Feature Tracking Process Analysis

Barron Henderson, William Vizuete [*], and Harvey Jeffries
Department of Environmental Sciences and Engineering
The University of North Carolina, Chapel Hill, North Carolina

1 SUMMARY

Air quality models determine air pollutant concentrations by calculating rates of atmospheric processes. Many models output only the spatial and temporal distribution of species concentrations, and rates of the individual processes that lead to these changes are not recorded. With only concentration fields, it is often difficult to infer why air pollutant concentrations change. A more detailed evaluation of modeled processes led to the development of a process analysis tool called pyPA (Process Analysis in python). The pyPA tool can quantitatively track physical and chemical processes that contribute to changing pollutant concentrations. The tool has been used to analyze stationary focus regions in California and Texas. pyPA has previously been limited when analyzing a moving feature such as a large petrochemical release or the transport of an urban plume. This presentation will detail the modifications made to our pyPA tool to aggregate data for a moving, resizing, and reshaping domain. We will illustrate an application of this modification with a petrochemical release in the Comprehensive Air quality Model with extensions (CAMx) simulation of the Houston, TX non-attainment area.

2 INTRODUCTION

Photochemical grid models use the finite difference method coupled with eularian continuity equations to efficiently calculate concentrations of chemical species and particulate matter within each grid cell. The chemical reaction and physical transport rates, or source and fate matrices, are calculated for a series of time-steps to approximate the actual pathways. Due to data storage impracticalities, many models output only the spatial and temporal distribution of species concentrations, and rates of the individual processes that lead to these changes are not recorded. When the model satisfactorily represents the modeled domain, the source and fate matrices have little post simulation value. When model formulation violates enough of the engineering assumptions and the model inaccurately represents the modeled environment, the source and fate matrices are invaluable. Without the source and fate matrices, the positive feedback, negative feedback, and non-linear equations would require recalculating species-specific continuity equations to diagnose a simulation that has gone awry. Process Analysis (PA), which has been reformulated and expanded into Python-based Process Analysis (pyPA), includes an in-model algorithm for aggregating model time-stepped source and fate matrices and outputting the averaged hourly values. These matrices include the separately integrated rates for individual chemical mechanism reactions and process pathways. The pyPA post-processor uses the output matrices to quantify radical budgets, source and fate of O_3 precursors, and the physical and chemical processes that affect each species. This data is used to compare the affect of chemical reactions and physical transport rates in O_3 production and has already been utilized to explain model phenomena in California and Houston, Texas. Useful insights gained from the application of this tool has prompted us to expand the application and to refine its operation. pyPA offers insights to the key variables for a specific region, but has previously been limited when analyzing a moving feature such as a large petrochemical release or the transport of an urban plume. This presentation will detail the modifications made to the pyPA tool to aggregate data for a moving, resizing, and reshaping domain and discuss refinements in focus domain definition that increase pyPA's accuracy.

3 EVOLUTION OF PYPA

pyPA, despite its new name, was originally completely Fortran based. Ease of use, future coding, and operational speed encouraged the reformulation in Python. Python, like Fortran, can be easily written to use POSIX style command line interface. Python, however, is easily integrated into a graphical user interface, which decreases learning speed for operation. A surprising result of conversion to Python was increased

[*] *Corresponding Author:* William Vizuete, Department ESE, UNC-Chapel Hill, 113 Rosenau Hall, CB 7431, Chapel Hill, NC 27599; e-mail: vizuete@unc.edu

operational speeds. This has more to do with the creation of CAMx input and output file classes and the strength of the python file object than actual computation or individual I/O speed. The Fortran version read each record and compared the received values to a search criteria. The Python CAMx integrated reaction rate and integrated process rate file classes are aware of the data structure and during initialization learn how to efficiently return records. Instead of requesting records and then comparing to the search criteria, the application requests just those records that meet the criteria. In the worst cases, extraction process can be reduced by over 95%.

4 MIXING HEIGHT VARIABILITY

The original PA developers realized that a time constant mixing height would skew the morning and evening results. As the earth warms in the morning and cools in the evening, the planetary boundary layer (PBL) grows and shrinks. To simulate the real environment, a time variable mixing height, allowing for vertical entrainment and detrainment, would reduce the unrepresentative dilution. There is still error due to irregular urban environment where anthropogenic activities can generate substantial amounts of heat and cause large variability in temperature and PBL. pyPA enhances the Fortran PA variable mixing height to allow for this spatial variability. As a post-processor, the resolution of the spatial variability is, by definition, limited by the resolution of the output data.

The pyPA algorithm for aggregation follows the original formulation, which assumes movement is instantaneous between hours. For each component of the source and fate matrix, a volumetric weighting factor is applied and the results summed. Initial concentration values combine unchanged and vertically detrained volumes. All other components use unchanged and vertically entrained. The aggregation schemes are outlined in Table 1. Vertical entrainment and detrainment terms are added to account for the initial concentrations of these volumes. The previous PA extraction output format assumed that the mixing height could either be rising, lowering, or remaining the same. This assumption allowed a single column, "En(De)trainment", to play double duty for chemical species. As the mixing height increases, the column contained the vertically entrained. As the mixing height decreases, it contained the vertically detrained volume. This format is insufficient for a spatially variable mixing height because at a given time step one cell may rise and another may fall. Although this may be infrequent, it will come up again for the variable geometric base and so was addressed here. The "En(De)trainment" column was split into 4 columns corresponding to the entrainment and detrainment definitions.

5 GEOMETRIC BASE VARIABILITY

The original PA used a stationary rectangular base for the reactor volume, but was quickly changed to a stationary convex polygon (e.g. excluding an "H" shape). pyPA takes this enhancement a step further by allowing for concave as well as convex shapes and permitting movement with time. A moving base is useful when analyzing a transient feature such as an industrial plume. The aggregation allows for asymmetrical horizontal entrainment and detrainment. In other words, a change in the leading boundary definition not necessarily offset by a change in the trailing boundary. In addition to the terms in spatial mixing height variability, horizontal entrainment and detrainment values are added to account for initial concentrations of these volumes.

	Un.	H.E.	H.D.	V.E.	V.D.
Volumetric Averaging					
Initial Concentration	X		X		X
Chemistry	X	X		X	
Area Emissions	X	X		X	
Pt source Emissions	X	X		X	
PiG change	X	X		X	
West Advection	X	X		X	
East Advection	X	X		X	
South Advection	X	X		X	
North Advection	X	X		X	
Bottom Advection	X	X		X	
Top Advection	X	X		X	
Dil. in the vert	X	X		X	
West Diffusion	X	X		X	
East Diffusion	X	X		X	
South Diffusion	X	X		X	
North Diffusion	X	X		X	
Bottom Diffusion	X	X		X	
Top Diffusion	X	X		X	
Dry Deposition	X	X		X	
Wet Deposition	X	X		X	
Aerosol chemistry	X	X		X	
Final Concentration	X	X		X	
Initial Contribution					
Horizontal Entrainment		X			
Horizontal Detrainment			X		
Vertical Entrainment				X	
Vertical Detrainment					X

Table 1: Summary of aggregation schemes

6 VERIFICATION

6.1 Control

Enhancing an existing analytic tool provides certain boundaries that are helpful. Unless a specific bug is identified, the new tool should results should match the old tool results with the same inputs and boundaries. During the course of development, outputs for a stationary non-spatially varying mixing height aggregated volume were compared to the original results for 4 cells corresponding to the Clinton monitor from the Houston Texas regulatory simulation (see Figure 1).

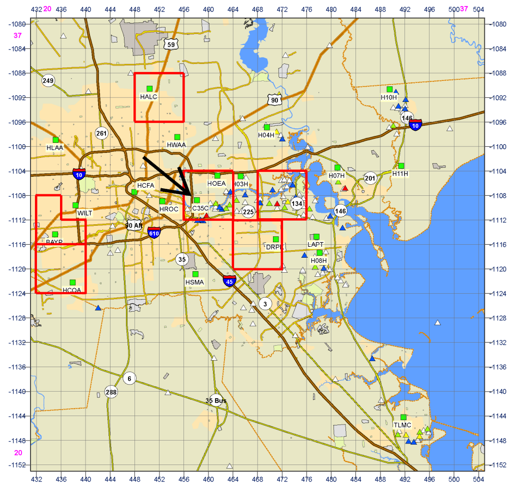

Figure 1: The control domain contains the Clinton monitor (Id: C35C)

6.2 Mixing Height Variability

A spatially variable mixing height is equivalent to using PA on multiple 1 by 1 grid cell focus domains and then volumetrically averaging the integrated rates. The same 4 cells from the control case are used with space and time variant mixing heights in the new pyPA. Those cells are also individually run with the old PA with time variant mixing heights each corresponding to the height for that section of the test run.

6.3 Geometric Base Variability

For a moving base, the test case is more complex. The test case will be described using a relative domain description based on the control. The initial horizontal volume definition starts -2 i, -2 j from the test case. Every other hour for 10 hours, the horizontal definition increments +1 i, +1 j and ends at +2 i, +2 j. The time-steps that do not include motion should match exactly the standard PA process for the same cells. The time-steps involving motion should match a volumetric average of the unchanged, the vertically entrained, and the horizontally entrained.

6.4 Differences

With few exceptions detailed below, pyPA is able to replicate PA outputs. PA only allowed for convex shapes, which facilitated the calculation of advection, diffusion, and displacement based on a leading edge only method. pyPA values for these processes differ because pyPA's more complex shapes required that a volumetric average method.