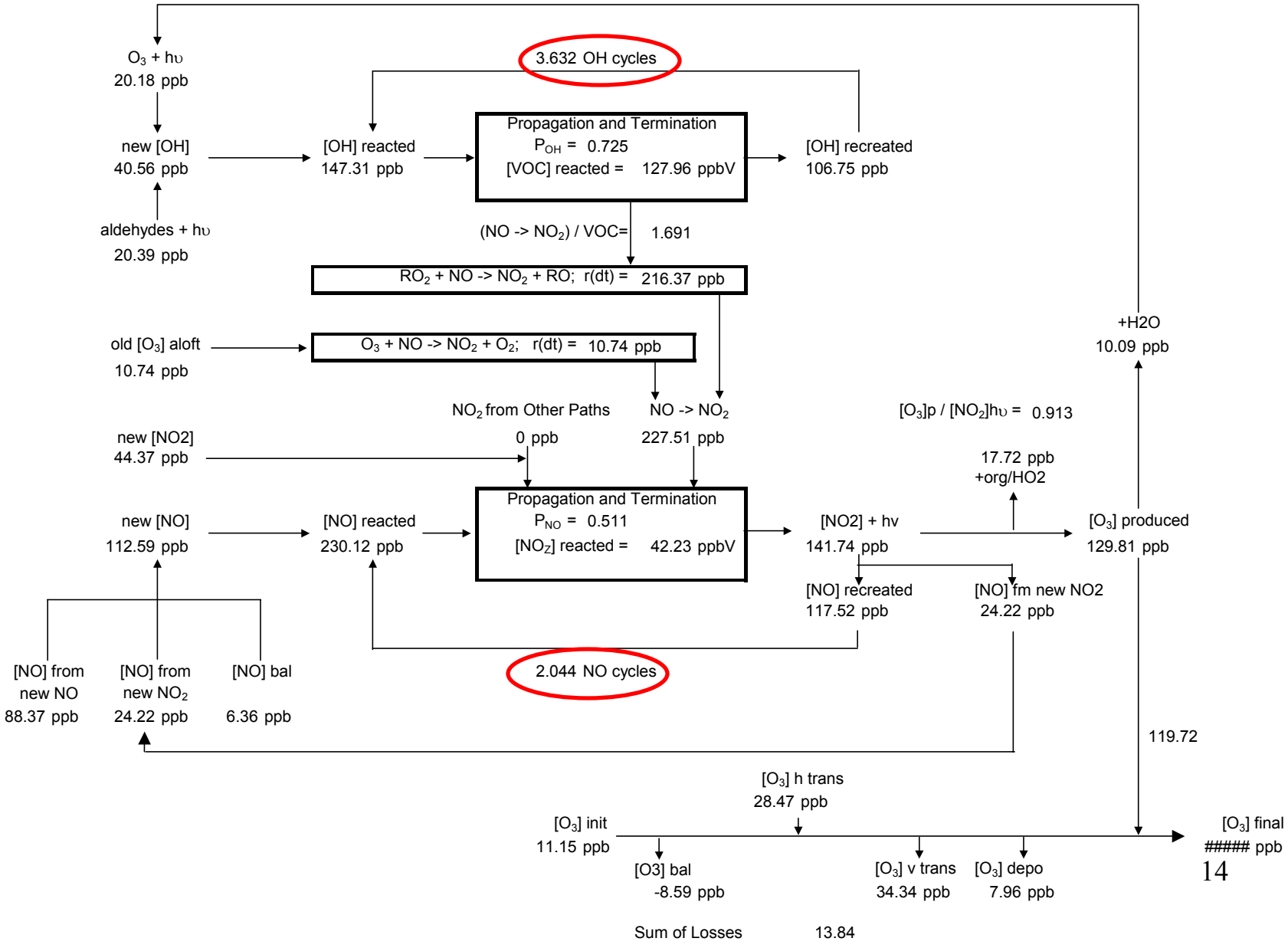
Process Analysis (grid model)



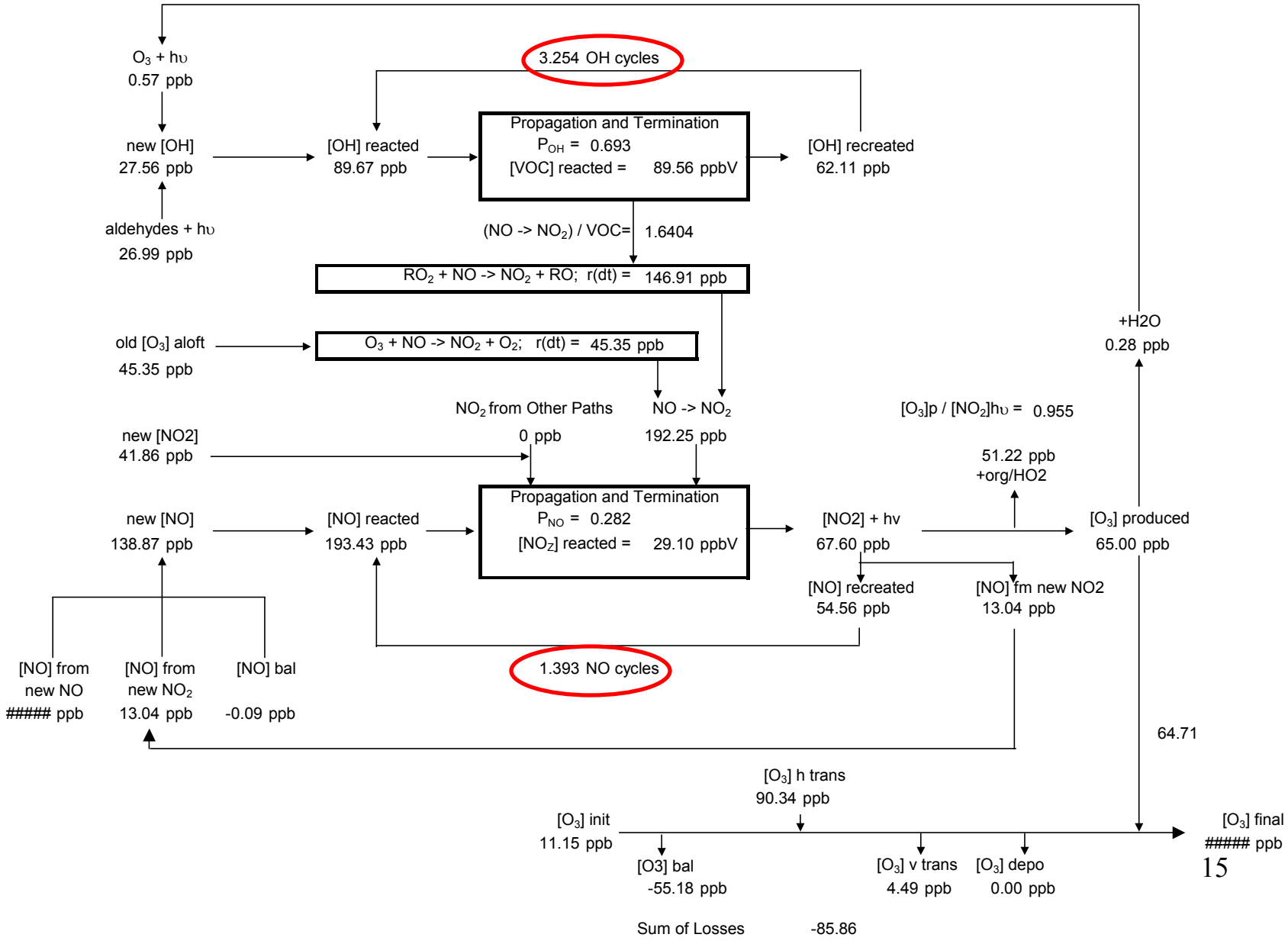
Process Analysis (box model)



Process Analysis (grid model)



Process Analysis (box model)

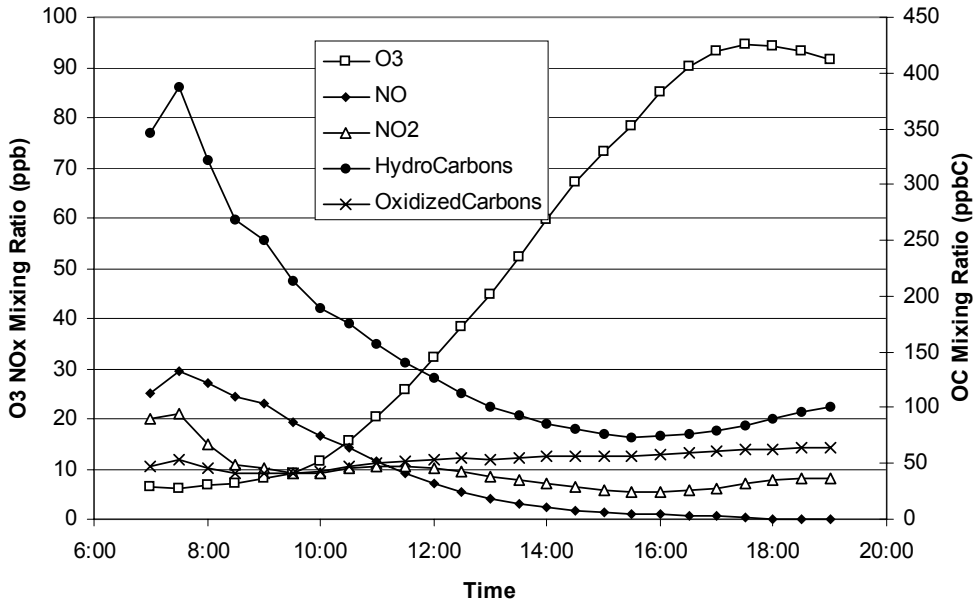


Stochastic Simulation

- Many instances of stochastic EI ("Snap-shots") are derived to drive a photochemistry model (i.e. Monte Carlo simulation)

Preliminary Results

- Box model and stochastic inventory was developed in simpler approaches
- Monte Carlo method was applied
- Ethylene, Propylene and Xylene emissions were independently perturbed



Preliminary Results