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Modeling Ozone Formation in a Central Texas Power Plant Plume

by

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Thesis

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Modeling Ozone Formation in a Central Texas Power Plant Plume

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The University of Texas at Austin, 2001

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ABSTRACT

Senate Bill 7, passed by the Texas Legislature in 1999, requires Electric Generating Utilities to reduce their NOx emissions to 50% of their 1997 levels by May, 2003. This control strategy does not take into account the diurnal variation in Ozone Production Efficiency (OPE) of NOx emissions. OPE is largely determined by meteorological mixing phenomenon and distinct diurnal differences in ozone chemistry. These differences are addressed in this research using the Comprehensive Air Quality Model with extensions (CAMx). Incremental increases in nighttime emissions from a rural power plant are found to form significantly more ozone (as measured during peak afternoon hours) than the same increases in afternoon emissions for all four This capability is quantified as both peak modeling days analyzed. concentration (and location) and total ozone present (spatially integrated) during sensitive afternoon hours. Nighttime OPE ranged from 4 to 10, while daytime emissions yielded from -1 to 4 (moles O₃ formed / moles NOx emitted). The range of high-impact emissions is from approximately 7 p.m. to 10 a.m. However, emissions from 7-9 p.m. and 8-10 a.m. are not consistently high-impact.

A limited validation of CAMx was performed using data collected by the Department of Energy's G-1 aircraft during the 2000 TEXas Air Quality Study (TEXAQS). On September 10, 2000, the U.S. Department of Energy's G-1 aircraft sampled the plume of emissions from the Fayette Power Project (FPP), located in Fayette County, Texas. The results of the aircraft plume sampling are compared with a similar day of a July 1995 CAMx modeling episode, namely July 9. Model predictions for FPP OPE are lower (1-4) than those measured by aircraft data (2-9). Domain-wide, threefold increases in the biogenic hydrocarbon emission inventory cause modeled OPEs to become comparable to measured OPEs.

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Chapter I: Introduction and Background

1.1 Ozone as an Air Pollutant

Ozone (O₃) is a gaseous pollutant which causes many adverse health effects, including inflammation and irritation of the respiratory tract (EPA, 1999). It is classified as a criteria pollutant by the United States Environmental Protection Agency (EPA). Control of ozone is difficult, however, because it is a secondary pollutant; it is formed in the atmosphere, by the reaction of nitrogen oxides (NOx) and volatile organic compounds (VOC) in the presence of sunlight.

As a criteria pollutant, Ozone is subject to a National Ambient Air Quality Standard (NAAQS). The current NAAQS for ozone is 0.12 parts per million (ppm), which is equivalent to 125 parts per billion (ppb) (one-hour average). Currently, a proposed NAAQS of 85 ppb (eight-hour average) has been successfully challenged in the court system, was upheld by the Supreme Court, and has been remanded to the EPA (D.C. Circuit Court, 1999). Until the proposed NAAQS is accepted, the one-hour, 125 ppb standard will remain in effect.

1.2 Ozone Status in Texas

Four urban areas in Texas exceed the current NAAQS for ozone under the one-hour standard: Houston-Galveston, El Paso, Dallas-Fort Worth, and Beaumont-Port Arthur. Four more areas are in danger of becoming non-attainment under the proposed 8-hour standard: Austin, San Antonio, Tyler-Longview-Marshall, and Victoria. To deal with non-attainment status, the State of Texas has developed a State Implementation Plan (SIP), in accordance with the requirements of the EPA.

1.3 Control Strategies

Recent land use studies indicate that biogenic VOC emissions comprise a large fraction of total VOCs in eastern Texas (Wiedinmyer et al., 2000). Therefore,

regulatory attention has focused on anthropogenic NOx emissions rather than anthropogenic VOC emissions (Sillman et al., 1990).

Recently, studies have also shown that a regional approach to ozone control may be necessary in Texas (Kasibhatla et al., 1998; Saylor et al., 1998; TNRCC, 2000). A regional approach to reducing ozone formation in eastern Texas will target large-scale regional NOx reduction. This necessarily includes reduction from some of the largest NOx producers in the state: electric generating utilities. Certain of these utilites have been allowed to operate without the new construction permits required from all sources beginning operation after 1971. This allowance is known as "grandfathering." Small sources (less than 250 Tons NOx/year) qualify for a Standard Exemption Permit; while all large, non-grandfathered sources must apply for a Title V Operating Permit.

Thus, NOx control by facilities in operation before 1971 has been optional. Recently, however, the Texas Legislature passed Senate Bill 7 (SB7), which requires all electric generating utilities to reduce NOx emissions to 50% of their 1997 levels by May 2003 (Texas Legislature, 1999). As part of the control strategy, emissions will be allocated to each facility based on the power generation, and a NOx trading program is undergoing further development. Figure 1 shows the 1997 contribution of grandfathered facilities (Gfr), Standard Exemption status facilities (Std. Ex.), and Title V Operating Permitted facilities (Perm.) to the total NOx emission inventory for the state. The total NOx inventory is the sum of the three contributions.

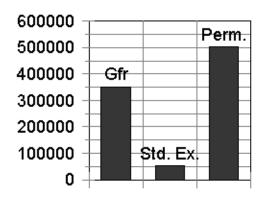


Figure 1-1. 1997 NOx Contribution (tons per year) by Source Category. (Std. Ex. = Standard Exemption, Gfr. = Grandfathered, Perm.=Title V Operating Permitted Facility) (All NOx-generating Facilities)

Recent development of a SIP for Houston involved some atmospheric modeling, which was performed using the Comprehensive Air quality Model with extensions (CAMx) (40 CFR, 2001). The State of Texas, in their evaluation of high O₃ in East Texas, noted from CAMx modeling that high background O₃ concentrations, combined with urban O₃ concentrations led to violations of the O₃ NAAQS. Sensitivity tests performed using a July, 1993 episode of CAMx indicated that a 50% reduction in NOx emissions from point sources in East Texas gave a consistent ozone reduction for some areas, such as Longview-Tyler-Marshall for most modeling days. However, ozone was not as consistently reduced in other areas, such as Austin (McDonald-Buller et al., 1999).

Further research using CAMx has illustrated that the ozone production of NOx point sources varies according to their location, and the time of their emissions (Nobel et al., 2000; Nowlin, 2001). Comparison of modeled data to aircraft data is needed to assess the ability of CAMx to predict NOx plume phenomena.

1.4 Diurnal Variations

Diurnal variations in ozone chemistry and meteorology give rise to the possibility that NOx emitted at night may have different ozone generating capacity than NOx emitted during the day.

1.4.1 Chemistry

Ozone chemistry is quite complex, and tends to be non-linear with respect to NOx. In general, ozone is generated during the day, and consumed at night, according to the following reactions.

Day

A photostationary cycle exists between NO_x (NO and NO_2) and O_3 , with no net change in ozone, as shown in Figure 1-2.

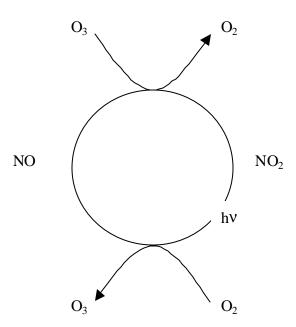


Figure 1-2. Photostationary State Between O_3 and NOx.

In the presence of reactive hydrocarbons, the conversion of NO-NO₂ by ozone is interrupted by a peroxy radical, as summarized in the following reactions.

$$RH + OH^{\bullet} \longrightarrow R^{\bullet} + H_2O$$
 (R1)

$$R^{\bullet} + O_2 \longrightarrow RO_2^{\bullet}$$
 (R2)

$$RO_2^{\bullet} + NO \rightarrow RO^{\bullet} + NO_2$$
 (R3)

The initiation of this step involves the hydroxyl radical, OH. The source of OH in these reactions is, in an initial phase, photolysis of ozone.

$$O_3 + h\mathbf{n} \to O_2 + O(^1D) \tag{R4}$$

$$O(^{1}D) + H_{2}O \rightarrow 2OH^{\bullet}$$
 (R5)

While the initiation of OH takes place by Reactions R4 and R5, propagation of OH is dominated by the conversion of NO to NO₂ by the alkylperoxyl radical, RO₂ (or its corollary, the hydroperoxy radical, HO₂), as in Reaction R3.

The daytime termination pathway is described by Reaction R6.

$$NO_2 + OH^{\bullet} \rightarrow HNO_3$$
 (R6)

Reaction R6 is significant in that nitric acid represents the only true termination product of NOx-VOC-O₃ chemistry. NOx which has formed nitric acid is no longer available for production of ozone.

Using an average urban mix of VOC, the rates of Reactions R1 and R6 are equal when NOx/VOC is 1:5.5 (Seinfeld, 1998). If isoprene dominates the VOC mix, the rates are equal at NOx/VOC $^{\sim}$ 1:0.25 (using k_{R6} =2.39x10⁻¹¹ cm³/molecule-

s, and k_{R1} =1.01x10⁻¹⁰ cm³/molecule-s, from Seinfeld, 1998). Since Reaction R6 represents removal of both NOx and OH, it contributes to retardation of O₃ formation. Thus, under high-NOx conditions (such as in a power plant plume, where NOx/VOC is much higher than 1:5.5), Reaction R6 will predominate, and retard O₃ formation. As NOx is depleted through Reaction R6, NOx/VOC becomes smaller, and accelerates O₃ formation. Emissions into an isoprene-rich region from a rural plant will begin to yield O₃ much more quickly than emissions from an urban plant. This leads to the formation of ozone "wings," or high-OPE zones at the edges of plumes. These are commonly recorded at the edges of large industrial NOx plumes (Gillani and Pleim, 1996; Sillman, 2000), and will be discussed further in Chapter III.

Night

Nighttime chemistry differs from daytime chemistry due to the absence of photolysis reactions that cannot take place during sunlight hours. Specifically, Reactions R7 through R9 are significant only in the absence of sunlight (Seinfeld, 1998).

$$NO_2 + O_3 \longrightarrow NO_3 + O_2 \text{ k=2.8e-3 ppb}^{-1}\text{hr}^{-1}$$
 (R7)

$$NO_3 + NO_2 + M \longrightarrow N_2O_5 + M$$
 (R8)

$$N_2O_5 + H_2O \longrightarrow 2HNO_3$$
 (R9)

During the day, NO_3 is rapidly photolyzed back to NO_2 and O_3 . However, during the night, this pathway provides the net sink for NOx (Platt et al., 1994). With negligible loss of NO_3 to other processes, the net loss is limited by the initial reaction with ozone and the first order rate constant with 50 ppb ozone is 0.28 hr^{-1} :

$$O_3 + 2 NO_2 + H_2O$$
? $2HNO_3$; $dNO_2/dt = 5.6e-3 hr^{-1}ppb-1 [O_3] [NO_2]$

1.4.2 Definitions

It is useful to define specific classes of the above species involved in nitrogen oxide chemistry.

NOy = NOx + NOz

Total Nitrogen Species =
$$NO + NO_2$$
 + Oxidized products of NOx (1-1)

Table 1 lists various species included in NOz for a power plant plume of emissions, and reports a typical daytime range of their fractional contributions to total oxidized species of NOx.

Table 1-1. NOz Species in the Fayette Power Project Plume of Emissions and Their Relative Daytime Contributions to NOz.

Specie Name	Fractional Contribution to NOz (Average model values from CAMx July 1995 modeling episode output)
Nitric Acid	65-70%
Peroxyacetyl Nitrate (PAN)	6-10%
Nitrous Acid	0
N _x O _y (e.g., N ₂ O ₅)	0
Organic Nitrates	15-25%

Nitrous Acid and N_xO_y do not exist during the day due to photooxidation. Organic nitrates include peroxyalkyl nitrates (ROONO₂), peroxyacyl nitrates (RC(O)OONO₂), and alkyl nitrates (RONO₂). All of the organic peroxynitrate species (including PAN) may thermally decompose back to a peroxy (or peroxyacetyl) radical and NO_2 .

A metric for determining ozone formation capability is known as Ozone Production Efficiency (OPE). OPE is defined, qualitatively, in Equation 1-2.

$$OPE = \frac{d[O_3]}{d[NOx]_{original}} \tag{1-2}$$

1.4.3 OPE

Because it is impossible to track the exact origin of a NOx molecule present in the atmosphere, other definitions have been proposed for OPE. Each of these definitions has been employed in this research. There is no universally accepted definition of OPE (Gillani et al., 1998b). A common alternative definition used is the ratio O₃/(NOy-NOx), or O₃/NOz (Olszyna et al., 1994).

$$OPE = \frac{d[O_3]}{d[NO_2]} \tag{1-3}$$

This definition accounts for ozone that has been produced by NOx that has been oxidized to form NOz. It will not, because of dry deposition of NOz, account for all of the "original NOx" emitted. The primary NOz specie involved in dry and wet deposition is nitric acid, HNO₃, which deposits from 2 to 10 times as fast as ozone (Seinfeld, 1998). One way to estimate this loss is to relate the ozone and NOz present at a given point in space to a "conserved" species, one which is not affected to such a great degree by dry deposition. Corrections can then be made to estimate concentrations based upon pre-loss circumstances. Corrections of this

nature have been employed for the OPE metric described in Equation 1-3 (Gillani et al., 1998a; Ryerson et al., 1998).

The use of total nitrogen species present, NOy, has also been employed as a convenient metric which relates to "original NOx" (Trainer et al., 1993).

$$OPE = \frac{d[O_3]}{d[NO_Y]} \tag{1-4}$$

However, it has been estimated that NOy is lost anywhere from 3-17% per hour, based upon an atmospheric mixing layer depth of 1 km. Few experiments have yielded reliable results (Gillani et al., 1998; Imhoff et al., 2001).

Still another way to represent OPE is to consider the ratio of the rise in ozone to the rise in nitric acid at a given point in space.

$$OPE = \frac{d[O_3]}{d[HNO_3]} \tag{1-5}$$

Nitric acid is the only true termination product of NOx oxidation, considering the thermal decomposition of other NOz species as described above. These oxidized nitrogen species can participate in regeneration of NOx, and therefore continue to play a role in the production of ozone. Because only a fraction (although up to 80%) of NOz is accounted for by using HNO₃ in Equation 1-5, values will be systematically higher than OPE as defined by Equation 1-3. The difference between dO₃/dNOz and dO₃/dHNO₃ will vary as the fraction of NOz as nitric acid varies.

OPE is affected greatly by NOx/VOC. In general, smaller NOx/VOC will yield higher OPE. This fact implies that smaller NOx sources, given equivalent background hydrocarbon concentrations, will have higher OPE

than larger NOx sources. This has indeed been confirmed in multiple studies (Gillani et al., 1998; Ryerson et al., 1998, 2001; Nunnermacker et al., 2000). OPE sensitivity to the NOx/VOC also implicates diurnal sensitivity to NOx emissions due to diurnal variation in atmospheric mixing.

1.4.4 Meteorology

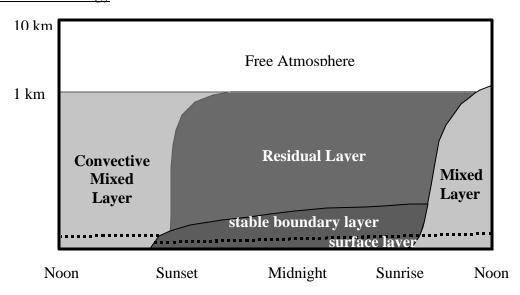


Figure 1-3. Diurnal Variation in Atmospheric Mixing.

Atmospheric mixing varies greatly due to the diurnal difference in heat supplied to the Earth's atmosphere. During the day, heat flows from the hot surface of the Earth into the atmosphere just above the surface through diffusive mechanisms. The warmed air parcel may be considered a "buoyant thermal," due to its higher temperature relative to surrounding air. As the heated air rises, the pressure surrounding the air parcel will drop, causing adiabatic expansion and cooling of the air parcel. The continual formation and vertical transport of these air parcels gives rise to the convective mixed layer, as depicted in Figure 1-3.

The Earth's surface cools upon sunset, and a temperature inversion forms during the night, as depicted in Figure 1-4.

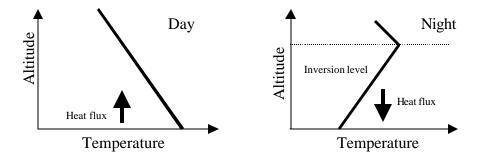


Figure 1-4. Nocturnal Temperature Inversion Formation.

The increase in temperature with elevation causes the formation of a stable nocturnal boundary layer, in which there is no opportunity for turbulent, buoyant transport of air. Very little mixing takes place in this circumstance, which, from an air pollution standpoint, is very significant (Seinfeld, 1998). The resulting nighttime plume tends to be quite slender and concentrated, and provides a high-NOx region where there is opportunity for chemical neutrilization of NOx by reaction with O₃, as in Figure 1, R6, and R7-R9.

1.5 Research Objectives

This research focuses on two major aspects of modeling the ozone problem in Texas, and proposes methods for further analysis.

- The ability of CAMx to accurately predict ozone production by a large NOx point source is validated by comparison to aircraft data taken in a plume of emissions from a grandfathered electric generating utility. Two different analysis techniques for performing such validation are proposed.
- The diurnal variability of ozone production by this large utility is examined, and new methods are proposed.
- Methods for further comparison of modeled data and aircraft data are proposed.

Chapter II. Atmospheric Modeling

2.1 The Comprehensive Air Quality Model with Extensions (CAMx)

CAMx was developed by Environ, and is available on-line at www.CAMx.com. The EPA requires that any model used for State Implementation Plan (SIP) development meet certain precision criteria (EPA, 1991). The Comprehensive Air Quality Model with extensions (CAMx) is one of only three or so models currently used by states to legislate State Implementation Plans. Others include UAM-IV and SARMAP (California). CAMx is used for SIP development in Texas, and is therefore the model employed in this research to investigate diurnal NOx control options (40 CFR, 2001).

CAMx utilizes a fixed-grid cell structure to report concentrations spatially in a specified domain. For the episode employed in this research, these grid cells have constant dimensions (although in some formulations, grid cell height can vary) throughout each modeling episode. CAMx allows the user to specify vertical and horizontal grid dimensions, the number of vertical layers, and the number of "nested grids." Figure 2-1 depicts the gridded domain used in this research. The domain was developed for use in regional modeling for the Austin and San Antonio urban areas. It contains 2 nested grids.

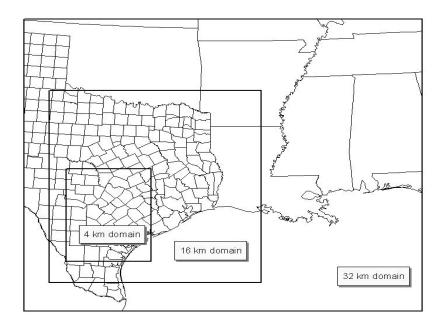


Figure 2-1. Grid Structure employed by CAMx.

The coarse grid pictured in Figure 2-1 utilizes 32x32 km grid cells; the nested grids contain 16x16 km and 4x4 km grid cells. For continuity, each grid cell structure must have the same number of layers, and the same layer heights.

Modeling episodes are typically chosen based upon occurrences of high ozone. The episode used in this research is from July 7-12, 1995, and will be described in detail later in this chapter. It is convenient at this point to define the days of the episode. Table 2-1 summarizes the episode days.

Table 2-1. July 1995 Modeling Episode Days.

Day	Referred to as:	Comments
July 7	Day 1	Model Initialization
July 8	Day 2	Model Initialization
July 9	Day 3	
July 10	Day 4	
July 11	Day 5	
July 12	Day 6	

Model initialization days are ones for which results are questionable. Results from Days 1 and 2 of the modeling episode are suspect due to the establishment of boundary conditions in the internal grids. For these days, there is too much dependence of model predictions on initial conditions. Day 3 utilizes boundary conditions calculated on Days 1 and 2 to model chemistry and transport. Days 1 and 2 do not have well-established boundary conditions; thus, they are not included in analysis.

In each of the grid cells, various routines are employed which eventually yield predictions for species of interest, including ozone. Table 2-2 has been adapted from the User's Guide for CAMx version 2.00 (Environ, December 1998). It summarizes the CAMx modules employed for description of key physical processes.

Table 2-2. Summary of the CAMx Modules for Key Physical Processes.

Module	Physical Model	Numerical Method	
Horizontal	Continuity equation	Smolarkiewicz (1983) or	
advection/diffusion	closed by K-theory		
	explicit diffusion		
Vertical	Continuity equation	Crank-Nicholson for	
transport/diffusion	closed by K-theory	transport, implicit	
		diffusion	
Chemistry	Carbon Bond IV (CB-	ENVIRON CMC Solver	
	IV)	(hybrid explicit/implicit/	
	steady-state)		
Dry deposition	Resistance model of	Specified as surface	
	Wesely (1989) boundary condition for		
	vertical diffusion		
Wet deposition	Scavenging model as in	Exponential decay in	
	CALPUFF (EPA,	each cell, each time step	
	1995)		
Plume-in-Grid	Continuous-leaking cylindrical plume segment		
	model with explicit inorganic chemistry		
Two-way grid nesting	Grids solved separately with one cell overlap at		
	boundaries to handle inter-grid pollutant flux via		
	boundary conditions. Fine grids sub-divide the		
	coarse grid time-step		

Of the processes listed above, the ones of greatest interest to this research are the processes for dry deposition and Plume-in-Grid. Both of these will directly affect predicted OPE of large point sources and, therefore, comparison with aircraft data.

2.2 Deposition

Because dry deposition has a direct effect on OPE (see Equation 1-3), it is important that CAMx reflect physical phenomenon effectively in its formulation. Typical CAMx values for O_3 and HNO_3 deposition velocity are tabulated in Table 2-3.

Table 2-3. Day and Night Deposition Velocities (cm/s) for Ozone and Nitric Acid.

	Modeled Values		Seinfeld, 1998
	Day	Night	Day
O_3	0.3	0.08	0.3
HNO ₃	0.4	0.25	0.4

It is convenient to show how model values were calculated. The physical model employed by CAMx is one developed by Wesely (Wesely, 1989; Environ, 1998). This model incorporates a 3-phase resistance mechanism which varies according to land use data. The three-phase resistance model is summarized in Equation 2-1.

$$v_d = \frac{1}{R_a + R_d + R_s} \tag{2-1}$$

Where R_a is the atmospheric resistance,

R_d is the deposition layer resistance, and

R_s is the surface layer resistance.

Atmospheric resistance describes the extent to which turbulent transport brings material from the convective mixed layer to the surface. It is based on mass transfer/momentum transfer similarity theory. Deposition layer resistance is a function of the diffusivity of a particular specie through an effective laminar boundary layer very near the surface. The surface layer resistance is a function of the surface type (water, land with or without dead or living vegetation, etc.), and incorporates an additional series resistance formula to include various levels of vegetative canopy. The methods employed in the Wesely model for dry deposition are not necessarily the best methods available for estimation; however, it is the model used most widely by regional photochemical models (Wesely, 1989; Seinfeld, 1998). Modifications proposed to Wesely's scheme have shown

significant (up to 23% for O₃ or NOz species) differences in surface resistances (Welmsley et al., 1996). Data confirming these calculated resistance values are not widely available; validation of the deposition model is outside the scope of this research. However, as Figure 2-2 indicates, deposition will likely have little effect on OPE between layers during the middle of the day.

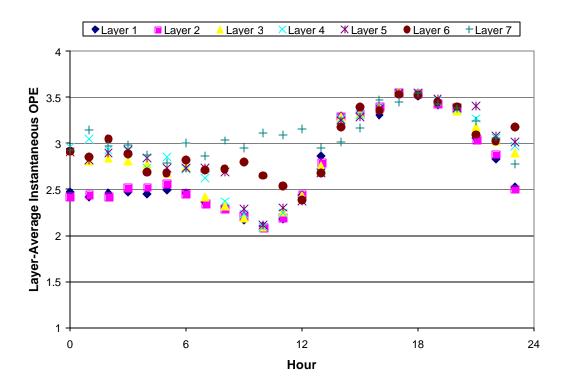


Figure 2-2. Average Instantaneous OPE (dO₃/dNOz) by Layer (CAMx Vertical Layers 1-7, Using [Plant On-Plant Off] Analysis and O₃ Threshold of 2.0 ppb, Day 3 of July 1995 Modeling Episode).

As seen in Figure 2-2, nighttime difference in model-predicted OPE is expected between layers. During the afternoon, however, when the atmosphere is well-mixed, deposition rates have a near equal effect (instantaneous OPE within 5%) at all layers. Data for Figure 2-2 is located in Appendix B.

2.3 Plume-in-Grid (the PiG)

The PiG is a puff model, which assumes a Gaussian distribution of mass in a puff with defined length and variable cross-sectional area. Each PiG puff is emitted to a final plume rise, and is added, at each time step of the model, to a particular vertical "layer of emission." The only species carried by PiG puffs are NO, NO₂, HNO₃, and O₃, and only O₃ is entrained during the life of the puff. The interaction between the background atmosphere and the NOx in the plume, is controlled by "leakage," which will be discussed in detail below.

The puff length is determined by the wind speed at the current time step, and the duration of the time step.

$$L_{ii} = u_{ii} \times dt \tag{2-2}$$

Where L_{ij} is the 2-dimensional length of the puff segment, u_{ij} is the 2-dimensional wind vector, and dt is the discrete time step employed in the Eulerian scheme.

The maximum length of a puff is defined by the user in the CAMx run control file (Appendix A). Should the potential length of a puff exceed the user-defined maximum length, multiple puffs are generated during the time step.

$$N_{puffs} = \inf\left(\frac{(u_{ij} \times dt)}{L_{\text{max}}}\right) + 1$$
(2-3)

Where N_{puffs} is the number of puffs formed per discrete time step, "int" is the truncation integer function, and L_{max} is the user-defined maximum puff length.

The PiG allows for simplified, inorganic chemistry (involving only the four species in each puff, noted above), and transport under a Lagrangian box model scheme. Figure 2-2 shows a simplified picture of PiG transport.

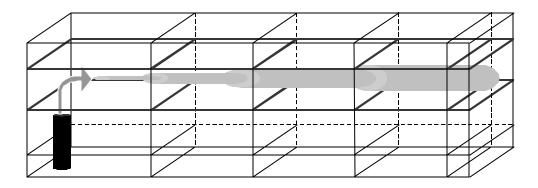


Figure 2-3. Simplified PiG Schematic.

The Lagrangian puffs are advected horizontally through CAMx grid cells, and experience growth and internal chemistry. As mentioned, the puffs will remain in their layer of emission, located at the final plume rise.

Each of the individual puff sections above, it must be noted, could very well be discontinuous with one another; in other words, there is a distinct possibility that an individual puff could find itself disjoined from any other puffs. During a single Eulerian time step within the CAMx framework, puffs may be emitted to different layers. Wind shears between different model layers may produce puffs from different hours of the same day which are transported to positions far from one another. An example is shown in Figure 2-3.

PiG Visualization

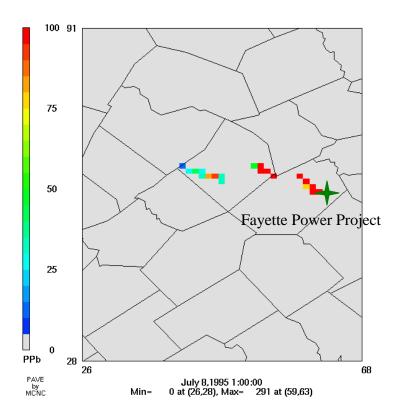


Figure 2-4. PiG NOy (NO + NO₂ + HNO₃) for Puffs Located in All Vertical Layers at 1:00 a.m, Day 2 of Modeling Episode, Base Case.

Figure 2-4 represents "PiG NOy" from a particular point source, namely the Fayette Power Project, located in Fayette County, Texas. PiG NOy is simply the concentration of the only three NOy species carried by the PiG: NO, NO₂, and HNO₃. We might use PiG NOy as a tracer to locate modeled puffs. Figure 2-3 clearly shows the potential for discontinuity between individual PiG puffs.

Such discontinuity may well represent the possibility for emissions from one source to have simultaneous impact at multiple receptor locations. This possibility was realized during the sixth day of the modeling episode utilized in this research, and will be discussed in Chapters 3 and 4.

2.3.1 PiG Growth

PiG growth is assumed to be the age-limiting factor in PiG puffs, as opposed to PiG chemistry. The implications of this choice are potentially huge. As the PiG puffs are advected downwind, they grow in cross-section, thereby diluting the concentration of the species inside the puff. Once the physical boundaries of the host grid cell have been reached (either layer height or horizontal grid cell dimension), the puff begins to "leak" its mass. The CAMx mechanism for PiG growth (piggrow.f) is included in Appendix A for reference.

To understand when puff mass is leaked, one must understand how PiG dimensions are defined. Upon initial release from the stack, the puffs have a volume equal to a cylinder with cross-sectional area equal to that of the stack from whence the emissions came. At the final plume rise, the puffs are assumed to have grown through adiabatic expansion, according to local pressure and temperature. This final plume volume is divided by the puff length, and the cross-sectional area is considered to be circular.

Once initial dimensions are established, the new puff is sent, along with all other puffs, to a growth routine at each time step. Cross-sectional growth occurs as a result of vertical and horizontal diffusivity, according to the following equation.

$$\mathbf{s}_{y}(t) = \sqrt{2 * K_{h} * t} + U_{xy} t \frac{d\mathbf{s}_{y}}{dx}$$
(2-4)

Where s_y is the horizontal dimension of the puff (m), K_h is the horizontal eddy diffusivity (m²/s), t is the time step (s), U_{xy} is the horizontal wind vector (m/s), and ds_y/dx is the change in dispersion parameter as a function of downwind distance (dimensionless).

The dispersion parameter is essentially an empirically derived estimation of the increased growth due to horizontal advection. In other words, plumes will tend to spread longitudinally in addition to cross-sectional growth. The fact that PiG puffs are assigned a constant length causes underestimation of actual dispersion; a fact which is accounted for by the second term of Equation 2-4. Correlations for this quantity are readily available (see, e.g., Seinfeld, 1998).

The example given in Equation 2-4 is for the horizontal growth. Vertical growth differs only in its use of a vertical eddy diffusivity and change in dispersion parameter.

After a certain amount of time, the puff dimensions will exceed those of their host grid cell. Because vertical diffusivities are typically on the order of 1% of horizontal diffusivities, horizontal growth will far exceed vertical growth. This leads to short, squat puffs. Also, growth in both directions occurs much more rapidly during the day than at night, for meteorological reasons summarized in Chapter 1. Thus, puffs may only exist for one hour during the day before reaching the physical limits of their host grid cell; while nighttime puffs tend to last much longer (on the order of 12 hours) before being dispersed by the morning time formation of the convective boundary layer.

The eventual "slaughter" of these puffs (rapid during day, slow at night) occurs as a result of "leakage." Basically, small amounts of a puff's NOx are removed from the puff and introduced to the grid cell in which the puff is located. This process begins after the puff outgrows the grid cell boundaries. When dumping the mass remaining in the puff will cause a grid cell concentration increase of less than 0.1 ppb, the puff is "slaughtered." "Slaughtering" a PiG is simply removing all of the remaining puff mass from the PiG puff and adding the

mass to the grid cell. A case study of a puff emitted at midnight is presented to assist with understanding of puff growth and leakage.

A typical mass of NOx is derived from emission rates from the Fayette Power Project, known to be approximately 0.5 tons / hour-stack. Using a wind velocity of 5 m/s (11 mph), and a 6 minute time step, the length of the puff will be 1800 m, according to Equation 2-2. Only one puff will be formed during this time step, considering a maximum puff length of 2000 m. The mass in this puff is simply the emission rate multiplied by the time step. Should there have been more puffs formed, the emissions would have been divided proportionally amongst the puffs. Using the fractions 85.5% NO and 14.5% NO₂, as provided by the emissions inventory, a total mass in the puff of 43 kg is calculated. Vertical and horizontal diffusivities and the change in dispersion parameter with downwind distance were derived from actual model input. Allowing for one hour of growth according to Equation 2-4, and assuming a Gaussian distribution of mass within the confines of the puff dimensions, the concentration profile can be developed. Allowing for another 1.5 hours of growth causes the puff to exceed the grid cell boundaries; the NOx within 1.5 s of the distribution and outside the grid cell boundaries is "leaked" to the host grid cell (NOT the cells on either side of the host grid cell). Figure 2-4 depicts growth and leakage for this case study.

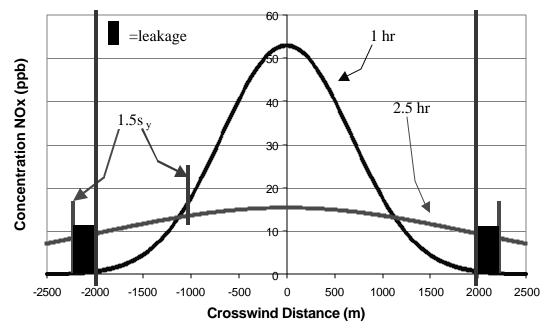


Figure 2-4. Growth and Leakage of a Midnight Puff of Emissions into the 4-km Grid Cell Structure (Concentration and 1.5s Inferred by Gaussian Distribution of Known Mass and Volume; "Snapshots" Taken at 1 and 2.5 hr after Puff Emission).

As can be seen from Figure 2-4, the mass leaked is within 1.5 s $_{y}$ of the mass distribution and outside the limits of the host grid cell. The significance of such a leaking process is that emissions are not allowed to interact with background air (including VOCs); in a word, they are "canned." Upon release by leakage, the NOx is free to interact with background VOCs and go about producing O_{3} by the mechanisms contained in the CB-IV chemical mechanism which is used for grid cell chemistry. Until that point, however, the emissions undergo a simplified inorganic chemistry, which is described below.

A way to describe the persistence of the "canned" nature of a PiG puff is by quantifying a "time delay." Nighttime releases will grow slowly, under stable nighttime atmospheric conditions; while daytime puffs will be quickly dispersed and slaughtered, due to the turbulence of the convective mixed layer. In general,

PiG puffs formed at night last from their time of emission until 9:00 a.m. PiG puffs formed during the day tend to last only on the order of an hour, or at most, two hours. The NOx that has been released will yield O₃, and its concentration upon introduction to the host grid cell will impact the efficiency with which O₃ will be formed.

This diurnal difference in puff life has direct relevance towards temporal sensitivity of O₃ formation to NOx emissions. Specifically, we might consider two puffs with the same initial mass; one originates at night, the other during the day. The nighttime puff will have a chance to leak a significant amount of its NOx before interacting with background VOCs. Its concentration in the host grid cell, when the puff is eventually slaughtered, will be smaller than that of the daytime puff. This will reduce the local NOx/VOC ratio, which will increase OPE in a NOx-limited region. However, this will hold true only if nighttime chemistry in the PiG does not completely remove NOx through conversion to HNO₃.

2.3.2 PiG Chemistry

PiG chemistry is simplified, inorganic chemistry. The FORTRAN code employed by CAMx is included in Appendix A, for reference. No reactions between NOx and hydrocarbons can take place in the PiG, because hydrocarbons are not carried by PiG puffs. Kumar and Russell have asserted that such simplifications do not impair model accuracy (Kumar et al., 1996); efforts are now being taken at the University of Texas at Austin to test this hypothesis.

Upon entry to the chemistry module, any NO present in the PiG puff is converted to NO₂, according to Reaction R10.

$$NO + NO + O_2 \longrightarrow 2NO_2$$
 (R10)

Any remaining NO is consumed via O₃ titration, as depicted in the photostationary cycle of Figure 1-2. If any O₃ is left after this titration, it is used in one of two ways, depending on whether the model considers it to be daytime, or nighttime. There is no in-between period for CAMx—it is either day, or night. A steady-state assumption is made for production and decay of N₂O₅, which is assumed to be limited by O₃ availability. Any N₂O₅ formed will react with available water, as stated in Section 1.4.1., to form HNO₃. During the day, O₃ photolysis generates OH radicals, which oxidize NO₂ to HNO₃, according to Reactions R4-R6.

Of specific interest to this research is the fact that only O_3 consumption is allowed by the chemistry, whether day or night. Consumption of O_3 happens by initial titration of O_3 with NO. Consumption of O_3 happens via formation of HNO₃ in the two ways mentioned above. Ozone entrainment is extremely critical in determining the daytime reactivity of the nighttime emissions. If the NOx is consumed by O_3 through the two pathways listed above, none will be left to react with background VOCs. If not enough O_3 is allowed to interact with PiG emissions, the amount of NOx present the next morning will be overpredicted.

Ozone entrainment occurs, in the model, as a result of PiG growth. Nighttime plumes last a significant amount of time and grow slowly. At each time step, O_3 is entrained according to the growth experienced during that time step. Equation 2-5 summarizes this entrainment.

$$O_{3,entrained} = C_{O_3,hostgridce\ ll} \times \Delta Volume$$
 (2-5)

Where $O_{3,entrained}$ is the quantity of O_3 entrained at each time step (mol), $C_{O3,hostgridcell}$ is the concentration of O_3 in the current grid cell (mol/m³), and ?Volume is the change in volume during the time step (m³).

The moles of O₃ entrained are added to the total moles of the puff, and future concentration distribution calculations account for both the increased size of the puff and the increased amount of O_3 . The extent of O_3 entrainment for the puff in the growth example above, over the life of the puff, considering a constant background concentration of 40 ppb, is approximately 8000 moles. According to the emission rate, 1300 moles NO would originally be in the puff. Thus, through entrainment, all of the NO would be converted to NO₂ through O₃-NO titration. The NO₂ still present upon sunrise, according to PiG chemistry, is limited by the O₃ entrained at each time step. If sufficient O₃ is present, the rate of HNO₃ formation by the NO₃/N₂O₅ pathway may become the limiting factor. For the growth example, there seems to be sufficient O₃; thus, Reaction R9 will limit the removal of NOx. The rate of Reaction R9 is highly dependent upon the local relative humidity (Platt et al., 1994). At RH > 50%, NO₃ lifetimes are on the order of a few minutes, whereas at lower RH, they are on the order of 40 minutes, implying slow removal of N₂O₅, and decomposition of N₂O₅ back to NO₂ and NO₃ (Seinfeld, 1998). CAMx includes this RH-dependence within the PiG chemistry module.

2.4 Episode Details

The particular episode used in this research was developed using data from July 7-12, 1995. The episode was developed for Dallas Attainment Plan Evaluation modeling, and is currently being used for air quality planning in Austin and San Antonio near non-attainment areas.

Grid setup for this episode is pictured in Figure 2-1. Layer heights were constant throughout the episode, and are summarized in Table 2-4.

Table 2-4. Layer Heights Used in July 1995 CAMx Modeling Episode.

	Height (m)
Layer 1	0-33
Layer 2	>33-100
Layer 3	>100-211
Layer 4	>211-390
Layer 5	>390-675
Layer 6	>675-1105
Layer 7	>1105-1815
Layer 8	>1815-2892
Layer 9	>2892-3600

The episode was unique due to its relatively calm wind speeds and varied wind direction by day. To expound upon this variation, ground-level wind directions near the Fayette Power Project are recorded in Figure 2-5 for each day. Ground-level wind velocities are reported for 15:00 on each day. This time is chosen because the plume data available from aircraft measurements was taken at approximately 15:00.

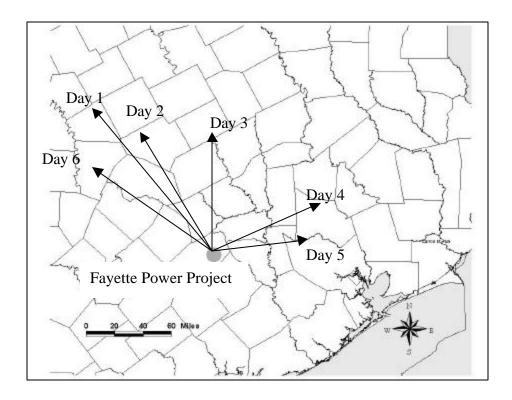


Figure 2-5. Wind Velocity (Scaled from 1.5-3.0 m/s) by Day for July 1995 CAMx Episode (Instantaneous Model Value at 15:00 on each day).

As Figure 2-5 bears out, winds varied greatly in their trajectory from day to day. The difference between Days 5 and 6 is nearly 150 degrees.

The emissions estimates given for the electric generating utilities in the episode were obtained from the Continuous Emissions Monitoring database, which provides hourly emissions data for various pollutants.

The biogenic VOC emissions database for Texas was developed by C. Wiedinmyer, and is based on the best available land use data for Texas (Wiedinmyer et al., 2000). Meteorological data was processed by and acquired from Environ and TNRCC (Environ, November 1998). The emission rate from the Fayette Power Project during the modeling episode is illustrated by Figures D1-6. The maximum O₃ concentrations modeled for each day are summarized in Figures

D7-D12. All modeling data has been archived to tape, and is available through Dr.

Gary T. Rochelle in the Department of Chemical Engineering.

Chapter III. Modeled / Aircraft Data Comparison

CAMx model outputs are compared to aircraft data collected during the Texas Air Quality Study undertaken August 15 to September 15, 2000 (TEXAQS 2000). The Department of Energy's G-1 aircraft was used to sample the plume of emissions from the Fayette Power Project (FPP), located in Fayette County, Texas on September 10, 2000. Data from this flight are archived in Appendix B, and are also available online, at ftp://aerosol.das.bnl.gov/pub/Houston00/.

3.1 Background

Although aircraft data are useful for estimation of plume OPE during certain periods, the data available for photochemical grid model validation is lacking. Intense efforts are required to acquire necessary data for an EPA-approved modeling episode, and it is difficult to arrange for collection of flight data that will coincide with these episodes. The recent study undertaken in Texas, the TEXas Air Quality Study (TEXAQS) will hopefully provide sufficient data to set up modeling episodes; the aircraft data available from the study should be sufficient for comparison to CAMx modeling results. In this way, the performance of the Plume-in-Grid submodel may be validated.

Until that time, it is useful to look at archived data to extract whatever meaningful lessons may be derived. In general, information on the processes of plume sampling and analysis may be gathered from existing plume data sets. One good source of data in Texas is the Baylor University Airborne Sampling Project (available online at http://www.utexas.edu/research/ceer/texaqs/baylorlinks.html). In concert with the Texas Natural Resource Conservation Commission and Sonoma Technology, Inc., some analysis of this data has been performed, and is available online (MacDonald et al., 1999).

In general, plume sampling is performed by flying in a transverse manner across a plume, perpendicular to the local wind direction. An example of this is seen in Figure 3-1, which represents a flight taken on August 25, 1997, by the Baylor Aircraft. This image is chosen because it is a good example of the extent of an industrial plume in East Texas.

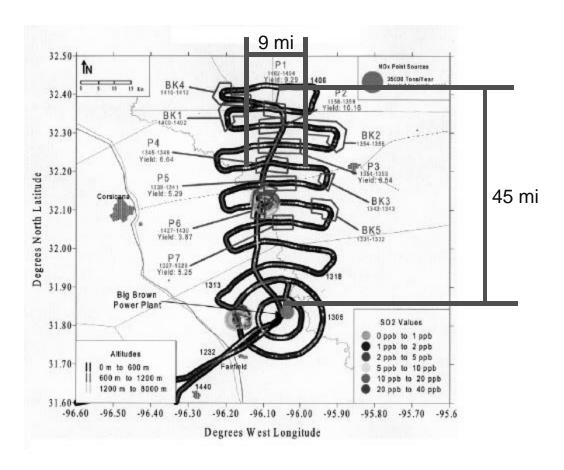


Figure 3-1. Typical Plume Sampling Flight Path and Large NOx Source Plume Dimensions (Baylor University Twin Otter, Flight 39, August 25, 1997). (Adapted from MacDonald et al., 1999)

The extent of the Big Brown Power Plant plume, pictured above, is typical for a large industrial source. The dimensions of plumes are often indicated by a sulfur dioxide, (SO₂) peak, which is a characteristic constituent of coal-fired power

plant emissions. Data taken by the aircraft at each transect of the plume can be plotted as a time series, to demonstrate dispersion and photooxidation of chemical species. Figure 3-2 shows a time series plot for a portion of the flight pictured in Figure 3-1.

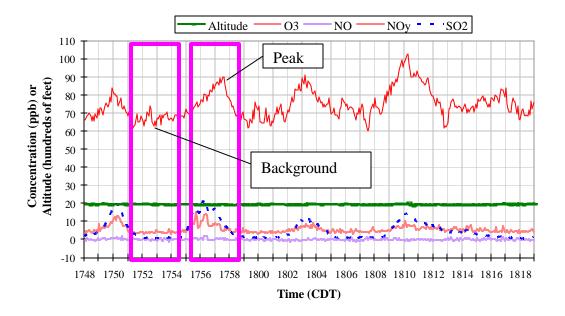


Figure 3-2. Time Series Plot of Flight 39 of the Baylor University Twin Otter, August 25, 1997. (Courtesy TNRCC).

As can be seen from Figure 3-2, O_3 peaks (red line) become quite clear within the plume (as defined by the SO_2 peak, blue dotted line). This is typical of a mature plume. Ozone titration is not captured by this portion of the time-series, which represents transects approximately 20-30 miles from the source.

Yields for the above data were calculated by MacDonald et al. by comparing the instantaneous peak O₃ to the instantaneous peak NOy for a given

transect. The boxed regions are considered to be the Peak (left box), and Background (right box) values for O₃ and NOy. Considering

$$O_{3,peak}$$
- $O_{3,bg} = 71.0-53.3 = 27.7$ ppb, and

$$NOy_{peak}-NOy_{bg} = 7.7-4.35 = 3.35 ppb,$$

The yield at this transect, according to MacDonald et al., is 5.3 moles O₃ per mole NOx emitted by Big Brown (NOy basis). Where NO and NO₂ data are available, the same analysis can be done for OPE as defined by dO₃/dNOz (NOz=NOy-NOx). The next section discusses other useful ways to derive OPE values for comparison.

3.2 Aircraft Data Analysis

3.2.1 Background

A number of uncertainties are implicit in comparisons of aircraft data to modeled data. First, aircraft data are instantaneous, while modeled data are hourly averages. Second, modeled data from all layers of the atmosphere are available; one must assume the presence of a well-mixed atmosphere when interpreting aircraft data. Third, it is rare to have a modeling episode for which aircraft data is available. It is this lack of data which will first be discussed.

Currently, there are a few models which adequately reflect the processes observed by aircraft in large industrial plumes (Karamchandani et al., 2000; Sillman, 2000). Most models still find difficulty in predicting O₃ "wings," the productive zones at the edges of plumes, where the NOx/VOC ratio has become sufficiently low to generate O₃ quickly. However, of the Baylor aircraft data collected in East Texas, there is only one flight which detected O₃ wings, Flight 7. A time series of Flight 7 from the Baylor aircraft data is shown in Figure 3-3. The

time series represents a transect taken approximately 2 km downwind from the City Public Service Power Plant in San Antonio.

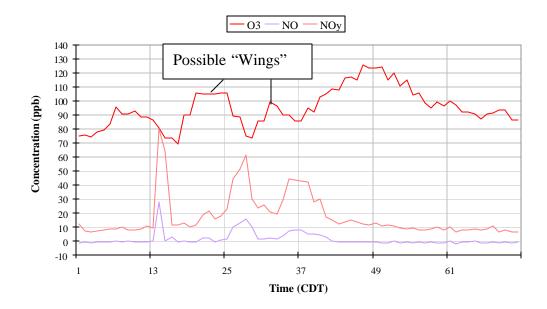


Figure 3-3. Time Series Plot of Flight 7 of the Baylor University Twin Otter, June 4, 1997. (Courtesy TNRCC).

Even these "wings" are not as prominent as some that have been witnessed in other areas, such as Tennessee (Gillani and Pleim, 1996; Sillman, 2000). Peaks on either side of the O₃ trough, where NO-O₃ titration is occurring in the plume, only reach approximately 15 and 10 ppb above background concentrations. The conditions on the day of Flight 7 included ground level temperatures of 35°C, wind from the SW at approximately 4 mph, and mostly sunny skies. These conditions do not appear to be particularly unique amongst other flights taken either near the San Antonio City Public Service Power Plant, or at other locations in East Texas. The FPP data collected during TEXAQS did not indicate any wings, either. This phenomenon seems to be unique to Texas data, and could possibly be explained by conditions that are unique to Texas, such as unique biogenic hydrocarbon mixtures

and levels, which would affect the extent and kinetics of reactions at the dilute edges of NOx plumes.

3.2.2 Approaches to Analysis and Comparison

There is fair agreement amongst the modelers mentioned so far (Karamchandani, Sillman, Ryerson, etc.) as to the methods to be employed for modeling validation. Both of these comparison methods are utilized in this research.

3.2.2.1 Concentration Ratio Approach—Entire Plume

One method of comparing values of OPE between model output and aircraft data, is to look at a cumulative value for OPE over the entire plume, rather than an instantaneous value (Ryerson et al., 2001). Sillman (2000) asserts that the cumulative value for OPE is to be favored "because it can be used more readily to estimate the amount of downwind transport of O₃ and contribution to global-scale photochemistry for a given NOx emission rate, and because the average lifetime can be related to measured quantities, such as O₃/(NOy-NOx)." The "concentration ratio" approach effectively combines all of the data from every transect into a "plume averaged" OPE. Ozone concentration at each point in the plume is plotted versus NOz concentrations at each point in the plume. The resulting slope is the OPE (Nunnermacker et al., 2000); it should be considered an upper limit, for reasons noted above. One can also use this approach to compare OPE at each transect to the plumes state of oxidation, or "chemical age," as discussed below.

3.2.2.2 Mass-Balance Approach

A second approach, employed by Ryerson et al. (1998) utilizes a "mass-balance approach" to deal with the fact that O₃/NOz may be considered an "upper limit" due to the longer atmospheric lifetime of O₃ relative to NOz (Trainer et al., 1993; Chin et al., 1994). Ryerson's mass balance approach compares the "flux"

(better termed "flow rate") of O_3 at a given transect to the reported plant NOx emission rate. "Flux," or flow rate, is calculated according to Equation 3-1.

$$net _flux = v \cos \mathbf{a} \int_0^z n(z) dz \int_{-v}^y X_m(y) dy$$
 (3-1)

Where net_flux is the flow rate of the component of interest (mol/s),

v is the wind velocity vector at the stack of interest (m/s),

a is the angle between the transect path and the direction normal to the wind vector,

n(z) is the number density of the atmosphere (mol/m³),

z is the height of the atmospheric mixed layer,

X_m(y) is the increase in mixing ratio of the component of interest above the background (mol/mol), and

y, -y are the crosswind plume positions, which define the plume dimension as observed by the transect (m).

This approach will yield a lower limit for OPE, as it does not account for loss of NOx through pathways other than participation in photochemical processes. OPE calculated by transect also varies temporally; each transect only provides a part of the picture which paints the overall impact of a NOx point source (and, therefore, its regional impact).

3.2.2.3 Chemical and Physical Age Calculation

Two methods of choosing *when* to compare modeled and measured OPEs have been reported. One draws comparison between transects of similar *physical* age, as calculated by wind speed and sampling location (Ryerson et al., 1998; Sillman, 2000). This method is summarized by Equation 3-2.

$$Physical_Age = \frac{Transect_Distance}{Wind_Speed}$$
 (3-2)

The other method compares transects of similar *chemical* age (Gillani et al., 1998b). Chemical age is defined in Equation 3-3, below.

$$Age_{chemical} = \frac{NOz}{NOy}$$
 (3-3)

Qualitatively, this ratio describes the extent to which the original NOx emissions (NOy) have been oxidized to NOz.

3.3 Fayette Power Project (FPP) Data

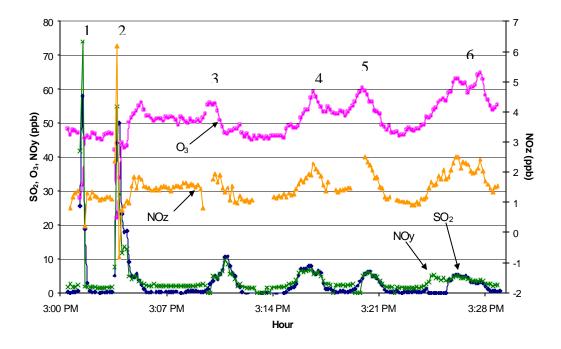


Figure 3-4. Time Series of FPP Data Acquired through TEXAQS (Number indicates transect).

FPP represented 2.3% of all NOx emissions in Texas in 1999, or nearly 20,000 tons. Only four other facilities emitted more NOx. Six transects were made through the FPP plume on September 10, 2000. Figure 3-4 is a time series representing those transects. As can be seen from Figure 3-4, no O₃ wings were

realized. The dip in O_3 concentration in transect 6 appears to depict wings. However, the dip is due to the aircraft turning parallel to the plume at that point. It essentially represents a half-transect, where the plane flew to the middle of the plume, and then turned downwind. Ozone generation was realized by the third transect.

Sulfur dioxide is a characteristic pollutant emitted by coal-fired electric generating utilities, and can be used to track the emissions plume. Therefore, "transects" throughout this section (the transition point from "outside the plume" to "inside the plume") will be defined as the point at which the SO₂ concentration changed threefold or better between successive data points.

3.3.1 Concentration Ratio Approach—Plume-Averaged OPE for FPP

Following Gillani et al. (1998b), OPE was calculated for the entire plume using the "concentration ratio" approach. OPEs were calculated by regression of O_{3,background corrected} versus NOz for each timestep for all transects, using

O_{3,original data}-O_{3,background} = O_{3,background corrected}.

Because the first transect (called the "fresh plume core") contained data points which were widely scattered, its data is not included in the analysis of the plume-averaged OPE. Figure 3-5 shows this analysis.

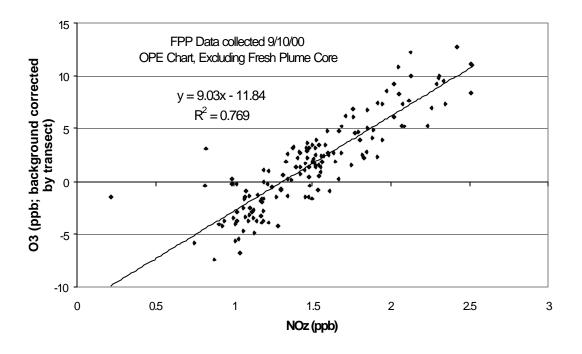


Figure 3-5. OPE for FPP, Derived from Aircraft Data Taken 9/10/2000 (all NOz assumed to be due to source).

Thus, a "plume-averaged" OPE of 9 was observed for FPP. This is within a reasonable range of OPEs reported for power plants the size of FPP located in rural areas in Tennessee (Ryerson et al., 1998). Comparison with model output is still desirable to further validate the result.

3.3.2 Concentration Ratio Approach—Transect-Averaged OPE for FPP

Again, following Gillani et al. (1998b), OPEs were calculated for *each* transect. OPEs were calculated by regression of O_{3,background corrected} versus NOz for each timestep for individual transects, using methods similar to those used in the OPE regression described above for the entire plume.

Because the first transect only yielded two data points, its regression is not included. Regressions were basically a sub-set of Figure 3-5, and can be seen in Figure 3-6. The data is located in Appendix B.

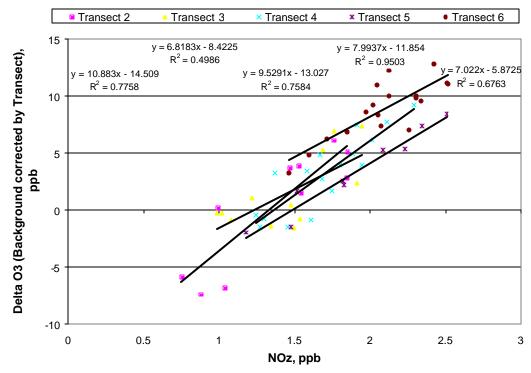


Figure 3-6. OPE by Transect for FPP Data Collected 09/10/2000.

3.3.3 Mass Balance Approach—Transect-Averaged OPE for FPP

OPE can be inferred from flux calculations. Flux is calculated following the approach of Ryerson et al. (1998), as summarized in Equation 3-1. A mixing height had to be assumed; thus the mixing height modeled in CAMx of 1105 m was used. Table 3-1 shows data used in these calculations.

Table 3-1. Flux (Flow rate) of NOy at Consecutive Transects; Calculation Based Upon Equation 3-1 (Data Taken by NOAA G-1 Aircraft from FPP Plume on 9/10/2000).

	V (m/s)	n(z) (mol/m³)	dz (m)	X _{m,NOy} (ppb above background)	dy (m)	ER _{NOx} (tons/hr)
Transect 1	4	37	1105	28	3,260	1.86
Transect 2	4	37	1105	10	11,420	2.28
Transect 3	4	37	1105	3.3	12,270	1.23

	V (m/s)	n(z) (mol/m³)	dz (m)	X _{m,NOy} (ppb above background)	dy (m)	ER _{NOx} (tons/hr)
Transect 4	4	37	1105	2.6	17,000	0.91
Transect 5	4	37	1105	2.5	11,800	0.59
Transect 6	4	37	1105	1.83	17,900	0.67

In this case, NOy was averaged for each transect, and assumed to reflect the original NOx emissions. These calculated emission rates match fairly well with the emission rate data used in the model, which averaged 1.5 tons/hr when all three boilers were in operation (see Appendix D). The assumptions of mixing layer height (1105 m) and molar density (40 mol/m³) of the atmosphere are conservative; this is likely a low estimate of the emission rate.

These calculated emissions correspond well with measured emission rates on the day of the aircraft sampling. Table 3-2 shows the NOx emission values for September 10, 2000. Data is courtesy LCRA.

Table 3-2. FPP NOx Emission Rate (tons/hr) for Each of Three Large Boilers (FPP-1,2, and 3) Reported by LCRA for 9/10/2000.

Time	FPP-1	FPP-2	FPP-3	Total
13:00	0.42	0.99	0.89	2.31
14:00	0.43	1.03	0.84	2.29
15:00	0.42	1.04	0.83	2.29
16:00	0.42	1.04	0.87	2.34

In order to ensure a lower bound for OPE, which is the purpose of the Mass Balance approach, the actual emission rate was chosen as the basis for OPE estimation. Thus, OPE for this approach will be defined according to Equation 1-3,

or the ratio of the flux of excess O₃ at a given transect to the flux of original NOx emissions.

Although no O_3 was generated until the third transect, all transects are included in this analysis. Negative O_3 fluxes should correlate to fresh (low chemical age) transects. Molar density of the atmosphere is based upon pressure data calculated during the flight (37 mol/m³). Mixing height was chosen as 1105 m, in the absence of mixing height data, to correspond to the mixing height modeled by CAMx. Calculated O_3 fluxes are summarized in Table 3-3.

Table 3-3. Ozone Flux (Flow Rate) Calculation Based Upon Equation 3-1.

	V (m/s)	$n(z)$ (mol/m^3)	dz (m)	X _{m,O3} (ppb)	dy (m)	Flux _{O3} (tons/hr)
Transect 1	4	37	1105	-9.15	3,260	-0.93
Transect 2	4	37	1105	-3.76	11,420	-1.34
Transect 3	4	37	1105	1.48	12,270	0.57
Transect 4	4	37	1105	3.19	17000	1.69
Transect 5	4	37	1105	3.84	11,780	1.41
Transect 6	4	37	1105	8.82	17,930	4.92

Now, dividing the O_3 flux at each transect by the original NOx emission rate gives an OPE for each transect. Table 3-4 summarizes these results.

Table 3-4. OPE by Transect Using Mass Balance Approach, NOx Flux Assumed from Data Obtained from LCRA for FPP, 9/10/2000.

	Flux _{O3} (tons/hr)	Flux _{NOx} (tons/hr)	OPE
			$(mol O_3/mol NOx)$
Transect 1	-0.93	2.29	-0.27
Transect 2	-1.34	2.29	-0.11
Transect 3	0.57	2.29	0.16
Transect 4	1.69	2.29	0.48
Transect 5	1.41	2.29	0.40
Transect 6	4.92	2.31*	1.40

^{*}Data from 13:00, as transect represented emissions from that time. All other data from 14:00.

Table 3-5 shows the same analysis, with one exception. In this calculation of OPE, the true Mass Balance Approach is employed, by calculating values for NOx flow rate at each transect in the same way as the O₃ fluxes were calculated.

Table 3-5. OPE by Transect Using Mass Balance Approach, NOx Flux Calculated.

	Flux _{O3} (tons/hr)	Flux _{NOx} (tons/hr)	OPE
			(mol O ₃ /mol NOx)
Transect 1	-0.93	1.86	-0.32
Transect 2	-1.34	2.28	-0.59
Transect 3	0.57	1.23	0.46
Transect 4	1.69	0.91	1.86
Transect 5	1.41	0.59	2.4
Transect 6	4.92	0.67	7.3

These instantaneous OPE values for each transect are most meaningful when correlated with the chemical and physical ages of the transect. For that reason, these ages were calculated for each transect.

3.3.4 Calculation of Chemical and Physical Age of FPP Transects

Chemical and physical ages of transects are useful for model comparison, for reasons mentioned in Section 3.2.2.3. To determine chemical age of each

transect, NOz concentrations were first inferred from (NOy-NOx) at each time step. NOz/NOy regressions were calculated for each transect by plotting NOz and NOy at each time step. The resulting regressions showed poor correlation between NOz and NOy. Figure B-1 illustrates this poor correlation.

From the original data, NOx and NOy data were regressed for each transect. These NOx/NOy regressions showed a good correlation. They are pictured in Figure 3-7.

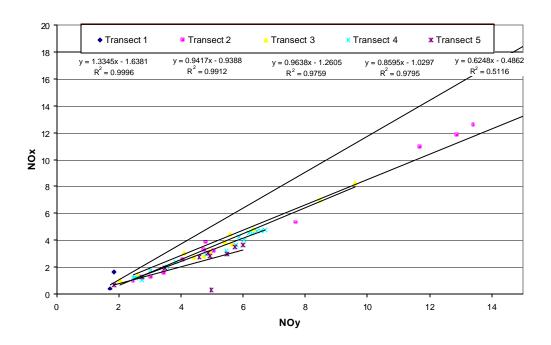


Figure 3-7. Regression of NOx and NOy for FPP G-1 Data 09/10/2000.

Due to the good correlation of NOx/NOy, NOy values were corrected by assuming the initial ratio of NOx/NOy reflected a pure-NOx plume. As seen from Figure 3-7, the initial ratio NOx/NOy (first transect) was approximately 1.3. A linear decrease in NOx/NOy can be see in Figure 3-8.

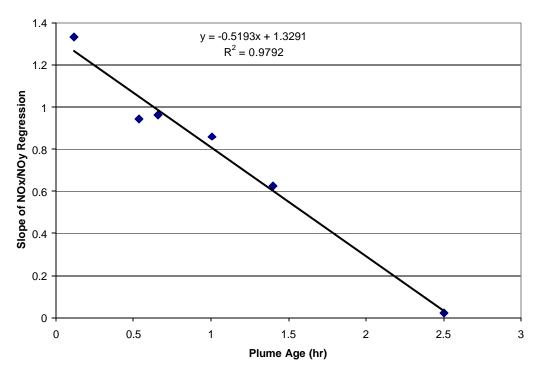


Figure 3-8. Cumulative Loss of NOx in FPP Plume (G-1 Data 09/10/2000).

From this constant loss of NOx, and the initial ratio NOx/NOy of 1.3, one might infer that NOy values are all artificially 30% low. To further investigate chemical age, all NOy values were increased by 30%, and called NOy_{corrected}.

$$NOy_{corrected} = NOy \times 1.3$$
 (3-4)

New NOz values (called NOz_{corrected}) were calculated based upon the NOy_{corrected} and original NOx values, as in Equation 3-5.

$$NOz_{corrected} = NOy_{corrected} - NOx_{original data}$$
 (3-5)

Next, to compute a corrected chemical age at each plume transect, $NOz_{corrected}$ and $NOy_{corrected}$ were plotted for each time step. The regressions calculated for $NOz_{corrected}/NOy_{corrected}$ can be seen in Figure 3-9.

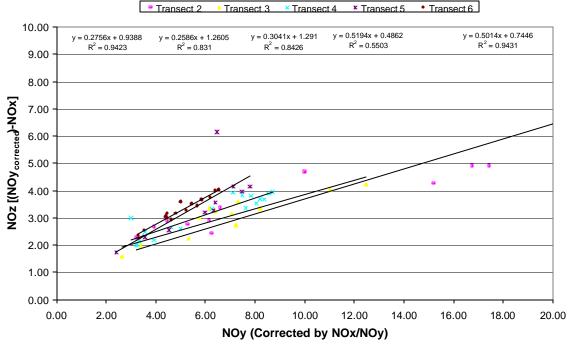


Figure 3-9. NOz/NOy (NOy Corrected Based Upon Initial NOx/NOy Ratio of 1.3)

With the exception of Transect 5, the regressions show good correlations. The chemical age for each transect is simply the corresponding slope of the line in Figure 3-9. Chemical ages for each transect are summarized in Table 3-6.

Table 3-6. Chemical Age (NOz_{corrected}/NOy_{corrected}) by Transect for FPP Plume (NOAA G-1 Data 09/10/2000).

	Chemical Age
Transect 1	0*
Transect 2	0.29
Transect 3	0.26
Transect 4	0.30
Transect 5	0.52
Transect 6	0.50

^{*}Chemical Age assumed 0 because of assumption that Transect 1 NOx/NOy = 1.0.

To relate aging of the plume to physical age, physical ages were calculated using the plume-average wind speed of 4 m/s (See Figure B-5), and the distance from the plant of each transect (See Table B-1), according to Equation 3-2. Table 3-7 summarizes the physical age of each transect.

Table 3-7. Physical Age of Transects for FPP Plume (NOAA G-1 Data 09/10/2000).

	Distance from Source (m)	Wind Speed (m/s)	Physical Age (hr)
Transect 1	1,680	4	0.12
Transect 2	7,700	4	0.53
Transect 3	9,540	4	0.66
Transect 4	14,590	4	1.0
Transect 5	19,980	4	1.4
Transect 6	36,040	4	2.5

Taking the regressed values for $NOz_{corrected}/NOy_{corrected}$ from Table 3-6 and plotting them versus the physical age of each transect implies stage-wise aging of the plume. Figure 3-10 illustrates this sequential oxidation.

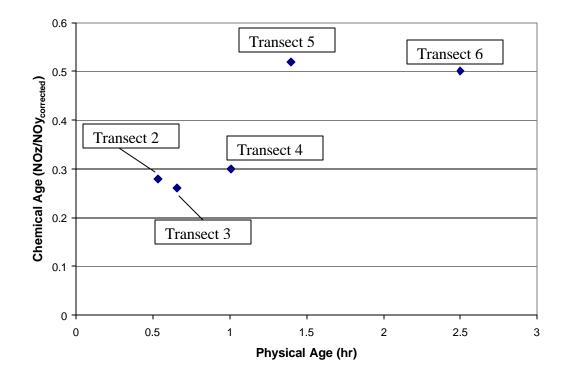


Figure 3-10. Regressed value of NOz_{corrected}/NOy_{corrected} Plots for Each Transect versus Physical Age of Each Transect (NOy Corrected by Assuming Initial NOx/NOy Ratio=1.0; Physical Age calculated by distance between transect and source, assuming a constant wind speed of 4 m/s).

If the plume had oxidized continuously after its emission from FPP, these points would lie in a straight line. Although there is clear stage-wise aging of the plume between transects 4 and 5, aging is not clear between the other transects.

Next, it is useful to relate the regressed OPE values derived in Figure 3-6 for each transect to the transect's chemical age, from Table 3-6. This relationship is

shown in Figure 3-11.

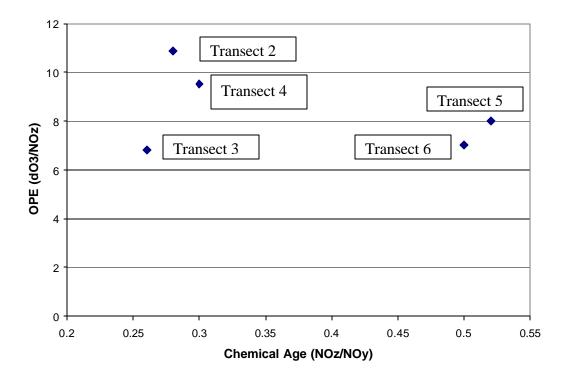


Figure 3-11. OPE (using Concentration Ratio Approach, by Transect) for Individual Transects versus Corresponding Chemical Ages.

Further comparison was done between transect chemical age and OPEs derived using the mass balance approach for each transect. Figure 3-12 shows the results of this analysis.

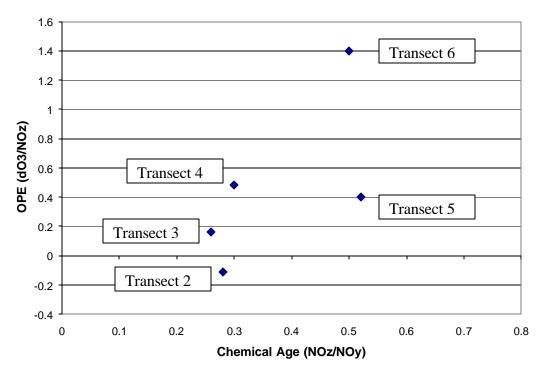


Figure 3-12. OPE (using Mass Balance Approach, by Transect) for Individual Transects versus Corresponding Chemical Ages.

With the exception of Transect 5, Figure 3-12 may show an increasing trend in OPE with increasing chemical age. However, there is no justification for discarding that point. Thus, Figures 3-11 and 3-12 show no clear correlation between OPE and chemical age. This is contrary to other findings (e.g., Gillani et al., 1998b); however, the data had to be severely manipulated to arrive at this conclusion. To summarize the data manipulation required to arrive at Figure 3-8, corrections of NOy were based upon the assumption that initial NOx/NOy was 1.0, rather than 1.3. New values for NOy were calculated simply by multiplying original data values by 1.3, which would correct the ratio NOx/NOy to 1.0. This manipulation was followed by re-calculation of NOz based upon this new value for NOy, simply by subtracting the corresponding original NOx datum.

NOx/NOy ratios higher than 1.0 (not possible, according to Equation 1-1) have been observed in other studies, yet they have not been addressed as being in serious error (Nunnermacker et al., 2000; Springston et al., 2000). These ratios are certainly not possible; they indicate either under estimation of NOy or over estimation of NOx. Under estimation of NOy could result from loss of species in the sampling inlet, such as HNO₃, which is notorious for doing so (Imhoff et al., 2000).

Finally, the NOz_{corrected}/NOy_{corrected} regressions (chemical ages) of the individual transects certainly carry a great deal of error. Any error present in the data measurements was propagated during each manipulation step, and should be viewed with caution. Data from the aircraft flight on September 10, 2000, did not yield reliable estimates of chemical plume age.

3.4 Comparison of Aircraft Data and Modeled Data

The data available from TEXAQS for FPP provides a source for model comparison. No modeling episodes are currently available for the days on which the aircraft data was taken. Thus, modeling days have been used from the existing modeling episode described in Chapter II to compare with the aircraft data.

The subsections following will 1) describe how modeling days were chosen, based upon finding similar meteorological and chemical conditions; and 2) show a comparison between modeled output and aircraft measurements using two different comparison methods. The first method of comparison utilizes modeled output for which a "virtual aircraft flight" is taken through the plume and directly compared to aircraft measurements. The second method of comparison utilizes a "difference method" between two runs. The difference between a modeling run with FPP

emissions turned on and another run with the emissions turned off reveals an effective O_3 impact for the source.

3.4.1 Relevant Parameters for Comparison

Wind direction is possibly the most important meteorological consideration when comparing modeled and aircraft data. Land use, and, therefore, biogenic and anthropogenic emissions of pollutants of chemical concern, shows wide spatial variation. On Day 3 of the modeling episode, at 15:00, as depicted in Figure 2-5, winds were from the south. Wind speeds and trajectories for the aircraft data collected September 10, 2000, can be seen in Figure B-5 (note that 180° means winds are from due south). Wind direction compares well between modeled and aircraft data. Thus, to minimize uncertainty between the modeled and aircraft comparison, Day 3 of the modeling episode was chosen.

Although wind direction was similar, wind speed measured by the G-1 aircraft was approximately double the speed input to the model for the available 1995 episode.

The emission rate modeled by CAMx for Day 3 was 0.8 tons/hr. Only one boiler was in operation during the afternoon. The emission rate on the day of the TEXAQS aircraft flight was approximately 2.3, as summarized in Table 3-2. This disparity would likely cause higher modeled OPE, because larger sources (higher NOx emission rates) tend to have lower OPE, as discussed in Chapter 1. Unfortunately, actual emission rates were not available when modeling commenced.

Temperature has significant effects on isoprene emissions (Weidenmeyer et al., 2001). The ground-level temperature on July 9, 1995 during the afternoon was approximately 33.5 °C, which correlates well with the temperature during the aircraft data collection, which ranged from 31.7 to 32.5 °C. Temperature data

(hourly for model, during FPP flight for aircraft; all ground-level) are plotted in Figure B-6. A linear interpolation was performed on model temperature data to show variation over the hours of interest; however, analysis for model validation will be confined to a single hour. Background O₃ concentrations for the modeling episode on July 9, 1995 were approximately 60 ppb (see Figure B-7), which compares with background O₃ values (on average, 50 ppb) observed on September 10, 2000, as seen in the time series below.

3.4.2 "Virtual Aircraft Flight" Comparison-Concentration Ratio Approach

Because chemical age inferences from the aircraft data did not correlate with OPE, a physical age comparison was made between the aircraft data and the model. This is a fair comparison, considering that physical growth criterion is the most significant in the formulation of the Plume-in-Grid submodel used by CAMx.

To choose a spatial extent of model results similar to that covered by the aircraft in obtaining the flight data, physical plume age was calculated for each transect flown by the aircraft, using the wind speed data available (located in Appendix B), and the position of the aircraft at each transect. Physical age ranged (as seen in Table 3-7) up to 2.5 hours, or about 36 km from the source.

These physical ages were transposed to ages for the plume in the modeling episode, where the wind speed was roughly half that of the aircraft data episode. This translated to a furthest approximate distance of 18 km from the source. All wind data was taken at corresponding heights of the atmosphere. The wind data for the aircraft sampling was taken at approximately 610 m above ground level. Thus, Layer 5 was chosen as the source for wind data from the model (see Table 2-4).

Modeled O₃ and NOz concentrations were sampled at distances corresponding to the NOAA G-1 transects' physical ages. These points were used

to generate a plume-averaged OPE, as in the aircraft data analysis in Section 3.3. The finest grid resolution in this modeling episode was only 4 km; thus, an extremely limited number of cells (21 total) were available to match the aircraft data. Figure 3-13 illustrates the extent of this analysis.

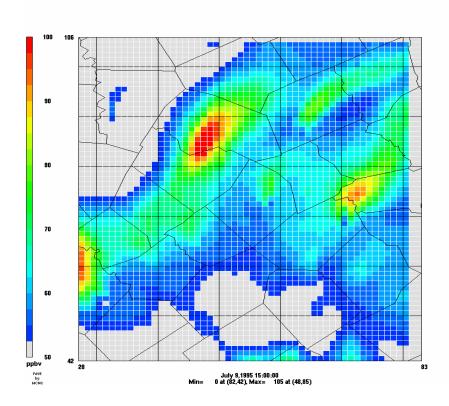


Figure 3-13. O₃ Concentrations in Modeled FPP Plume at Comparable Physical Age and Altitude (CAMx Layer 5) to FPP G-1 Data collected 9/10/2000 (Model Day 3, 15:00 data, wind speed = 2.0 m/s).

It should be noted that the extent to which the physical age of the modeled plume matches the physical age the above plot is only within the boxed area. The plot is also from level 5 of the model output, which corresponds to atmospheric heights between 400 and 670 m. The aircraft data were taken at approximately 600 m altitude. An area of high O₃ concentrations north of FPP is apparent beyond the extent of analysis. It may be that the aircraft data were not gathered far enough

downwind to pick up the peak O_3 in the plume, as well. The time series plot of the aircraft data in Figure 3-4 shows the O_3 concentration still rising from transect 5 to transect 6, which was the final transect. However, as the plane turned parallel to the wind direction during the middle of transect 6, no higher O_3 values were noted; thus, it is assumed that the peak in transect 6 represents the maximum O_3 concentration realized in the sampled plume.

NOz was measured in the same manner as listed above for O_3 . OPE was then calculated as was done for the aircraft data (using the "concentration ratio" approach); the result is shown in Figure 3-14.

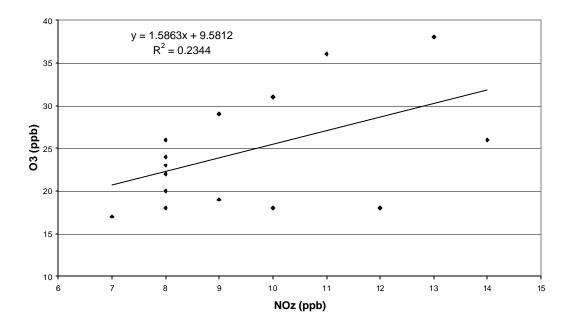


Figure 3-14. OPE for Modeled Data with Similar Physical Age and Altitude to FPP G-1 Data Collected 9/10/2001.

Again, the data is quite limited due to a coarse grid cell resolution. A background O_3 value of 50 ppb was assumed, as there is no apparent break in the plume (ref. Figure 3-13). The slope of the line is not affected by the choice of

background values for O_3 , however, so the predicted OPE within this short plume age is 1.6. This is notably lower than that observed by the aircraft.

3.4.3 "Virtual Aircraft Flight" Comparison-Mass Balance Approach

The above analysis utilizes the "concentration ratio" approach, as described in Section 3.2.2. In order to analyze the model output using the "mass balance approach," data is needed at each transect, for calculation of "flux" according to Equation 3-1. Specifically, average O₃ and NOy concentrations above background are needed for each transect. This is not possible under the analysis using the "Virtual Aircraft Flight," because plume boundaries are not apparent. As mentioned, the "concentration ratio" approach is not affected by choice of background O₃ concentration.

3.4.4 Dimensional Analysis of the "Virtual Aircraft Flight"

As noted in Chapter II, the PiG is "slaughtered" to the host grid within one grid cell (4km) of the source during the day. The first aircraft transect was approximately 3 km across, at a distance of 2 km downwind from the source. The widest the plume was observed was 17 km, or about 10 miles, which compares well with the Big Brown Power Plant Plume, depicted in Figure 3-1. Modeled data, as in Figure 3-13, shows a distinct plume as much as 40 km (10 grid cells) across (green area on either side of the O₃ peak). A comparison between the ozone plume dimensions of the two data sets, interpolated using the Krieging method within the Golden Surfer Software, is depicted in Figure 3-15.

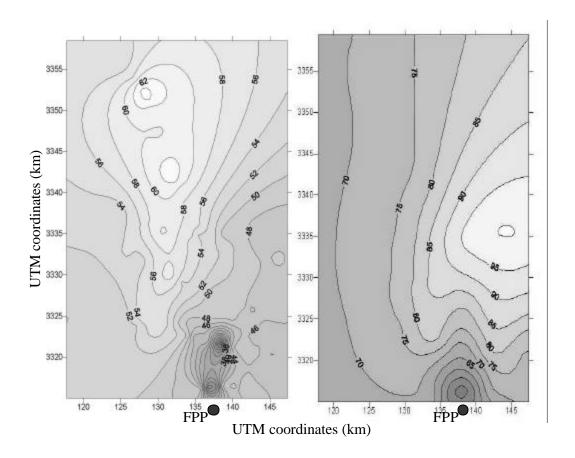


Figure 3-15. Ozone Concentrations (ppb) from Aircraft and Modeled data (Aircraft on left, FPP data collected by NOAA G-1, 9/10/2000; Modeled on right, CAMx, July 9, 1995, 15:00; both interpolated using Krieging method and plotted using Golden Surfer Software).

The ozone plume predicted by the model is much greater in both magnitude and width than that measured by the aircraft data, as described above. Note that the isopleth lines are at intervals of 2 ppb for the aircraft data, and 5 ppb for the modeled data. The reason for this is simple: background concentrations are different for each case.

Sources totaling approximately 10% of FPP's full-load emission rate dot the countryside within 40 km to the north of FPP. Figure 3-16 illustrates this fact.

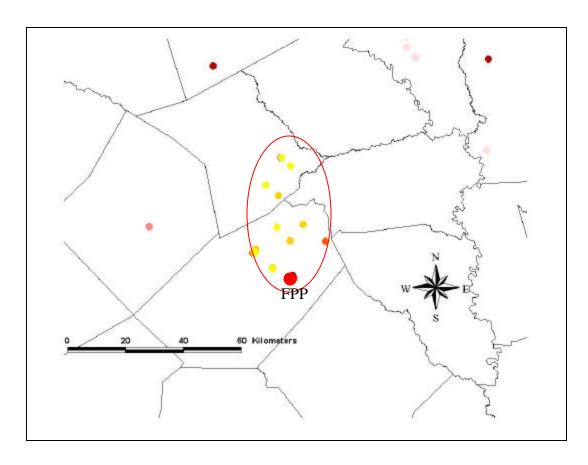


Figure 3-16. NOx Sources within 40 km of FPP (Total NOx contribution ~10% of FPP source strength).

As mentioned in Chapter 2, CAMx utilizes a 4km x 4km grid cell structure around FPP. All NOx emission introduced to grid cells within this structure are immediately distributed amongst the host grid cell, which is 4km x 4km, and has a height corresponding to the level of release, as tabulated in Table 2-4. Thus, it is difficult to extract from plumes, such as the ones in Figures 3-13 and 3-15, what emissions (and therefore, ozone production) are due to FPP, and what emissions are due to other sources. This process may have been easier for the aircraft, as there was an available tracer, SO₂, which defined clear boundaries for the plume. To deal with the lack of modeled plume boundaries, methods were developed to isolate the emissions from a particular source.

3.4.5. "Plant On – Plant Off" Comparison-Concentration Ratio Approach

Another method of comparison for these plumes was developed in concert with the temporal sensitivity studies performed and discussed in Chapter IV as part of this research. By turning FPP's emission on and off, O₃ formed from FPP can be isolated, and compared with the actual emission rate (or increase, from case to case). In addition, the removal of all other emissions and O₃ from the background allows for calculation of dO₃ instead of having to assume a background concentration where there are no clear plume boundaries, as in Figures 3-13 and 3-15. Delta O₃ (or NOz) is calculated according to the following equation.

$$[O_3]_{plant_on} - [O_3]_{plant_off} = dO_3$$
 (3-6)

Equation 3-6 can be viewed as an " O_3 puff." Figure 3-17 demonstrates an O_3 puff, while Figure 3-18 portrays an OPE puff.

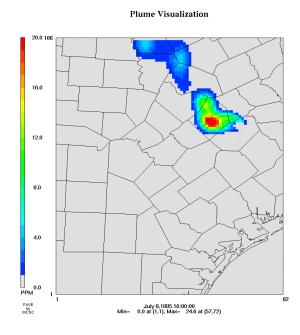
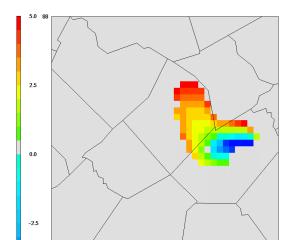


Figure 3-17. O₃ "Puff" (Plant On – Plant Off Difference Plot) Due to Emissions from FPP at 2:00 p.m. on July 8, 1995.



Layer 1 OPE

Figure 3-18. OPE "Puff" (Plant On – Plant Off Difference Plot) Due to Emissions from FPP at 2:00 p.m. on July 8, 1995.

July 8,1995 14:00:00 Min= -17.8 at (69,69), Max= 5.0 at (68,72)

PAVE by MCNC

Figure 3-18 shows an interesting result: the appearance of productive "wings" at the outside of the OPE puff. As mentioned, wings were observed in only one flight of the Baylor aircraft, and in none of the aircraft data available so far from the TEXAQS study. It is unclear *why* the model predicts wings. We may assume that it is due to the lower concentrations located near the outside of the plume, as noted in the background of Chapter I. Why the aircraft data do not show wings is outside the scope of this research, but deserves investigation.

It is necessary to confine the analysis of these modeled plumes to only those cells which show a difference between model runs with full emissions and model runs with no emissions. We may define this dimension by points exceeding a threshold in the difference between $NOy_{Emissions_On}$ and $NOy_{Emissions_Off}$:

$$\sum_{grid} [NOy_{emissions_on} - NOy_{emissions_off}] > 0.1 \text{ ppb }? \text{ "in the plume"}$$

$$\sum_{all_grid_cells} [NOy_{emissions_on} - NOy_{emissions_off}] = 0.1 \text{ ppb ? "outside the plume"}$$

Using Equation 3-6 to derive the same type of OPE plot as was used previously, there appear to be productive areas within the plume. Figure 3-19 shows OPE results for FPP over the region covered by the aircraft data. All of the following plots limit the plumes to the same physical age as that observed in the data collected by the G-1 aircraft.

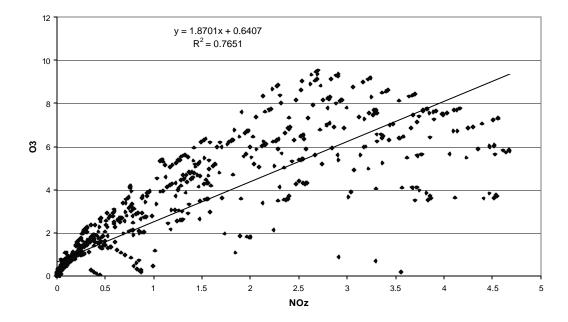


Figure 3-19. OPE of FPP at 3:00 p.m. on July 9, 1995; Plant On – Plant Off Analysis.

Again, the predicted OPE is significantly less (2) than the measured OPE collected by the G-1 aircraft (9). Areas of OPE as high as 4 can be seen within the larger data set, just as in Figure 3-17. A clear difference should be noted between

Figure 3-19 and Figure 3-15. Whereas only an additional 9 ppb O_3 is formed due to FPP emissions according to the Plant On-Plant Off analysis, Figure 3-15 shows, from the base case, a peak of >95 ppb—easily 30 ppb over the background O_3 concentration outside the plume.

Sensitivity tests with biogenic emissions can be tested, to determine if artificially low inventories are the reason for the overall low OPE. To test this hypothesis, the biogenic inventory over the entire 32x32 km domain (pictured in Figure 2-1) was increased by a factor of three. The anticipated result was an increase in OPE for the plume; Figure 3-20 shows the results of this analysis.

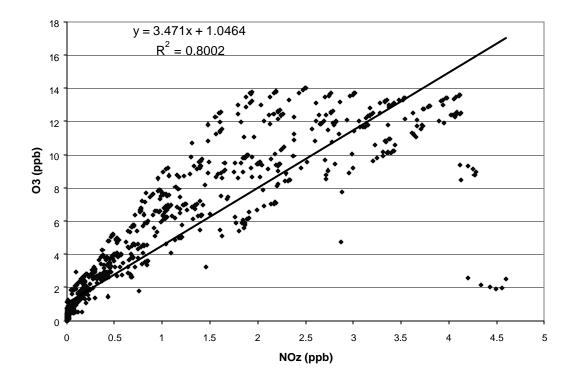


Figure 3-20. OPE of FPP at 3:00 p.m. on July 9, 1995; Plant On – Plant Off Analysis; Three Times Original Biogenic Hydrocarbons.

As can be seen from Figure 3-20, a threefold increase in OPE is predicted when biogenic hydrocarbons are increased threefold. Additionally, a few zones can be seen in Figure 3-20 which show OPEs of up to 7 (upper bound). Further increase of the biogenic inventory to six times its original value was performed and modeled to see if an upper limit could be reached on hydrocarbon productivity. The VOC-limiting plateau was not reached by that estimate, and OPE for FPP was closer to aircraft data predictions than either of the other two runs. Figure 3-21 shows the result of the 6-times biogenic runs.

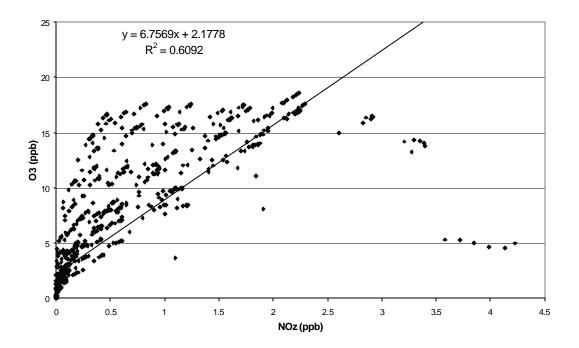


Figure 3-21. OPE of FPP at 3:00 p.m. on July 9, 1995; Plant On – Plant Off Analysis; Six Times Original Biogenic Hydrocarbons.

The slope value shown above (6.8) is obviously a lower bound; zones in this plume can reach OPEs as high as 25. This is an indication that the region is extremely NOx-limited, implying the presence of many reactive hydrocarbons. The region which demonstrates extremely low OPE (points to the far right in Figure 3-

17) is located within approximately 20 km of the source, and contributes to formation of up to 5 ppb O₃.

3.4.6. "Plant On – Plant Off" Comparison-Mass Balance Approach

Transect data was obtained in the following manner: dO₃ and dNOz in cells in the horizontal (East-West) direction were averaged; each "transect" was assumed to be 1 cell in length in the downwind direction. The widths of "transects," dO₃, dNOz, fluxes, and Mass Balance Approach OPE are summarized in Table 3-8.

Table 3-8. Data used for Calculation of Integrated Ozone over FPP Plume (based on aircraft data collected by NOAA G-1 9/10/2000, height assumed 1105 m, wind speed 2 m/s, atmospheric density 37 mol/m³).

	dO_3	dNOy	Crosswind	O ₃ Flux	NOx Flux	OPE
	(ppb)	(ppb)	Width (m)	(tons/hr)	(tons/hr)	
Transect 1	-3.28	0.124	8,000	-0.41	0.01	-26
Transect 2	-2.16	0.36	16,000	-0.54	0.058	-6.1
Transect 3	0.64	0.56	20,000	0.20	0.11	1.14
Transect 4	1.0	0.90	32,000	0.50	0.30	1.10
Transect 5	1.12	1.22	44,000	0.76	0.55	0.91
Transect 6	2.55	1.66	48,000	1.91	0.81	1.54
Transect 7	3.43	1.90	52,000	2.78	1.01	1.81
Transect 8	4.5	2.21	48,000	3.37	1.08	2.03
Transect 9	4.6	2.0	52,000	3.72	1.06	2.3

Other transects (further distances downwind) were analyzed; however, the ones listed above represent the peak within the plume. Other OPEs ranged up to 5.0, but did not represent a dO₃ over that listed above. This approach is intended to provide a lower bound for OPE; however, it is apparent from comparison with the concentration ratio approach that it does not. Reasons for this likely include the assumptions that must be made to come up with "transects" in the model output. This method is not to be trusted above the concentration ratio approach.

3.4.7. "Plant On – Plant Off" Comparison-Ozone Production Approach

In addition to the above OPE analysis, it is also possible, through the Plant On-Plant Off method, to define plume boundaries, and perform a gross macroscopic comparison of total ozone production between model output and aircraft measurement. Downwind distances analyzed for the model are one-half the distances measured by the aircraft, due to the fact that the modeled wind speed was one-half the wind speed measured by the aircraft. Crosswind plume boundaries were defined by a nitric acid difference: if at least 0.07 ppb more HNO₃ was reported in a cell for the modeling run with the emissions turned on than for the modeling run with no emissions, the O₃ value of that cell was included in the analysis. This metric allows for inclusion of cells with negative O₃ production (which would occur through titration with NO). All layers were included in the analysis. One hundred twenty cells (over 9 layers) returned a value, and most were negative, implying an extremely fresh plume. Thus, the total ozone "production" by FPP, for a comparable distance downwind, was -53,000 moles.

It is likely that the above result is due to the fact that the additional NOx from FPP, when introduced to the background NOx from the other sources in the area, caused initial titration of ozone ("Plant On" relative to "Plant Off" modeling runs). This caused a localized ozone disbenefit upon addition of more NOx. Analysis further downwind would be necessary to quantify the overall impact of the plume.

If the plume is left unbounded, that is, all cells are considered if they meet the HNO₃ threshold requirement, no matter how far downwind they are, an ozone production of 58,150,000 moles is predicted. This may be a fair comparison to data from the aircraft flight, the final transect of which appears to have picked up the peak plume O₃ concentration. It is uncertain why the peak occurs so much

further downwind (in terms of physical plume age, or time since emission) for the model than the aircraft. Again, this may be a function of the incorporation of many sources into large grid cells, such as the other small NOx sources in the background of the FPP plume. It seems the dispersion of the plume is also accelerated by the model, due to the introduction of emissions into large grid cells upon leakage and slaughter from the PiG puffs, as described in Chapter 2. Sensitivity tests are recommended to determine whether retaining the integrity of the PiG puffs for longer periods of time will improve the prediction of downwind distance to peak ozone concentrations.

To spatially integrate ozone production for the aircraft data, plume boundaries must be interpolated between transect widths. Mixing height data must be assumed, as there is no upper air sounding data available near Fayette County, Texas, for September 10, 2000. Thus, a mixing height equal to that modeled by CAMx, 1105 m, will be assumed. Background values for O₃ concentration for the aircraft data are inferred from the time series plot of the aircraft data (Figure 3-4). Again, the aircraft did not appear to reach the "end" of the plume, as defined by a peak O₃ concentration. Thus, the plume extent was defined only by what data was available. Table 3-9 summarizes the calculations performed for the aircraft data.

Table 3-9. Data used for Calculation of Integrated Ozone over FPP Plume (based on aircraft data collected by NOAA G-1 9/10/2000, height assumed 1105 m).

	Avg. Conc.	Distance from	Crosswind	O ₃ present
	(ppb)	Source (m)	Width (m)	(moles)
Transect 1	-9.15	1,680	3,260	-2.48×10^6
Transect 2	-3.76	7,700	11,400	-1.28×10^7
Transect 3	1.48	9,540	12,270	1.64×10^6
Transect 4	3.19	14,590	17,000	1.35×10^7
Transect 5	3.84	19,980	11,780	1.20×10^7
Transect 6	8.82	36,040	17,930	1.25×10^8

The total ozone present according to aircraft measurements and assumed dimensions, is 137,180,000 moles (STP). The major differences in aircraft versus modeled data predictions for ozone production are summarized in Table 3-10.

Table 3-10. Summary of Comparisons of Modeled Data (July 9, 1995 CAMx Episode, 15:00) to Aircraft Data (NOAA G-1 9/10/2000).

	Modeled Data	Modeled Data	Aircraft
	(Virtual Aircraft Flight)	(Plant On-	Data
		Plant Off)	
Ozone Production Efficiency	1.6	1.9	9
(moles O ₃ /moles NOx)			
Magnitude of Ozone	n/a	58,150,000	137,180,000
Production (moles)	(no boundaries apparent)		
Maximum Width of	> 40	> 40	18
Ozone Plume (km)	(may be due to multiple		
	sources)		
Downwind Distance to	~ 50	~ 57	36
Peak (km)			

It is apparent that the model over predicts dispersion in both the downwind and crosswind directions. Even with wind speeds ½ the magnitude of those sampled by the G-1 aircraft, the ozone peak within the FPP plume is predicted to occur between 50 and 57 km downwind. In the crosswind direction, a maximum plume width of 18 km, noted by the aircraft, compares with a modeled maximum plume width o more than 40 km.

Three horizontal advection schemes are available in CAMx: one developed by Smolarkiewicz in 1983, and two more recent improvements to the scheme by Bott, 1989, and Colella and Woodward (known as Piecewise Parabolic Method, or PPM), 1984 (Environ, 1998). The horizontal advection scheme utilized in this research was PPM. Because of the disparity in modeled and aircraft-measured

plume dimensions, sensitivity analyses are recommended for this point source, to determine if other advection schemes improve the prediction.

3.5 Conclusions

Tools have been developed to compare aircraft plume measurement data to modeled data. First, a tool known as PSET, the Point Source Evaluation Tool, is included in Appendix A. PSET is to be used in Plant On-Plant Off analyses to isolate O₃ formed due to a particular source. PSET analyzes modeled output to give plume-averaged OPE, transect-averaged OPE, chemical age, loss of NOx, and other relevant plume parameters. The desired spatial extent of analysis can be limited to plume dimensions as measured in aircraft plume sampling.

For direct comparison, without Plant On-Plant Off analysis, AIRCOMP (also included in Appendix A) is a program which will generate spatially-assigned O₃ values for modeled output, which can then be interpolated (using Golden Surfer software, for example) to aircraft plume measurement data. This allows the user to perform a "virtual air craft flight" through the plume, taking samples at locations corresponding to aircraft measurements.

CAMx under predicts Ozone Production Efficiencies, according to these two different types of analysis. In the Plant On-Plant Off analysis, an OPE of 1.9 was observed. Using the "virtual aircraft flight" method, an OPE of 1.6 was predicted. Data taken by the NOAA G-1 aircraft on September 10, 2000, a similar day in terms of wind direction and temperature, indicated a plume-averaged OPE of 9 (upper bound). A mass-balance approach (lower bound) to OPE calculation yields OPEs ranging from -0.27 (fresh plume) to 1.4 (sixth and final transect, plume supposed to be at highest maturity).

Of these values, the best approach to be taken for comparing aircraft data to model output is using the Plant On-Plant Off comparison, combined with the "concentration ratio" approach. This approach requires much less manipulation of data than the "concentration ratio" approach for the "virtual aircraft flight" comparison and the mass balance approach for either comparison. The "concentration ratio" approach for the Plant On-Plant Off comparison requires boundaries to be set by corresponding physical age of the aircraft plume. As seen in this research, such limitations cause much of the plume attributable to the source to be excluded from the analysis. Transect data is needed for the mass balance approach, and is not available in either comparison, except through data manipulation and assumption.

The cause of OPE under prediction by CAMx may lie in over dispersion of emissions in both the downwind and crosswind directions. This is proposed because of the great disparity in plume dimensions between modeled data and aircraft measurement data. Aircraft data indicate a peak at 36 km downwind, and a maximum plume width (as defined by both O₃ and SO₂ concentrations above background) of only 18 km. For a similar set of meteorological conditions (although not identical), CAMx predicts a peak ozone concentration 50-57 km downwind (at ½ the wind speed measured by the aircraft), and a maximum plume width of more than 40 km. For this reason, sensitivity tests employing different horizontal advection schemes are recommended.

Biogenic inventory shortcomings may be the culprit in the appearance of lower-than-measured OPEs. Increasing the biogenic inventory caused a rise in potential OPEs to levels near and beyond those observed in the aircraft data. A more directly correlated modeling episode will be useful for drawing more substantial results, however. Data do not support similar emission rates nor wind

speeds. These disparities may explain the lack of comparability between the modeled and aircraft data.

Finally, the different emission rates between modeled and aircraft data will have an effect on the resulting comparison. On the day of the aircraft flight, 9/10/2000, FPP was emitting 2.3 tons/hr NOx. The modeling performed in this research used an emission value of 0.8 tons/hr NOx on Day 3, because actual emission rate values were not yet available. However, this fact should have caused an over prediction of OPE by the model, since smaller sources tend to have higher OPE. It is uncertain, however, how great the sensitivity to this parameter may be. Additional modeling is required to further investigate this matter. When possible, the modeled emission rate of the source being examined should match the emission rate on the day aircraft data is collected.

<u>Chapter IV: Temporal Sensitivity of O₃ Formation to NOx Emissions</u> from a Large, Rural Point Source in Eastern Texas.

This chapter summarizes research started with modeling approaches previously developed at The University of Texas at Austin. The goal is to answer the following two questions:

- 1) What time of the day is most likely to contribute emissions that will cause spikes in O_3 concentration by sensitive afternoon hours?
- 2) What time of the day is most likely to contribute emissions that will cause high overall O_3 production (e.g., total moles O_3) by sensitive afternoon hours?

4.1 Modeling Approach

The methods of Nowlin et al., originally developed by McDonald-Buller and Nobel, were utilized to create temporal variations in NOx emissions from a single point source in Central Texas, the Fayette Power Project (FPP). In each case, modifications were made to CAMx-ready emissions files using the ptmodpig.f program (located in Appendix A) and a factor file, which was generated using Microsoft Excel (also in Appendix A). First, a "base case" modeling run was performed which normalized emissions for FPP for each day of the modeling episode. Original and normalized emission rates are plotted in Appendix D. The normalizing emission factor was calculated according to the following equation.

$$\frac{ER_{new} \times profile}{ER_{old}} = factor$$
 (4-1)

Where ER_{new} is the hourly average emission rate (tons/hr), profile is the fraction of original emissions desired for the run, ER_{old} is the original hourly emission rate (tons/hr), and factor is the factor calculated by Excel to modify emissions files.

The next step was to reduce the NOx emission rate for FPP to half its normalized emission rate. For the base case, "profile," in Equation 3-1, was considered to be 100%; in the case of half emissions, the "profile" for each hour was changed to 50%. Finally, emissions files with two-hour increases of NOx emissions were created by changing the "profile" to 100% for a given two-hour time period, while leaving the other 22 hours at 50%. This was meant to simulate the NOx reduction to be realized by Senate Bill 7, as mentioned in Chapter 1.

By examining the impacts of each two-hour increase in NOx, we see the impact of having no NOx control for that two-hour time period. A period of the day which is shown to form little O₃ may be suitable for "environmental dispatching." This method of NOx control shifts the power load from coal-fired power plants to gas-fired power plants, which exhibit lower NOx emissions per Btu of energy produced. FPP is a base-loaded plant, which means that it carries a full power load all day, every day. If some of the load on FPP could be shifted to a gas-fired plant during times of the day when NOx emissions have the highest OPE, regional O₃ formation could be effectively reduced. Nowlin's results indicated nighttime emissions were most efficient at producing ozone. Nighttime would be the most suitable time to employ environmental dispatching, as the power load reaches a minimum.

4.2 Receptor Site Analysis

Nowlin's analysis examined four large NOx sources and performed simultaneous reductions and temporal sensitivity analyses. To quantify impact, Nowlin chose receptor sites, urban areas which exceeded a daily O₃ threshold of 110 ppb, based on reasoning described in that work. The change in O₃

concentrations at those sites due to NOx increases at the four NOx sources was quantified by an "impact index," which was developed by Nobel, and is defined by Equation 4-2.

$$OzoneIndex = \frac{\sum_{cells > threshold} ([O_3]_{run} - [O_3]base_case)}{Daily_NOx_Increase * \#Cells_in_Re\ gion}$$
(4-1)

units:
$$\frac{ppb}{\Delta ton_NOx/day}$$

The indices were designed to offer a qualitative comparison between impact at different sites and on different days by normalizing the indices to the NOx increase and the number of cells in each site. Integration over the time of day during which high O₃ concentrations are witnessed is accomplished by Equation 4-2.

$$IntegratedIndex = \sum_{\substack{2d \ hours}} ([t_{n+1} - t_n] * AverageOzoneIndexValue_{t_n \rightarrow t_{n+1}})$$
 (4-2)

$$units: \frac{ppb-hour}{\Delta ton_NOx/day}$$

The integrated index was used to derive a single impact value for emissions from a particular time of day. Plotting these single values together illustrates the relative impact of emissions from different times of the day. Some of Nowlin's results are shown in Figure 4-1.

INTEGRATED INDEX Houston, Day 4 110ppb Threshold

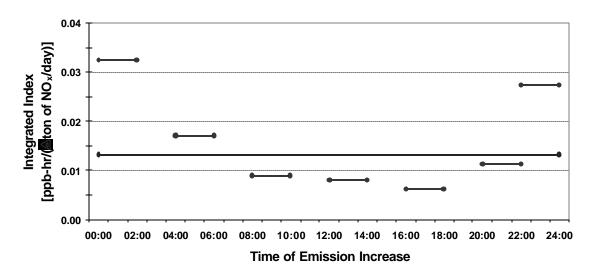


Figure 4-1. Diurnal Impact of NOx Emissions (Nowlin, 2001).

As can be seen from Figure 4-1, nighttime NOx emissions produce more O₃ at the receptor site in Houston than daytime NOx emissions. Clarification is needed from Nowlin's results, to be sure that selection of "receptor sites" to quantify impact did not slant the results. It was discovered during research with FPP that selection of a "receptor site" can cause a particular time of emissions to seem significant, when in fact, only the emissions during that time made it to the receptor site. It is important to consider the spatial location of emissions as well as their chemical capacity to produce O₃. We will refer to these issues as "meteorology vs. chemistry."

In choosing Austin as a receptor site for FPP studies, for example, on July 12, the emissions which were in Austin were from the previous afternoon.

Although these emissions showed the highest impact by far, the impact itself was insignificant. Figure 4-2 illustrates these results.

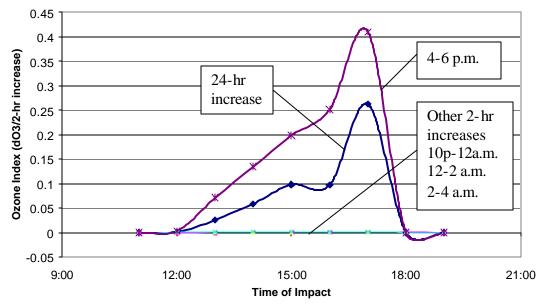


Figure 4-2. FPP Impact (dO₃/Two Hours of Increased Emissions) in 6- grid cell (4x4 km) Region Surrounding Austin, TX for Emissions Increases (Day 6 of Modeling Episode).

According to Figure 4-2, afternoon emissions will have the greatest impact in Austin. The index used, however, points to the fact that the change in O₃ concentration due to the 4-6 pm doubling of NOx emissions was less than 0.5 ppb. Further analysis shows that nighttime emissions dominate O₃ production, no matter where the emissions have gone. This points to "chemical" reasons as to why nighttime emissions are significant, as opposed to misleading transport issues like the one shown in Figure 4-2.

4.3 Plume Location Analysis

To address the issue of transport, one must "follow the plume." First, the difference between two modeling runs isolates the O₃ which is solely due to a two-hour NOx increase, according to Equation 4-3.

$$[O_3]_{2-hr_increase_case} - [O_3]_{base_case} = dO_3$$

$$(4-3)$$

Puffs can be followed by both their absolute O₃ concentrations or their instantanteous OPEs (O₃/NOz). Puffs locations are assigned according to their maximum O₃ concentration, as pictured in Figure 4-3. By tracking the peak concentration, one can answer the first of the two questions stated as objectives to this research. Figure 4-3 represents a "typical puff." Puffs for other time periods are depicted in Appendix C.

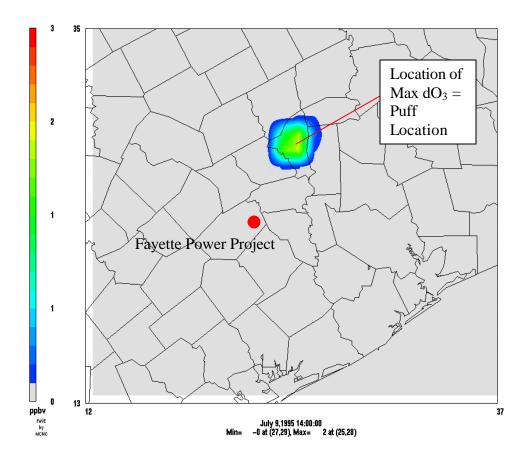


Figure 4-3. Ozone "Puff" (Difference plot of [2-hr Increase – Base Case]) for a Midnight-2am NOx Increase on July 9, 1995, snapshot taken at 14:00, ground layer.

To further the analysis, a relative impact of *moles of ozone present at a certain time of the day* was calculated for each puff at a given time of day. The time of most interest is the afternoon, when high ozone events will typically occur. Two o'clock p.m. was chosen as an analysis time. Three and five o'clock p.m. analyses are also included, to provide a more complete picture. Results of this analysis will answer the second question proposed at the beginning of this chapter.

The total number of moles of O₃ carried by each puff at STP (for a given instant in time) was calculated by simply integrating the concentrations of O₃ in each grid cell over the volume of the cells. Layer heights were obtained from CAMx input files, and are summarized in Table 2-4.

Because cumulative effects of O_3 production (for a given instant in time) were assessed by integrating spatially, no anomalous spikes in O_3 concentrations were assigned undue weight. Figure 4-4 shows the relative impacts of emissions from different times of the day and night on O_3 production. The time selected for analysis is 2:00 p.m. on the afternoon following the emissions. Thus, the emissions from 4:00-6:00 p.m. are emissions that originated the previous day.

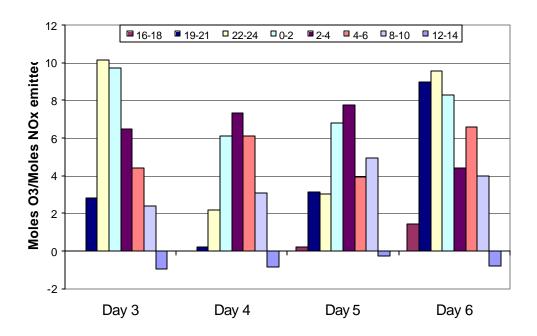


Figure 4-4. Relative Impacts of Two-Hour Emissions Increases; 14:00 Analysis.

As Figure 4-4 bears out, nighttime NOx emissions produced more O_3 than morning or afternoon emissions by 2:00 p.m. on a given day. Although emissions from noon-2 p.m. are not expected to have an impact at 2 p.m., this result is useful in its quantification of that fact. Analysis later in the day, at 5 p.m., yields similar results.

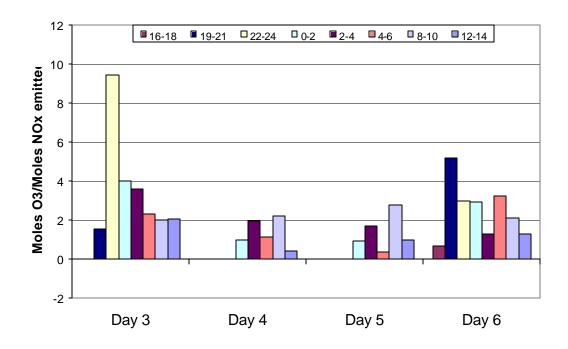


Figure 4-5. Relative Impacts of Two-Hour Emissions Increases; 17:00 Analysis.

The relative impact of emissions from 8-10 a.m. increases significantly depending on which window is examined. The 10 p.m.-midnight emissions from Day 2 of the modeling episode are still quite chemically active at 5:00 p.m. the next day; most of the other nighttime emissions have been neutralized, presumably through photooxidation. Indeed, most of the impacts are much lower than those measured for the 2:00 p.m. analysis. This is likely because photochemically active NOx is consumed through O₃ chemistry.

Analysis performed at 3:00 p.m. indicates a significant reduction in photochemically active NOx between the hours of 2:00 and 3:00 p.m. Again, the peak O_3 production is approximately one-fifth of the production at 2:00. Figure 4-6 demonstrates these results.

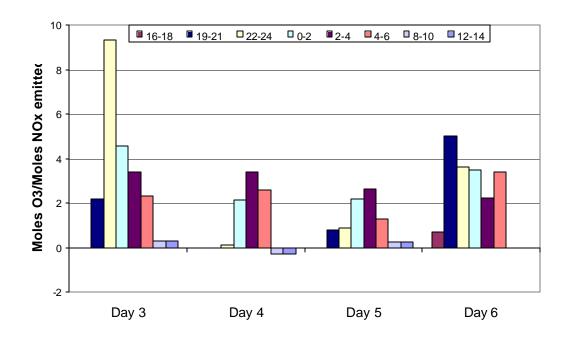


Figure 4-6. Relative Impacts of Two-Hour Emissions Increases; 15:00 Analysis.

Again, the nighttime emissions contribute more O_3 by 3:00 p.m. than emissions from other times of the day. These results must be correlated with the location of impact. Conclusions can be drawn about control strategies for emissions with potential impact in urban areas only when the potential spatial extent of those emissions can be quantified. Figure 4-7 quantifies the impacts as well as their location (defined by maximum $?O_3$ in the puff).

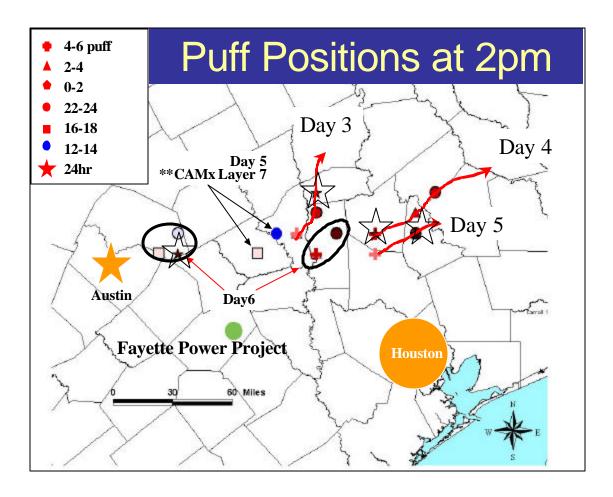


Figure 4-7. Positions of Maximum ?O₃ for Two-Hour Emissions Increases, all Layers; 14:00 Analysis (darker symbol color indicates higher impact; blue indicates negative impact, open star locates maximum impact of all-day, 50% reduction).

Analysis of Figure 4-7 is quite significant to this research. Although the symbols have been color-coded according to their relative impacts (as quantified in Figures 4-4 through 4-6; darker color indicates higher impact), it is not necessary to know their exact values. Qualitatively, it is equally useful to examine where the two-hour impacts occur relative to where the maximum 24-hour impact occurs. The 24-hour impact was calculated in the same manner as the other impacts, only the emissions "increase" was considered to be the difference in emissions between the full, normalized emissions case, and the half-emissions case, as mentioned in

section 4.1. The location of an O₃ maximum for the 24-hour emission increase reflects the position of the overall maximum impact for that particular day. On Day 4, for instance, the maximum 24-hour impact lies at the same position as the maximum impact for the 2-4 a.m. emissions increase case. This implies that the 2-4 a.m. emissions were the main contributor to maximum O₃ concentrations on that day. In fact, from looking at Figures 4-4 and 4-6, that particular time period of emissions did dominate for Day 4.

By locating the puffs at their point of maximum concentration, one can consider the potential impact of emissions as both ozone concentration and total ozone production. The first metric is significant to work currently being done in Houston, to address high ozone events which arise from rapid formation of ozone. The second metric addresses regional control strategies, and the potential of the plant to contribute to high background concentrations of ozone.

Another important observation from Figure 4-7 is the separation of puffs from one another on Days 5 and 6. On these days, some emissions from higher levels in the CAMx grid structure were carried in those upper layers (presumably out of the modeled convective mixed layer) in a different direction than the prevailing ground-level winds. This reflects the meteorological phenomenon of wind shearing, which, as mentioned in Chapter I, can lead to transport of emissions in different directions, and discontinuity of plumes.

Finally, a potential control strategy development could arise from this type of analysis. It is obvious from the above plot, that nighttime emissions could have a large impact on urban areas such as Austin or Houston, depending on prevailing wind direction during the night. Minimizing these emissions is crucial to efficient regional control of O₃ formation. This could be accomplished through

environmental dispatching, or in a more sophisticated way, through predictive control.

4.4 Conclusions

Methods have been developed in this research to compare ozone production capability of emissions from different times of the day. Specifically, the Point Source Evaluation Tool for Temporal sensitivity (PSETTEMP, available in Appendix A), is useful for integrating ozone production over a given period of time and space. This tool applies to the Plant On-Plant Off technique, and emissions can be scaled between 0 and 100% for user-defined time periods using the point source summarization and modification programs also located in Appendix A.

According to this research, incremental increases in afternoon emissions from a rural point source will not have an impact on urban areas during sensitive times of the day. Different results will likely arise for urban point sources, for theories summarized in Chapter 1. This research has provided effective analysis methods for such investigations. The rural point source studied showed high impact of emissions during the night, viewed as both ozone concentration contribution, and spatially integrated ozone formation (total moles ozone formed by a single set of emissions).

For the particular rural point source studied, the location of the O₃ attributable to the source during peak hours of the day is such that it could potentially impact an urban area during peak O₃ hours, and thereby cause an exceedance of the O₃ NAAQS. The emissions most likely to cause such an exceedance originate during the night, and are transported for release in Austin or Houston during sensitive hours. Further consideration should be given to determine

statistically when such events are likely to occur (by historical wind rose), and to determine the feasibility of predictive control.

The impact potential of a source on an urban area is a function of wind speed, wind direction, and source strength. Based on a given wind speed and direction, the source strength could potentially be tuned (or environmental dispatching could be employed) during different periods of the day to minimize ozone production.

Chapter V: Summary and Conclusions

Modeling of power plant plumes (PPPs) is a subject which has been approached on a submodel level; rarely has it been investigated within a larger framework, such as a regional photochemical grid model. The photochemical grid model investigated, CAMx, overestimates crosswind plume dispersion, and under predicts OPE in a power plant plume relative to aircraft plume sampling on a similar day. The large NOx source under examination, Fayette Power Project, located in Fayette County, Texas, was sampled on September 10, 2000 by the National Oceanic Aviation Administration's G-1 aircraft. Analysis of the data acquired indicates an Ozone Production Efficiency (OPE) of approximately 9 (moles O₃ produced per mole NOx emitted). Analysis of a similar CAMx modeling day, July 9, 1995, indicates an OPE of only 1.6-1.8.

Tools have been developed to compare aircraft plume measurement data to modeled data. First, a tool known as PSET, the Point Source Evaluation Tool, is included in Appendix A. PSET is to be used in Plant On-Plant Off analyses to isolate O₃ formed due to a particular source. PSET analyzes modeled output to give plume-averaged OPE, transect-averaged OPE, chemical age, loss of NOx, and other relevant plume parameters. The desired spatial extent of analysis can be limited to plume dimensions as measured in aircraft plume sampling.

For direct comparison, without Plant On-Plant Off analysis, AIRCOMP (also included in Appendix A) is a program which will generate spatially-assigned O₃ values for modeled output, which can then be interpolated (using Golden Surfer software, for example) to aircraft plume measurement data. This allows the user to perform a "virtual aircraft flight" through the plume, taking samples at locations corresponding to aircraft measurements.

CAMx under predicts Ozone Production Efficiencies, according to these two different types of analysis. In the Plant On-Plant Off analysis, an OPE of 1.9 was observed. Using the "virtual aircraft flight" method, an OPE of 1.6 was predicted. Data taken by the NOAA G-1 aircraft on September 10, 2000, a similar day in terms of wind direction and temperature, indicated a plume-averaged OPE of 9 (upper bound). A mass-balance approach (lower bound) to OPE calculation yields OPEs ranging from -0.27 (fresh plume) to 1.4 (sixth and final transect, plume supposed to be at highest maturity).

Of these values, the best approach to be taken for comparing aircraft data to model output is using the Plant On-Plant Off comparison, combined with the "concentration ratio" approach. This approach requires much less manipulation of data than the "concentration ratio" approach for the "virtual aircraft flight" comparison and the mass balance approach for either comparison. The "concentration ratio" approach for the Plant On-Plant Off comparison requires boundaries to be set by corresponding physical age of the aircraft plume. As seen in this research, such limitations cause much of the plume attributable to the source to be excluded from the analysis. Transect data is needed for the mass balance approach, and is not available in either comparison, except through data manipulation and assumption.

The cause of OPE under prediction by CAMx may lie in over dispersion of emissions in both the downwind and crosswind directions. This is proposed because of the great disparity in plume dimensions between modeled data and aircraft measurement data. Aircraft data indicate a peak at 36 km downwind, and a maximum plume width (as defined by both O₃ and SO₂ concentrations above background) of only 18 km. For a similar set of meteorological conditions (although not identical), CAMx predicts a peak ozone concentration 50-57 km

downwind (at ½ the wind speed measured by the aircraft), and a maximum plume width of more than 40 km. For this reason, sensitivity tests employing different horizontal advection schemes are recommended.

Biogenic inventory shortcomings may be the culprit in the appearance of lower-than-measured OPEs. Increasing the biogenic inventory caused a rise in potential OPEs to levels near and beyond those observed in the aircraft data. A more directly correlated modeling episode will be useful for drawing more substantial results, however. Data do not support similar emission rates nor wind speeds. These disparities may explain the lack of comparability between the modeled and aircraft data.

Afternoon emissions from a rural point source will not have an impact on urban areas, according to this research. Different results will likely arise for urban point sources. This research has provided effective analysis methods for such investigations.

Comparison of Chapters III and IV should be approached with caution. Note that the maximum contribution of the 24-hour "puffs" from Chapter IV, Figure 4-7, occurs far downwind of the maximum ozone concentration reported from the base case, in Figure 3-18 from Chapter III. This is likely due to non-linearity in ozone chemistry. The 24-hour puff of Chapter IV originates in a region which already contains the same quantity of NOx emissions (as it results from an increase in emissions from half- to full-strength). The ozone generation in Figure 3-18 is from a source being emitted into a region with essentially no background NOx. Those emissions have higher OPE and realize their chemical maturity at a more rapid rate. In other words, the ozone production in Chapter IV is, in every case, due to *incremental* increases in NOx emissions. In Chapter III, the ozone production measured is based on the *absolute* emission rate of the power plant.

Chapter VI: Recommendations

In order to address the over dispersion of emissions, the PiG may be modified to "can" emissions longer. This would cause a further delay in the introduction of emissions to the coarse grid. It is quite possibly this introduction which causes the overestimation. This is also a good first step to see whether the under predicted OPE is caused by the overestimation of dispersion. Furthermore, the horizontal advection scheme used in the model was the PPM scheme, as defined by CAMx. Two other schemes are available within CAMx, based on research by Bott and Smolarkiewicz (Environ, 1998), and should be examined alongside the PPM scheme to test the sensitivity of the model.

Other factors potentially causing under prediction of plume OPE, as mentioned, are under prediction of biogenic emissions local to FPP. Steps continue to be taken to address the uncertainty surrounding the biogenic emissions inventory in Central and Eastern Texas.

The absence of wings in Central Texas plumes sampled by aircraft is an interesting phenomenon. This is contrary to findings in other parts of the country, for example, Tennessee. This phenomenon should be noted and further explored.

The diurnal sensitivity of Ozone formation to NOx emissions observed for a rural source should be compared with modeling for an urban source, using the experimental procedure developed during this research. By following the plumes, an impact analysis should be performed to estimate the potential for a given source to impact an urban area which is either non-attainment or near non-attainment. Using these results to develop control strategies will increase the effectiveness of NOx control implementation in Central and Eastern Texas.

APPENDICES

APPENDIX A: Computer code

- 1. CAMx run control file
- 2. PiG growth subroutine
- 3. PiG chemistry subroutine
- 4. Point Source Modification Program (ptsumpig, ptmodpig.f and pigoff.f)
- 5. Point Source Evaluation Tool, PSET
- 6. Temporal Sensitivity Evaluation Tool, PSETTEMP
- 7. Aircraft Data Comparison Code, AIRCOMP

1. CAMx run control file (3 pages)

```
#!/bin/csh
# CAMx 2.0 run for Central TX 1995 07/07 - 07/12
#
# NOTES
#
# July 1995 Base Case with one exception
#
  Emissions have been normalized for the Fayette Power Plant
#
   to a steady daily emission rate.
set verbose
date
set RUN = "Fayettebase"
rm -rf $RUN
mkdir $RUN
set EXEC = "/usr/local/models/CAMx2.03/CAMx"
set INPUT = "/yo/modeling/july95/camx"
set EMIS = "/yo/emissions/july95/eps2/16km/emiss"
set EMIS2 = "/yo/emissions/july95/eps2/4km/emiss"
set POINT = "/yo/hamlin/ptsrce"
set OUTPUT = "/yo/hamlin/outputs/$RUN"
rm -rf $OUTPUT
mkdir $OUTPUT
# run the first day
cat << ieof > CAMx.in
CAMx2.03 CTX, 950707, 32-16-4km Run: $RUN
Root output name | $OUTPUT/CAMx2.ctx.950707.$RUN
Start yr/mo/dy/hr | 95 07 07
                             0.
    yr/mo/dy/hr | 95 07 07 2400.
End
dtmx,dtin,dtem,dtou 0.5 1. 1. 1.
nx,ny,nz
                  147 41 9
                 UTM
Coordinate ID
xorg, yorg, dx, dy, zon | -300. 2824. 32. 32. 15
time zone
PiG parameters
                  2000. 24.
Avg output species |6
                           NO NO2
                                               PAN
                  03
                                                          NXOY
HNO3
                  | 2
Num fine nest
il,i2,j1,j2,nz,mesh 4 28 5 31 9 2
i1,i2,j1,j2,nz,mesh | 6 15 8 20 9 8
SMOLAR, BOTT, PPM? | PPM
```

```
Restart
                   false
Chemistry
                   ltrue
Dry dep
                   ltrue
Wet dep
                   false
PiG submodel
                   true
Staggered winds
                   false
Treat area emiss
                   true
Treat point emiss | true
1-day emiss inputs | true
3-D average file
                 true
Source Apportion
                   |false
Chemparam
                   |$INPUT/common/CAMx2.chemparm.3
Photolysis rates
                   |$INPUT/common/camx.rates.ctx.jul95
Landuse
                   |$INPUT/common/landuse.32km
Height/pressure
                   |$INPUT/met/32km/camx.zp.950707.32km
Wind
                   |$INPUT/met/32km/camx.uv.950707.32km
Temperature
                   |$INPUT/met/32km/camx.tp.950707.32km
Water vapor
                   |$INPUT/met/32km/camx.qa.950707.32km
Cloud cover
Rainfall
Vertical diffsvty | $INPUT/met/32km/camx.kv.950707.32km.kvpatch
Initial conditions |$INPUT/icbc/ic.ctx.950707
Boundary conditions | $INPUT/icbc/bc.ctx.950707
Top concentration | $INPUT/icbc/tc.ctx
Albedo/haze/ozone | $INPUT/common/alhzoz.ctx.950707-12.a0
Point emiss
                   | $POINT/ptsrce.aacog.$RUN.950707
Area emiss
                    $EMIS/emiss.aacoq.32km.950707
Landuse
                #1 | $INPUT/common/landuse.ctx_16km
Landuse
                #2 | $INPUT/common/landuse.ctx_04km
Height/pressure #1 | $INPUT/met/16km/camx.zp.950707.16km.ctx
Height/pressure #2 |$INPUT/met/4km/camx.zp.950707.4km.ctx
Wind
                #1 | $INPUT/met/16km/camx.uv.950707.16km.ctx
Wind
                #2 | $INPUT/met/4km/camx.uv.950707.4km.ctx
Temperature
                #1 | $INPUT/met/16km/camx.tp.950707.16km.ctx
Temperature
                #2 | $INPUT/met/4km/camx.tp.950707.4km.ctx
Vertical diff
                #1 | $INPUT/met/16km/camx.kv.950707.16km.ctx.kvpatch
Vertical diff
                #2 | $INPUT/met/4km/camx.kv.950707.4km.ctx.kvpatch
Area emiss
                #1 | $EMIS/emiss.aacoq.16km.950707
Area emiss
                #2 | $EMIS2/emiss.4km.run2.wbuf.950707
ieof
$EXEC | & tee $RUN/CAMx2.ctx.950707.$RUN.out
date
# run remaining days
foreach today (08 09 10 11 12 )
set yesterday = `echo $today | awk '{printf("%2.2d",$1-1)}'`
cat << ieof > CAMx.in
```

```
CAMx2.03 CTX, 950707, 32-16-4km Run: $RUN
Root output name | $OUTPUT/CAMx2.ctx.9507$today.$RUN
Start yr/mo/dy/hr
                   |95 07 $today
                                     0.
                   |95 07 $today 2400.
     yr/mo/dy/hr
dtmx,dtin,dtem,dtou | 0.5 1. 1. 1.
nx,ny,nz
                    47 41
Coordinate ID
                   UTM
xorg, yorg, dx, dy, zon | -300. 2824. 32. 32. 15
time zone
                   16
PiG parameters
                   2000. 24.
Avg output species |6
                    03
                              NO
                                         NO2
                                                   PAN
                                                             NXOY
HNO3
Num fine nest
                   | 2
i1,i2,j1,j2,nz,mesh| 4 28 5 31 9 2
i1,i2,j1,j2,nz,mesh | 6 15 8 20 9 8
SMOLAR, BOTT, PPM? | PPM
Restart
                   ltrue
Chemistry
                    ltrue
Dry dep
                    ltrue
                   |false
Wet dep
PiG submodel
                   true
Staggered winds
                   |false
Treat area emiss
                   ltrue
Treat point emiss | true
1-day emiss inputs | true
3-D average file
                   Itrue
                    lfalse
Source Apportion
                    |$INPUT/common/CAMx2.chemparm.3
Chemparam
Photolysis rates
                   |$INPUT/common/camx.rates.ctx.jul95
                    |$INPUT/common/landuse.32km
Landuse
                    $INPUT/met/32km/camx.zp.9507$today.32km
Height/pressure
Wind
                    $INPUT/met/32km/camx.uv.9507$today.32km
Temperature
                    $INPUT/met/32km/camx.tp.9507$today.32km
Water vapor
                    |$INPUT/met/32km/camx.qa.9507$today.32km
Cloud cover
Rainfall
Vertical diffsvty | $INPUT/met/32km/camx.kv.9507$today.32km.kvpatch
Initial conditions
Boundary conditions | $INPUT/icbc/bc.ctx.9507$today
                   |$INPUT/icbc/tc.ctx
Top concentration
Albedo/haze/ozone
                   |$INPUT/common/alhzoz.ctx.950707-12.a0
Point emiss
                   | $POINT/ptsrce.aacog.$RUN.9507$today
Area emiss
                   |$EMIS/emiss.aacoq.32km.9507$today
Landuse
                #1 | $INPUT/common/landuse.ctx_16km
                #2 | $INPUT/common/landuse.ctx_04km
Landuse
Height/pressure #1 | $INPUT/met/16km/camx.zp.9507$today.16km.ctx
Height/pressure #2 | $INPUT/met/4km/camx.zp.9507$today.4km.ctx
Wind
                #1 | $INPUT/met/16km/camx.uv.9507$today.16km.ctx
Wind
                #2 | $INPUT/met/4km/camx.uv.9507$today.4km.ctx
```

```
Temperature
                #1 | $INPUT/met/16km/camx.tp.9507$today.16km.ctx
Temperature
                #2 | $INPUT/met/4km/camx.tp.9507$today.4km.ctx
Vertical diff
                #1
|$INPUT/met/16km/camx.kv.9507$today.16km.ctx.kvpatch
Vertical diff
              #2
|$INPUT/met/4km/camx.kv.9507$today.4km.ctx.kvpatch
Area emiss
                #1 | $EMIS/emiss.aacog.16km.9507$today
Area emiss
                #2 | $EMIS2/emiss.4km.run2.wbuf.9507$today
Coarse grid restart | $OUTPUT/CAMx2.ctx.9507$yesterday.$RUN.inst.2
Fine grid restart | $OUTPUT/CAMx2.ctx.9507$yesterday.$RUN.finst.2
PiG restart
                   |$OUTPUT/CAMx2.ctx.9507$yesterday.$RUN.pig
ieof
$EXEC | & tee $RUN/CAMx2.ctx.9507$today.$RUN.out
#
end
exit
```

2. PiG growth subroutine

```
subroutine
piggrow(n,dt,rkv,axiszmx,axisymx,o3amb,wind,dumpmass)
c----CAMx v2.03 000229
     PIGGROW performs the following functions:
C
C
              (1) grows puffs
              (2) calculates the mass to dump if growth restricted
С
              (3) entrains grid mass if growth allowed
      Copyright 1996, 1997, 1998, 1999, 2000 ENVIRON International
Corporation
С
     Modifications:
С
С
       none
С
     Input arguments:
С
С
                             puff index
С
        dt
                             time step (s)
        rkv
С
                             vertical diffusivity (m2/s)
        axiszmx
                             maximum allowable vertical depth (m)
С
C
        axisymx
                            maximum allowable lateral size (m)
С
        o3amb
                             ambient ozone concentrations (umol/m3)
С
        wind
                             ambient wind (m/s)
С
С
    Output arguments:
        dumpmass
                            NO, NO2, HNO3 mass to dump (umol)
С
C
    Subroutines called:
С
С
        none
С
     Called by:
С
        PIGDRIVE
С
С
      include "camx.prm"
      include "pigsty.com"
      include "filunit.com"
С
      dimension dumpmass(3)
      data pi/3.1415926/
      data dsydx /2.66e-2/
      data dszdx /4.95e-4/
C
c----Entry point
c----Calculate horizontal diffusivity from Kv, and grow puff in
cross-section
```

```
only
С
      zscore = 1.5
      rkh = 46.4*rkv**(2./3.)
      rkh = amax1(rkh, 10.)
      volold = xlength(n)*axisy(n)*axisz(n)*pi
      sigzo = sigz(n)
      sigyo = sigy(n)
      sigz(n) = sqrt(sigz(n)*sigz(n) + 2.*rkv*dt) + wind*dt*dszdx
      sigy(n) = sqrt(sigy(n)*sigy(n) + 2.*rkh*dt) + wind*dt*dsydx
C
      if (lnewg(n)) then
        axisy(n) = zscore*sigy(n)
        axisz(n) = zscore*sigz(n)
        fmspig(n) = 1. - exp(-zscore*zscore/2.)
        goto 900
      endif
c----Limit puff dimensions by axiszmx and axisymx
      fmsold = fmspig(n)
      axisz(n) = zscore*sigz(n)
      if (2.*axisz(n).qt.axiszmx) then
        axisz(n) = axiszmx/2.
        zscore = axisz(n)/sigz(n)
        fmspig(n) = 1. - exp(-zscore*zscore/2.)
      endif
      axisy(n) = zscore*sigy(n)
C
      if (2.*axisy(n).gt.axisymx) then
        axisy(n) = axisymx/2.
        zscore = axisy(n)/sigy(n)
        axisz(n) = zscore*sigz(n)
        fmspig(n) = 1. - exp(-zscore*zscore/2.)
      endif
C
c----Artificially shrink puffs older than agemax so that 10% of
puff mass
C
      is released each timestep
      if (agepig(n).ge.agemax) then
        fmspig(n) = amax1(0., fmsold - 0.1)
        zscore = sqrt(-2.*alog(1. - fmspig(n)))
        axisy(n) = zscore*sigy(n)
        axisz(n) = zscore*sigz(n)
      endif
c----Pump out puff mass due to expansion
      delms = (fmsold - fmspig(n))/fmsold
```

```
if (delms.gt.1.e-5) then
        do 1=1,3
          dumpmass(1) = puffmass(1,n)*delms
          puffmass(l,n) = puffmass(l,n) - dumpmass(l)
        enddo
      else
        do 1=1,3
          dumpmass(1) = 0.
        enddo
      endif
900 volnew = xlength(n)*axisy(n)*axisz(n)*pi
      if (volnew.lt.0.0) then
        write(iout,'(//,a)') 'ERROR in PIGGROW:'
        write(iout,*) 'Negative puff volume'
        write(iout,*) 'Puff#,length,axis_x/y/z:'
       write(iout,*) n,xlength(n),axisy(n),axisz(n),axiszmx
       write(iout,*) 'Size/mass parameters:'
       write(iout,*) zscore,fmspig(n),fmsold
       write(iout,*) 'CAMx Stopping'
        stop
      endif
c----Update ozone puff mass due to entrainment
      if (lnewg(n)) then
        puffmass(4,n) = o3amb*volnew
      elseif (volnew.gt.0.) then
       dvol = volold*(sigy(n)*sigz(n)/(sigyo*sigzo) - 1.)
        if (volnew.le.volold) dvol = amin1(dvol,volnew)
        conpig = puffmass(4,n)/volnew
        if (o3amb.gt.conpig) puffmass(4,n) = puffmass(4,n) +
o3amb*dvol
      endif
С
     return
      end
```

3. PiG chemistry subroutine (3 pages)

```
subroutine pigchem(dt,ldark,bdnlo3,bdnlno,h2o,pk,
                         convfac,conpig,o3dif)
С
c----CAMx v2.03 000229
      PIGCHEM updates NOx and O3 concentrations in the puff
С
С
      Copyright 1996, 1997, 1998, 1999, 2000 ENVIRON International
Corporation
С
     Modifications:
С
        none
С
С
      Input arguments:
С
С
                             time step (s)
С
         ldark
                             darkness flag (logical)
        bdnlo3
                             lower bound ozone concentration (ppm)
С
С
        bdnlno
                             lower bound NO concentration (ppm)
                             water vapor concentration (ppm)
С
        h2o
С
        pk(1)
                            rate constant for NO2 + O3 -> NO3
                            rate constant for
                                                       03 -> 0(1D)
С
        pk(2)
С
        pk(3)
                            rate constant for
                                                    O(1D) -> O(3P)
С
        pk(4)
                            rate constant for
                                                    O(1D) -> 2 OH
                             rate constant for NO3 + NO2 -> NO +
С
        pk(5)
NO2
С
        pk(6)
                            rate constant for NO3 + NO2 -> N2O5
                            rate constant for N2O5 + H2O -> 2 HNO3
C
        pk(7)
                                                     N2O5 -> NO3 +
C
        pk(8)
                            rate constant for
NO2
                             rate constant for
                                                  NO + NO -> 2 NO2
C
         pk(9)
                             conversion factor from ug/m3 to ppm
         convfac
С
                             concentrations of NO, NO2, HNO3, O3
         conpig
(umo1/m3)
      Output arguments:
                            concentrations of NO, NO2, HNO3, O3
С
         conpig
(umol/m3)
                           ozone reduction due to chemistry
C
        o3dif
(umo1/m3)
С
     Routines Called:
С
С
        none
С
     Called by:
С
        PIGDRIVE
С
С
      dimension conpig(4), pk(9)
```

```
real no, no2, no3, n2o5
      logical ldark
С
c----Entry point
c----Convert umol/m3 to ppm
С
     no = conpig(1)/convfac
     no2 = conpig(2)/convfac
     hno3 = conpig(3)/convfac
     o3 = conpig(4)/convfac
     o3old = o3
     o3dif = 0.
С
c----NO-NO self reaction
      tmpno = no/(1. + pk(9)*dt*no/3600.)
     no2 = no2 + (no - tmpno)
     no = tmpno
c----NO-O3 titration
      if (no.le.bdnlno .or. o3.le.bdnlo3) goto 10
      if (o3.le.no) then
       tmp = o3 - bdnlo3
       o3 = bdnlo3
       no2 = no2 + tmp
       no = amax1((no-tmp),bdnlno)
      else
       tmp = no - bdnlno
       no = bdnlno
       no2 = no2 + tmp
       o3 = amax1((o3-tmp),bdnlo3)
      endif
 10
     o3dif = o3 - o3old
C
c----HNO3 production
      if (o3.gt.bdnlo3) then
        if (ldark) then
C
      Nighttime: Generate nitric acid via the N2O5+H2O channel;
С
                 after calculating a steady-state N2O5
concentration,
                 assume the process is limited by ozone
availability
                 and use this rate to calculate the decay of ozone;
                 note that loss of one N2O5 removes two ozone
molecules
```

```
flux1 = pk(1)*no2*o3
          flux5 = pk(5)*no2
          flux6 = pk(6)*no2
          flux7 = pk(7)*h2o
          flux8 = pk(8)
С
          ssratio = flux6/(flux7 + flux8)
          no3 = flux1/(flux5 + flux6 - ssratio*flux8 + 1.e-20)
С
          n2o5 = no3*ssratio
          flux7 = n2o5*flux7
С
          do3 = o3 * (1.0 - exp(-flux7*dt*2.0/(o3*3600.)))
          do3 = amin1(o3,do3,no2)
          03 = 03 - d03
          no2 = no2 - do3
          hno3 = hno3 + do3
          o3dif = o3 - o3old
        else
     Daytime: ozone photolysis generates OH radicals, which
C
oxidize NO2
               to nitric acid
С
          alpha = (dt/3600.)*pk(2)*pk(4)*h2o/(pk(3) + pk(4)*h2o)
          do3 = amin1(o3,alpha*o3,no2/2.)
          03 = 03 - d03
          no2 = no2 - 2.*do3
          hno3 = hno3 + 2.*do3
          o3dif = o3 - o3old
        endif
      endif
c----Convert from ppm to umol/m3
С
      conpig(1) = no*convfac
      conpig(2) = no2*convfac
      conpig(3) = hno3*convfac
      conpig(4) = o3*convfac
      o3dif = o3dif*convfac
С
      return
      end
```

4. Point Source Summarization Program

C234567890123456789012345678901234567890123456789012345678901234567

- C Program: PTSUM.F
- C Program goal: This program reads binary point source emissions files and creates an
- C output file with the NOx emissions (total in tons/hr) summarized for all point $\,$
- ${\tt C}$ sources within $2{\tt km}$ of user specified set of coordinates. The user can specify up to
- ${\tt C}$ 50 coordinate pairs. They must be in the same system and units of the coordinates in the file
- C file. THIS PROGRAM ASSUMES THAT THE NUMBER AND ORDER OF SOURCES IS IDENTICAL IN
- C THE MASTER AND HOURLY STACK LISTS. THIS MUST BE TRUE FOR CAMX PIG SIMULATIONS OVER
- C MULTIPLE DAYS. FUTHURMORE IT IS ASSUMED THAT NO IS THE FIRST SPECIES AND NO2 IS THE
- C SECOND SPECIES IN THE SPECIES LIST.
- C The format of the userin file for the coordinate pairs x and y is: I7,1x,I7
- C Each pair sits on a separate line. The last line must have 0 0 as the entry.
- C Language: Fortran
- C Programmers: Matt Russell and Amy Baron
- C Last modification date: 6/19/00

C234567890123456789012345678901234567890123456789012345678901234567

C MAIN PROGRAM:

parameter (NUMSPECIES=15, NUMSOURCES=20000, MAXIN=50)

character*125 INFILE.OUTFILE

real NOX(2,NUMSOURCES), DUM(NUMSOURCES), HT(NUMSOURCES)

real XC(NUMSOURCES), YC(NUMSOURCES), DIA(NUMSOURCES)

real BEGT, ENDT, REFORX, REFORY, XLOC, YLOC, TEMP(NUMSOURCES)

real XSIZE, YSIZE, SHGT, MINSD, MINDT, VEL(NUMSOURCES)

integer FILETYPE(10),FILENAME(60),NAMESPE(10,15)

integer SPECIE(10),numsrc

integer SEG, NUMSPE, BEGD, ENDD, HRNUMPT

integer ZONE,NUMXCELL,NUMYCELL,NUMZCELL

integer SD, DT, SEGX, SEGY, SCELLX, SCELLY

integer NUMPT,index(maxin,maxin),X(MAXIN),Y(MAXIN)

integer numcoord(maxin),molw

integer DUM2(NUMSOURCES) C Open input and output files WRITE(*,'(A)')' Enter the EMISSIONS file to be examined: ' READ (*,'(A)') INFILE open (unit=25, file=INFILE, status='old',FORM='UNFORMATTED') WRITE(*,'(A)')' Enter the USERIN file: ' READ (*,'(A)') INFILE open (unit=10, file=INFILE, status='old',FORM='FORMATTED') WRITE(*,'(A)')' Enter the output file: ' READ (*,'(A)') INFILE open (unit=30, file=INFILE, status='new',FORM='FORMATTED') C Read in coordinate pairs from userin file 10 read(10,*,end=30) x(j),y(j)j=j+1goto 10 C25 format(I7,1x,I7)30 continue numsrc=j-1 write(30,*) "number of sources in userin file: ",numsrc write(*,*) "x-coordinate=",X(1) C Read header info read(25) FILETYPE,FILENAME,SEG,NUMSPE,BEGD,BEGT,ENDD,ENDT write(30,*) "julian date of emissions: ",BEGD read(25) REFORX,REFORY,ZONE,XLOC,YLOC,XSIZE,YSIZE, \$ NUMXCELL, NUMYCELL, NUMZCELL, SD, DT, SHGT, MINSD, MINDT read(25) SEGX, SEGY, SCELLX, SCELLY read(25) ((NAMESPE(K,J), K=1,10), J=1,NUMSPE) read(25) SEG, NUMPT read(25) (XC(K), YC(K), HT(K), DIA(K), TEMP(K), VEL(K), K=1, NUMPT)C Scan master stack list and record number of stacks per source (max is 50) C and the record number of each stack

C Criteria for including stack is to be within 2000 meters of input coordinate

do j=1,numsrc numcoord(j)=0 do k=1,NUMPT

```
if (ABS(XC(K)-X(J)).LE.2000 .AND. ABS(YC(K)-Y(J)).LE.2000)
then
        numcoord(j)=numcoord(j)+1
        index(j,numcoord(j))=k
С
         write(30,*) "Source ",j,", stack ",numcoord(j)," is
",HT(K)
         write(30,*) "meters tall, has a stack diameter of ",DIA(K)
C
С
         write(30,*) "with its gas at ",TEMP(K)," degrees K,"
С
         write(30,*) "and is moving at ",VEL(K)," meters per hour."
         write(30,*) "its index, for CAMx, is ",k
С
        endif
         enddo
         write(30,*) "Source ",j," has ",numcoord(j)," stacks."
C
        enddo
C Read hourly data and summarize NOx emissions
          write(30,*) "hour, source, stack, emissions (tons/hr)"
        do i=1.24
         read(25) BEGD, BEGT, ENDD, ENDT
          read(25) SEG, HRNUMPT
           read(25) (DUM2(M),DUM2(M),DUM2(M),DUM(M),DUM(M),
M=1,HRNUMPT)
C Read the first 2 species, ASSUMED TO BE NO AND NO2 !!!
           do k=1,2
            read(25) SEG,SPECIE,(NOX(K,M),M=1,HRNUMPT)
           enddo
C Convert to tons and write out NOx emissions for each stack.
          do j=1, numsrc
           do m=1,numcoord(j)
         write(30,"(3(i2,','),2(E12.6,','))") i,j,m,
            (NOX(1,index(j,m))*30/454/2000),
            (NOX(2,index(j,m))*46/454/2000)
           enddo
          enddo
C Read the rest of the species
         do k=3, numspe
            read(25) SEG,SPECIE,(NOX(1,M),M=1,HRNUMPT)
         enddo
        enddo
        end
```

Point Source Modification Program (5 pages)

**ptmodpig.f and pigoff.f differ only in the emboldened part of the code below. ptmodpig.f does not turn off the PiG for sources (does not include the part in bold, which changes the diameter of the stack to a negative value).

C234567890123456789012345678901234567890123456789012345678901234567

```
C Program:
              PIGOFF.F
C Program goal: This program reads binary point source emissions
files and creates a new
C file with modified NOx emissions for PiGed point sources within
2km of user specified set
C of coordinates. The modification is accomplished by factoring
original hourly emissions.
C *****This program also turns the PiG off for those specified
sources.****
C The user can specify up to
C 50 coordinate pairs. They must be in the same system and units of
the coordinates in the file
C file. THIS PROGRAM ASSUMES THAT THE NUMBER AND ORDER OF SOURCES
IS IDENTICAL IN
C THE MASTER AND HOURLY STACK LISTS. THIS MUST BE TRUE FOR CAMX PIG
SIMULATIONS OVER
C MULTIPLE DAYS. FUTHURMORE IT IS ASSUMED THAT NO IS THE FIRST
SPECIES AND NO2 IS THE
C SECOND SPECIES IN THE SPECIES LIST.
C The format of the userin file for the coordinate pairs x and y
is: I7,1x,I7
C Each pair sits on a separate line.
C The format of the factor file for the NOx emissions is text tab
delimited real
C numbers, one entry for each hour, separate lines for each source.
Program assumes
C same number of sources in factor file as in userin file. The
factor is applied
C to the hourly NOx emission.
C Language:
            Fortran
```

```
C Original Programmers: Matt Russell and Amy Baron
C Significant Modifications made by Dyron Hamlin for PiG on/off
sensitivity analyses
C Last modification date: 5/07/01
C234567890123456789012345678901234567890123456789012345678901234567
89012
C MAIN PROGRAM:
        parameter (NUMSPECIES=15, NUMSOURCES=20000, MAXIN=50)
        character*125 INFILE,OUTFILE
        real EMISS(NUMSOURCES),HT(NUMSOURCES)
        real XC(NUMSOURCES),YC(NUMSOURCES)
        real BEGT, ENDT, REFORX, REFORY, XLOC, YLOC
        real FLRT(NUMSOURCES), EHT(NUMSOURCES)
        real XSIZE, YSIZE, SHGT, MINSD, MINDT, fac(maxin, 24)
        real DIA(NUMSOURCES), TEMP(NUMSOURCES), VEL(NUMSOURCES)
        integer FILETYPE(10),FILENAME(60),NAMESPE(10,15)
        integer SPECIE(10),numsrc
        integer SEG, NUMSPE, BEGD, ENDD, HRNUMPT
        integer ZONE, NUMXCELL, NUMYCELL, NUMZCELL
        integer SD, DT, SEGX, SEGY, SCELLX, SCELLY
        integer NUMPT,index(maxin,maxin),X(MAXIN),Y(MAXIN)
        integer numcoord(maxin),count(maxin)
        integer RECX(NUMSOURCES), RECY(NUMSOURCES), RECZ(NUMSOURCES)
        character*30 str
C Open input and output files
      WRITE(*,'(A)')' Enter the EMISSIONS file to be converted: '
      READ (*,'(A)') INFILE
      open (unit=25, file=INFILE, status='old',FORM='UNFORMATTED')
      WRITE(*,'(A)')' Enter the USERIN file: '
      READ (*,'(A)') INFILE
      open (unit=10, file=INFILE, status='old',FORM='FORMATTED')
      WRITE(*,'(A)')' Enter the factor file: '
      READ (*,'(A)') INFILE
      open (unit=11, file=INFILE, status='old',FORM='FORMATTED')
      WRITE(*,'(A)')' Enter the output file: '
      READ (*,'(A)') INFILE
      open (unit=30, file=INFILE, status='new',FORM='UNFORMATTED')
C Read in coordinate pairs from userin file
        j=1
15
        read(10,*,end=30) x(j),y(j)
          j=j+1
        goto 15
```

```
C25
           format(I7,1x,I7)
30
          continue
        numsrc=i-1
        write(*,*) "number of sources in userin file: ",numsrc
C Read in the factor file. PROGRAM ASSUMES SAME NUMBER OF SOURCES
C IN FACTOR FILE AS IN USERIN FILE
        do j=1, numsrc
        read(11,*) (fac(j,k),k=1,24)
        enddo
C Read and write header info
        read(25) FILETYPE, FILENAME, SEG, NUMSPE, BEGD, BEGT, ENDD, ENDT
        write(*,*) "julian date of emissions: ",BEGD
        write(30) FILETYPE, FILENAME, SEG, NUMSPE, BEGD, BEGT, ENDD, ENDT
        read(25) REFORX, REFORY, ZONE, XLOC, YLOC, XSIZE, YSIZE,
     $
                  NUMXCELL, NUMYCELL, NUMZCELL, SD, DT, SHGT, MINSD, MINDT
        write(30) REFORX,REFORY,ZONE,XLOC,YLOC,XSIZE,YSIZE,
                  NUMXCELL, NUMYCELL, NUMZCELL, SD, DT, SHGT, MINSD, MINDT
        read(25) SEGX, SEGY, SCELLX, SCELLY
        write(30) SEGX,SEGY,SCELLX,SCELLY
        read(25) ((NAMESPE(K,J), K=1,10), J=1,NUMSPE)
        write(30) ((NAMESPE(K,J), K=1,10), J=1,NUMSPE)
        read(25) SEG, NUMPT
        write(30) SEG, NUMPT
        read(25)
(XC(K), YC(K), HT(K), DIA(K), TEMP(K), VEL(K), K=1, NUMPT)
C Need to determine where the stack of interest is. The diameter
of this
C stack must be changed from negative to positive. This change
turns off
C the PiG for that stack. This must be done before writing the
DIA(K)
C array to the new emissions file.
```

```
C Scan master stack list and record number of stacks per source (max
C is 50) and the record number of each stack

do j=1,numsrc
    count(j)=0
    numcoord(j)=0
    do k=1,NUMPT

C Criteria for including stack is to be within 2000 meters of input coordinate

if (ABS(XC(K)-X(J)).LE.2000 .AND. ABS(YC(K)-Y(J)).LE.2000)then
    numcoord(j)=numcoord(j)+1

C Change the diameter of any stacks given negative diameter to a positive dia.

if (DIA(K).LE.0) then
```

```
DIA(K) = -DIA(K)
count(j) = count(j) + 1
index(j,count(j)) = k
```

endif

C Keep track of the stack number for changing emissions

```
endif
          enddo
          write(*,*) "Source ",j," has ",numcoord(j)," stacks."
          write(*,*) count(j)," have negative diameter."
         enddo
C
         do j=1, numsrc
           do k=1,count(j)
            write(*,*) "coord's of stacks w/ neg
C
dia",XC(index(j,k))
           write(*,*) YC(index(j,k))
           enddo
С
          enddo
С
```

C Write modified emissions file

```
write(30)
(XC(K), YC(K), HT(K), DIA(K), TEMP(K), VEL(K), K=1, NUMPT)
C Read hourly data, for NOx apply factor and write new file
        do i=1,24
        read(25) BEGD, BEGT, ENDD, ENDT
        write(30) BEGD, BEGT, ENDD, ENDT
        read(25) SEG, HRNUMPT
        write(30) SEG, HRNUMPT
        read(25) (RECX(M),RECY(M),RECZ(M),FLRT(M),EHT(M),
M=1,HRNUMPT)
write(30)(RECX(M),RECY(M),RECZ(M),FLRT(M),EHT(M),M=1,HRNUMPT)
C Read the first 2 species, ASSUMED TO BE NO AND NO2 !!!
          do k=1,2
           read(25) SEG,SPECIE,(EMISS(M),M=1,HRNUMPT)
C Apply NOx factor for each stack. This is not being done for
C PiG off analysis.
C The code will be left here for future use with the PiG.
            do j=1, numsrc
C This changes emissions on PiGed stacks
             do m=1,count(j)
              EMISS(index(j,m))=fac(j,i)*EMISS(index(j,m))
             enddo
            enddo
C Write new NOx emissions. Write un-modified emissions if just
turning off PiG.
           write(30) SEG,SPECIE,(EMISS(M),M=1,HRNUMPT)
          enddo
C Read and write the rest of the species
          do k=3,numspe
             read(25) SEG,SPECIE,(EMISS(M),M=1,HRNUMPT)
             write(30) SEG,SPECIE,(EMISS(M),M=1,HRNUMPT)
          enddo
        enddo
       end
```

5. Point Source Evaluation Tool

c234567890123456789012345678901234567890123456789012345678901234567

```
PROGRAM pset
c This program reads 2 UAM format .AVRG files
c and subtracts species, and writes an ASCII format file
c which is useful for analyzing point source data.
c Dyron Hamlin, August 2001.
c Define Variables
       integer SEG, NUMSPE, BEGD, ENDD, ZONE, NUMXCELL, NUMYCELL, M
       integer NUMZCELL, SD, DT, SEGX, SEGY, SCELLX,
SCELLY, I, J, L, Z, H
       integer NUMCELLS, kount(24), SPECMOD,
GRIDCELL, k, count(9), hr, X, Y
       real BEGT, ENDT, REFORX, REFORY, XLOC, YLOC, XSIZE, YSIZE
       real SHGT, MINSD, MINDT, THRESH
       real hropenoz(24),hravope
       real DELO3(82,106,9,24), DELNOZ(82,106,9,24)
       real OPENOZ(82,106,9,24), PERCOX(82,106,9,24)
       real PERCORG(82,106,9,24)
       real DELPAN(82,106,9,24), DELNTR(82,106,9,24)
       real DUMM(82,106,9,24), DELNOX(82,106,9,24), DUMMY(82,106)
       real DELNA(82,106,9,24), avgopenoz
       real layopenoz(9)
       dimension MFILETYPE(10), MFILENAME(60)
       dimension MDUMMY(10), MSPECIES(10,30), MSPECIE2(10,30)
       integer SPECIE(10)
       character*100 IPATH
89012c Open files and make new output file
     WRITE(*,'(A)')' Enter the first .avrg file to be converted:'
     READ (*,'(20x,A)') IPATH
     open (unit=11, file=IPATH, status='old',FORM='UNFORMATTED')
     WRITE(*,'(A)')' Enter the .avrg file to be subtracted: '
     READ (*,'(20x,A)') IPATH
     open (unit=12, file=IPATH, status='old',FORM='UNFORMATTED')
```

```
READ (*,'(20x,A)') IPATH
      open (unit=13, file=IPATH, status='unknown',FORM='FORMATTED')
      WRITE(*,'(A)')' Enter the O3 threshold which defines the
plume: '
      READ (*,'(20x,F5.2)') THRESH
      WRITE(*,'(a,F5.2)') 'Threshold= ',THRESH
      WRITE(*,'(A)')' Enter the gridcell of the source of interest:
     READ (*,'(20x,i2,1x,i2)') X,Y
      WRITE(*,'(a,i2,'','',i2)') 'Gridcell= ',X,Y
       DO H=1,24
        DO Z=1, NUMZCELL
         DO I=1, NUMXCELL
          DO J=1, NUMYCELL
           DELNOZ(I,J,Z,H)=0.
           DELNOX(I,J,Z,H)=0.
          ENDDO
          ENDDO
         ENDDO
           kount(h)=0
           hropenoz(h)=0.
        ENDDO
       READ(11) MFILETYPE, MFILENAME, SEG, NUMSPE, BEGD, BEGT
        , ENDD, ENDT
       READ(11) REFORX, REFORY, ZONE, XLOC, YLOC, XSIZE
     & , YSIZE, NUMXCELL, NUMYCELL, NUMZCELL, SD, DT, SHGT, MINSD
          , MINDT
        READ(11) SEGX, SEGY, SCELLX, SCELLY
        READ(11) ((MSPECIES(M,L),M=1,10),L=1,NUMSPE)
c Put the species list into a dummy array that can be changed for
c reading.
       do L=1, NUMSPE
       do M=1,10
       MSPECIE2(M,L)=MSPECIES(M,L)
```

WRITE(*,'(A)')' Enter the OUTPUT file to be created: '

```
enddo
C Bswap the name and number of species to allow the flag index to
C the "integer" MSPECIE2 as characters when converted to big endian
          call bswap(MSPECIE2,10,30)
          do l=1, numspe
          WRITE(*,'(I5,A,10A1)') L,' ',(MSPECIE2(M,L),M=1,10)
          enddo
C Flag indices of O3, HNO3, PAN, and NXOY.
C - These will be used later to ensure that correct data is read.
        iflag=0
        do i=1,NUMSPE
           IF(MSPECIE2(1,i).EQ.'O'.AND.MSPECIE2(2,i).EQ.'3') then
           IFLAG=i
           write(*,'(a,i1)') 'found some O3. Species = ',iflag
           ENDIF
        end do
        jflag=0
        do j=1,NUMSPE
           IF(MSPECIE2(1,j).EQ.'H'.AND.MSPECIE2(2,j).EQ.'N'
            .AND.MSPECIE2(3,j).EQ.'O'.AND.MSPECIE2(4,j).EQ.'3')
then
           JFLAG=j
           write(*,'(a,i2)') 'found some HNO3. Species = ',jflag
           ENDIF
        end do
c Currently, for some reason, I can't recognize PAN using this same
c bswap technique. Thus, one should make sure that PAN is indeed
  species #4.
С
        iiflag=4
         do ii=1,NUMSPE
С
С
            IF((MSPECIE2(1,ii).EQ.'P')) then
С
            IIFLAG=ii
           write(*,'(a,i2)') 'found some PAN. Species = ',iiflag
            ENDIF
C
         end do
С
        jjflag=0
        do jj=1,NUMSPE
           IF((MSPECIE2(1,jj).EQ.'N'.AND.MSPECIE2(2,jj).EQ.'X'.AND.
     $
               MSPECIE2(3,jj).EQ.'O')) then
```

enddo

write(*,'(a,i2)') 'found some NXOY. Species = ',jjflag

JJFLAG=jj

```
ENDIF
        end do
       kkflag=0
        do kk=1, NUMSPE
           IF((MSPECIE2(1,kk).EQ.'H'.AND.MSPECIE2(2,kk).EQ.'O'.AND.
               MSPECIE2(3,kk).EQ.'N')) then
          KKFLAG=kk
           write(*,'(a,i2)') 'found some HONO. Species = ',kkflag
        end do
        llflag=0
        do ll=1,NUMSPE
           IF((MSPECIE2(1,11).EQ.'N'.AND.MSPECIE2(2,11).EQ.'T'.AND.
               MSPECIE2(3,11).EQ.'R')) then
          LLFLAG=11
          write(*,'(a,i2)') 'found some NTR. Species = ',llflag
          ENDIF
        end do
        iiiflag=0
        do iii=1,NUMSPE
IF((MSPECIE2(1,iii).EQ.'N'.AND.MSPECIE2(2,iii).EQ.'O'.AND.
               MSPECIE2(3,iii).NE.'2')) then
     $
           IIIFLAG=iii
           write(*,'(a,i2)') 'found some NO. Species = ',iiiflag
          ENDIF
        end do
        jjjflag=0
        do jjj=1, NUMSPE
IF((MSPECIE2(1,jjj).EQ.'N'.AND.MSPECIE2(2,jjj).EQ.'O'.AND.
               MSPECIE2(3,jjj).EQ.'2')) then
           JJJFLAG=jjj
           write(*,'(a,i2)') 'found some NO2. Species = ',jjjflag
           ENDIF
        end do
c READ in headers from second record.
        READ(12) MFILETYPE, MFILENAME, SEG, NUMSPE, BEGD, BEGT
         , ENDD, ENDT
        READ(12) REFORX, REFORY, ZONE, XLOC, YLOC, XSIZE
       , YSIZE, NUMXCELL, NUMYCELL, NUMZCELL, SD, DT, SHGT, MINSD
          , MINDT
```

```
READ(12) SEGX, SEGY, SCELLX, SCELLY
        READ(12) ((MSPECIES(M,L),M=1,10),L=1,NUMSPE)
c Read hourly stuff.
          DO 9 H = 1,24
            READ(11) BEGD, BEGT, ENDD, ENDT
            READ(12) BEGD, BEGT, ENDD, ENDT
c Read the two files, checking to see if the specie is either O3 or
c HNO3. If the specie is Ozone, read it into CONC arrays.
            DO 12 S=1, NUMSPE
            if (S.EQ.IFLAG) then
             DO Z = 1, NUMZCELL
              READ(11) SEG,SPECIE,((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                    J=1, NUMYCELL)
     &
              DO I=1, NUMXCELL
               DO J=1, NUMYCELL
              DELO3(I,J,Z,H) = DUMM(I,J,Z,H)
               ENDDO
              ENDDO
              READ(12) SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
     &
                                    J=1, NUMYCELL)
              DO I=1, NUMXCELL
               DO J=1, NUMYCELL
              DELO3(I,J,Z,H) = DELO3(I,J,Z,H) - DUMM(I,J,Z,H)
              ENDDO
             ENDDO
c If the specie is Nitric Acid, read it into DELNA arrays.
            elseif (S.EQ.JFLAG) then
             DO Z = 1, NUMZCELL
              READ(11) SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
     &
                                    J=1, NUMYCELL)
              DO I=1, NUMXCELL
               DO J=1, NUMYCELL
              DELNA(I,J,Z,H) = DUMM(I,J,Z,H)
               ENDDO
              ENDDO
              READ(12) SEG,SPECIE,((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                    J=1, NUMYCELL)
              DO I=1, NUMXCELL
               DO J=1, NUMYCELL
              DELNA(I,J,Z,H) = DELNA(I,J,Z,H) - DUMM(I,J,Z,H)
               ENDDO
```

```
ENDDO
c If the specie is PAN, read it into DELPAN arrays.
            elseif (S.EQ.IIFLAG) then
             DO Z = 1, NUMZCELL
              READ(11) SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
     &
                                     J=1, NUMYCELL)
              DO I=1, NUMXCELL
               DO J=1, NUMYCELL
              DELPAN(I,J,Z,H) = DUMM(I,J,Z,H)
               ENDDO
              ENDDO
              READ(12) SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                     J=1, NUMYCELL)
              DO I=1, NUMXCELL
               DO J=1, NUMYCELL
              DELPAN(I,J,Z,H) = DELPAN(I,J,Z,H) - DUMM(I,J,Z,H)
               ENDDO
              ENDDO
             ENDDO
c If the specie is NTR, read it into DELNTR arrays.
            elseif (S.EQ.LLFLAG) then
             DO Z = 1, NUMZCELL
              READ(11) SEG,SPECIE,((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                     J=1, NUMYCELL)
     &
              DO I=1, NUMXCELL
               DO J=1, NUMYCELL
              DELNTR(I,J,Z,H) = DUMM(I,J,Z,H)
               ENDDO
              ENDDO
              READ(12) SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                     J=1, NUMYCELL)
     &
              DO I=1, NUMXCELL
               DO J=1, NUMYCELL
              DELNTR(I,J,Z,H) = DELNTR(I,J,Z,H) - DUMM(I,J,Z,H)
               ENDDO
              ENDDO
             ENDDO
c If the specie is part of NOz, read it into DELNOZ arrays
            elseif ((S.EQ.JJFLAG).OR.(S.EQ.KKFLAG)) then
                 DO Z = 1, NUMZCELL
                    READ(11)
SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
```

ENDDO

J=1, NUMYCELL)

&

```
DO I=1, NUMXCELL
                    DO J=1, NUMYCELL
                     DELNOZ(I,J,Z,H) = DUMM(I,J,Z,H) + DELNOZ(I,J,Z,H)
                    ENDDO
                   ENDDO
                     READ(12)
SEG,SPECIE,((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                     J=1, NUMYCELL)
                   DO I=1, NUMXCELL
                    DO J=1, NUMYCELL
                     DELNOZ(I,J,Z,H) = DELNOZ(I,J,Z,H) - DUMM(I,J,Z,H)
                    ENDDO
                   ENDDO
                  ENDDO
c If the specie is NOx (NO or NO2), save the difference as DELNOX.
c TO AVOID NEGATIVE VALUES, JUST REPORT THE NOX FROM THE FIRST
FILE???
            elseif ((S.EQ.IIIFLAG).OR.(S.EQ.JJJFLAG)) then
                  DO Z = 1, NUMZCELL
                     READ(11)
SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
     &
                                     J=1, NUMYCELL)
                   DO I=1, NUMXCELL
                    DO J=1, NUMYCELL
                     DELNOX(I,J,Z,H) = DUMM(I,J,Z,H) + DELNOX(I,J,Z,H)
                    ENDDO
                   ENDDO
                     READ(12) SEG, SPECIE, ((DUMMY(I,J), I=1, NUMXCELL),
                                     J=1, NUMYCELL)
     &
                    DO I=1, NUMXCELL
С
С
                     DO J=1, NUMYCELL
                      DELNOX(I,J,Z,H) = DELNOX(I,J,Z,H) - DUMM(I,J,Z,H)
С
                     ENDDO
С
                    ENDDO
С
                  ENDDO
c If the specie is none of these things, read it into a dummy
array.
            else
                  DO Z = 1, NUMZCELL
                     READ(11) SEG, SPECIE, ((DUMMY(I,J), I=1, NUMXCELL),
                                     J=1, NUMYCELL)
     &
                     READ(12) SEG,SPECIE,((DUMMY(I,J),I=1,NUMXCELL),
                                     J=1,NUMYCELL)
                  ENDDO
            endif
```

```
c Loop through all of the Layers
12
            CONTINUE
c Loop through all of the Hours
            write(*,'(a,2I)') 'Done reading Hour # ',H
9
           CONTINUE
         write(*,'(a)') 'done with all the reading stuff'
c Now, we wish to find the difference in ozone and the differences
in
c nitric acid or NOz for the two runs. These values, when
combined,
c can give us an estimate for OPE.
write(13,"(12(',',a))")'CELL','O3','NOx','PAN','NTR',
                                       'HNO3', 'NOz', 'OPENOz', 'Lay
Av',
                                       'Hrly Av','% Ox', '% Org'
             DO H=13,21
              DO Z=1, NUMZCELL
               layopenoz(z)=0.
               count(z)=0
               DO J=1, NUMYCELL
                DO I=1, NUMXCELL
                 lprint=.false.
                 GRIDCELL=I*100+J
c If we're not in the "plume," set all values = 0. Note, also,
c flag for printing the values to the output files defaults to
.false.
С
                  if ((1000.*(delo3(i,j,z,h))).le.THRESH) then
                    delo3(i,j,z,h)=0.
                    delna(i,j,z,h)=0.
                    delnoz(i,j,z,h)=0.
                    delnox(i,j,z,h)=0.
                    delpan(i,j,z,h)=0.
                    delntr(i,j,z,h)=0.
                    openoz(i,j,z,h)=0.
                    percox(i,j,z,h)=0.
                    percorg(i,j,z,h)=0.
c If we are in the "plume," meaning there is at least THRESH delta
03
```

c between the two runs being processed, then store the following

```
c values only for cells within 28 km of the stack
c This allows for comparison with data taken in the NOAA aircraft
c during TEXAQS, 2000, when the aircraft flew only to an extent of
c 25 km.:
С
                  else
                    if (I.lt.(X-13).OR.I.gt.(X+13).OR.
                        J.lt.(Y-13).OR.J.gt.(Y+13)) then
     ۶
                    lprint=.false.
                    else
                    lprint=.true.
c The number of grid cells in the current layer
C
                    count(z) = count(z) + 1
c The total delta NOz (update it to include nitric acid, PAN, and
NTR)
                    delnoz(i,j,z,h) = delnoz(i,j,z,h) + delna(i,j,z,h)
+delpan(i,j,z,h)+delntr(i,j,z,h)
c The percent oxidation of the plume (NOz/NOy) and the percent of
c oxidation products which are organic nitrates.
percox(i,j,z,h) = delnoz(i,j,z,h) / (delnoz(i,j,z,h) +
                                    delnox(i,j,z,h)+.000000001)
percorg(i,j,z,h)=(delntr(i,j,z,h)+delpan(i,j,z,h))/
(delnoz(i,j,z,h)+.000000001)
c The OPE on NOz basis for this cell
                    OPENOZ(i,j,z,h) = delo3(i,j,z,h) / (delnoz(i,j,z,h))
     &
+.000000001)
c The cumulative OPE for this layer. These values will be used to
c compute a layer average.
                    layopenoz(z)=layopenoz(z)+OPENOZ(i,j,z,h)
                    endif
                  endif
c Then print the data for this cell, this layer.
```

if (lprint) then

```
write(13, "(',',i5,7(',',f6.3),',',',',2(',',f6.3))")
                                  gridcell,
     &
                                  (1000.*delo3(i,j,z,h)),
                                  (1000.*delnox(i,j,z,h)),
     &
     ď
                                  (1000.*delpan(i,j,z,h)),
     &
                                  (1000.*delntr(i,j,z,h)),
     &
                                  (1000.*delna(i,j,z,h)),
                                  (1000.*delnoz(i,j,z,h)),
     &
                                  openoz(i,j,z,h),percox(i,j,z,h),
     &
                                  percorg(i,j,z,h)
                 endif
С
c Now go back and check the next cell.
                ENDDO
               ENDDO
c Let the fun begin. Find the LAYER AVERAGE OPE on both bases
                  if(count(z).gt.0) then
                    avgopenoz=layopenoz(z)/count(z)
                    kount(h)=kount(h)+count(z)
                    hropenoz(h)=hropenoz(h)+layopenoz(z)
                  else
                    avgopenoz=0.
                  endif
c This is the end of the layer loop...go back and start a new
layer.
                write(13, "(a,i2,9(','),F6.3)")'LAYER ',Z,avgopenoz
              print*,'finished writing layer',z
              ENDDO
c Let the fun begin. Find the HOUR AVERAGE OPE on both bases
                  if(kount(h).gt.0) then
                    hravope=hropenoz(h)/kount(h)
                  else
                    hravope=0.
                  endif
c This is the end of the hourly loop...go back and start a new
hour.
С
                  hr=h-1
                write(13, "(a,i2,10(','),F6.3)")'HOUR ',hr,hravope
```

```
print*,'finished writing hour',h
            ENDDO
         WRITE(*,'(A)')' COMPLETE '
89012
       END
c function to convert big-endian character strings stored as
integers
c to little endian character strings stored as integers
С
c arguments: integer string array to be converted
            number of elements in array along 1st dimension
            number of elements along second dimension
С
C
     Subroutine bswap (instring, num1, num2)
     logical*1 instring(*), tmp1, tmp2
     integer*4 num1,num2
     integer*4 i,j,k
c process in row major order
     if (num2 .ne. 0) goto 200
C
c Single dimension array
100 do 150 i=1, num1
     j=(i-1)*4+1
     tmp1 = instring(j)
     instring(j) = instring(j+3)
     instring(j+3) = tmp1
     tmp2 = instring(j+1)
     instring(j+1) = instring(j+2)
     instring(j+2) = tmp2
150 continue
     goto 300
c Double dimension array
200 continue
     do 250 i=1, num2
     do 240 j=1, num1
     k = (i-1)*(num1*4)+(j-1)*4+1
     tmp1 = instring(k)
```

instring(k) = instring(k+3)

```
instring(k+3) = tmp1
tmp2 = instring(k+1)
instring(k+1) = instring(k+2)
instring(k+2) = tmp2
240   continue
250   continue
300   return
c
   end
```

6. Temporal Sensitivity Evaluation Tool

c234567890123456789012345678901234567890123456789012345678901234567

```
PROGRAM psettemp
c This program reads 2 UAM format .AVRG files
c and subtracts species, and writes an ASCII format file
c which is useful for analyzing point source data.
c Dyron Hamlin, August 2001.
c Define Variables
        integer SEG, NUMSPE,
BEGD, ENDD, ZONE, NUMXCELL, NUMYCELL, M, NUMSPE2
        integer NUMZCELL, SD, DT, SEGX, SEGY, SCELLX,
SCELLY, I, J, L, Z, H
        integer NUMCELLS, kount(24), GRIDCELL, k, count(9), hr, X, Y
        integer gridmax, diff
        real BEGT, ENDT, REFORX, REFORY, XLOC, YLOC, XSIZE, YSIZE
        real SHGT, MINSD, MINDT, THRESH
        real layo3(9), masso3, hrmass, maxo3
        real DELO3(82,106,9,24)
        real DUMM(82,106,9,24)
        real DELNA(82,106,9,24), height(9)
        dimension MFILETYPE(10), MFILENAME(60)
        dimension MSPECIES(10,30), MSPECIE2(10,30)
        integer SPECIE(10)
        character*100 IPATH
        data height(1)/33./
        data height(2)/100./
        data height(3)/211./
        data height(4)/390./
        data height(5)/675./
        data height(6)/1105./
        data height(7)/1815./
        data height(8)/2892./
        data height(9)/3600./
c234567890123456789012345678901234567890123456789012345678901234567
89012c Open files and make new output file
      WRITE(*,'(A)')' Enter the first .avrg file to be converted:'
      READ (*,'(20x,A)') IPATH
      open (unit=11, file=IPATH, status='old',FORM='UNFORMATTED')
```

```
WRITE(*,'(A)')' Enter the .avrg file to be subtracted: '
      READ (*,'(20x,A)') IPATH
      open (unit=12, file=IPATH, status='old',FORM='UNFORMATTED')
      WRITE(*,'(A)')' Enter the OUTPUT file to be created: '
      READ (*,'(20x,A)') IPATH
      open (unit=13, file=IPATH, status='unknown',FORM='FORMATTED')
      WRITE(*,'(A)')' Enter the HNO3 threshold which defines the
plume: '
      READ (*,'(20x,F5.2)') THRESH
      WRITE(*,'(a,F5.2)') 'Threshold= ',THRESH
      WRITE(*,'(A)')' Enter the gridcell of the source of interest:
      READ (*,'(20x,i2,1x,i2)') X,Y
      WRITE(*,'(a,i2,'','',i2)') 'Gridcell= ',X,Y
        READ(11) MFILETYPE, MFILENAME, SEG, NUMSPE, BEGD, BEGT
        , ENDD, ENDT
        READ(11) REFORX, REFORY, ZONE, XLOC, YLOC, XSIZE
     & , YSIZE, NUMXCELL, NUMYCELL, NUMZCELL, SD, DT, SHGT, MINSD
         , MINDT
        READ(11) SEGX, SEGY, SCELLX, SCELLY
        READ(11) ((MSPECIES(M,L),M=1,10),L=1,NUMSPE)
c Put the species list into a dummy array that can be changed for
reading.
        do L=1, NUMSPE
        do M=1,10
        MSPECIE2(M,L)=MSPECIES(M,L)
        enddo
        enddo
C Bswap the name and number of species to allow the flag index to
read the
\ensuremath{\mathtt{C}} "integer" MSPECIE2 as characters when converted to big endian
```

call bswap(MSPECIE2, 10, 30) (see pset.f)

```
do l=1, numspe
          WRITE(*,'(I5,A,10A1)') L,' ',(MSPECIE2(M,L),M=1,10)
          enddo
C Flag indices of O3, HNO3, PAN, and NXOY.
C - These will be used later to ensure that correct data is read.
        iflag=0
        do i=1,NUMSPE
           IF(MSPECIE2(1,i).EQ.'O'.AND.MSPECIE2(2,i).EQ.'3') then
           write(*,'(a,i1)') 'found some O3. Species = ',iflag
           ENDIF
        end do
        jflag=0
        do j=1, NUMSPE
           IF(MSPECIE2(1,j).EQ.'H'.AND.MSPECIE2(2,j).EQ.'N'
            .AND.MSPECIE2(3,j).EQ.'O'.AND.MSPECIE2(4,j).EQ.'3')
then
           JFLAG=j
           write(*,'(a,i2)') 'found some HNO3. Species = ',jflag
           ENDIF
        end do
        iiflag=4
         do ii=1,NUMSPE
С
С
            IF((MSPECIE2(1,ii).EQ.'P')) then
С
            IIFLAG=ii
           write(*,'(a,i2)') 'found some PAN. Species = ',iiflag
            ENDIF
C
         end do
С
        jjflag=0
        do jj=1,NUMSPE
           IF((MSPECIE2(1,jj).EQ.'N'.AND.MSPECIE2(2,jj).EQ.'X'.AND.
     $
               MSPECIE2(3,jj).EQ.'O')) then
           JJFLAG=jj
           write(*,'(a,i2)') 'found some NXOY. Species = ',jjflag
           ENDIF
        end do
        kkflag=0
        do kk=1,NUMSPE
            \texttt{IF((MSPECIE2(1,kk).EQ.'H'.AND.MSPECIE2(2,kk).EQ.'O'.AND.} \\
               MSPECIE2(3,kk).EQ.'N')) then
           KKFLAG=kk
           write(*,'(a,i2)') 'found some HONO. Species = ',kkflag
           ENDIF
        end do
```

```
llflag=0
       do ll=1,NUMSPE
           IF((MSPECIE2(1,11).EQ.'N'.AND.MSPECIE2(2,11).EQ.'T'.AND.
              MSPECIE2(3,11).EQ.'R')) then
          LLFLAG=11
          write(*,'(a,i2)') 'found some NTR. Species = ',llflag
          ENDIF
        end do
        iiiflag=0
       do iii=1,NUMSPE
IF((MSPECIE2(1,iii).EQ.'N'.AND.MSPECIE2(2,iii).EQ.'O'.AND.
              MSPECIE2(3,iii).NE.'2')) then
     $
          IIIFLAG=iii
          write(*,'(a,i2)') 'found some NO. Species = ',iiiflag
          ENDIF
        end do
        jjjflag=0
       do jjj=1,NUMSPE
IF((MSPECIE2(1,jjj).EQ.'N'.AND.MSPECIE2(2,jjj).EQ.'O'.AND.
              MSPECIE2(3,jjj).EQ.'2')) then
          JJJFLAG=jjj
          write(*,'(a,i2)') 'found some NO2. Species = ',jjjflag
          ENDIF
        end do
c READ in headers from second record.
       READ(12) MFILETYPE, MFILENAME, SEG, NUMSPE2, BEGD, BEGT
       , ENDD, ENDT
       READ(12) REFORX, REFORY, ZONE, XLOC, YLOC, XSIZE
       , YSIZE, NUMXCELL, NUMYCELL, NUMZCELL, SD, DT, SHGT, MINSD
          , MINDT
       READ(12) SEGX, SEGY, SCELLX, SCELLY
       READ(12) ((MSPECIES(M,L),M=1,10),L=1,NUMSPE2)
       diff=numspe-numspe2
c Read hourly stuff.
         DO 9 H = 1,24
           READ(11) BEGD, BEGT, ENDD, ENDT
            READ(12) BEGD, BEGT, ENDD, ENDT
```

```
c Read the two files, checking to see if the specie is either 03 or
c HNO3. If the specie is Ozone, read it into CONC arrays.
            DO 12 S=1, NUMSPE2
            if (S.EQ.IFLAG) then
             DO Z = 1, NUMZCELL
              READ(11) SEG,SPECIE,((DUMM(I,J,Z,H),I=1,NUMXCELL),
     &
                                    J=1, NUMYCELL)
              DO I=1, NUMXCELL
               DO J=1, NUMYCELL
              DELO3(I,J,Z,H) = DUMM(I,J,Z,H)
               ENDDO
              ENDDO
              READ(12) SEG,SPECIE,((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                    J=1, NUMYCELL)
              DO I=1, NUMXCELL
               DO J=1, NUMYCELL
              DELO3(I,J,Z,H) = DELO3(I,J,Z,H) - DUMM(I,J,Z,H)
               ENDDO
              ENDDO
             ENDDO
c If the specie is Nitric Acid, read it into DELNA arrays.
            elseif (S.EQ.JFLAG) then
             DO Z = 1, NUMZCELL
              READ(11) SEG,SPECIE,((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                    J=1, NUMYCELL)
     &
              DO I=1, NUMXCELL
               DO J=1, NUMYCELL
              DELNA(I,J,Z,H) = DUMM(I,J,Z,H)
               ENDDO
              ENDDO
              READ(12) SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                    J=1, NUMYCELL)
     &
              DO I=1, NUMXCELL
               DO J=1, NUMYCELL
              DELNA(I,J,Z,H) = DELNA(I,J,Z,H) - DUMM(I,J,Z,H)
               ENDDO
              ENDDO
             ENDDO
c If the specie is PAN, read it into dummy arrays.
            elseif (S.EQ.IIFLAG) then
             DO Z = 1, NUMZCELL
              READ(11) SEG,SPECIE,((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                    J=1, NUMYCELL)
     &
              READ(12) SEG, SPECIE, ((DUMM(I,J,Z,H), I=1, NUMXCELL),
```

```
J=1, NUMYCELL)
     &
             ENDDO
c If the specie is NTR, read it into dummy arrays.
            elseif (S.EQ.LLFLAG) then
             DO Z = 1, NUMZCELL
              READ(11) SEG,SPECIE,((DUMM(I,J,Z,H),I=1,NUMXCELL),
     &
                                    J=1, NUMYCELL)
              READ(12) SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                    J=1, NUMYCELL)
     &
             ENDDO
c If the specie is part of NOz, read it into dummy arrays
            elseif ((S.EQ.JJFLAG).OR.(S.EQ.KKFLAG)) then
                 DO Z = 1, NUMZCELL
                    READ(11)
SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                    J=1, NUMYCELL)
                    READ(12)
SEG,SPECIE,((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                    J=1, NUMYCELL)
                 ENDDO
c If the specie is NOx (NO or NO2), read it into a dummy array.
            elseif ((S.EQ.IIIFLAG).OR.(S.EQ.JJJFLAG)) then
                 DO Z = 1, NUMZCELL
                    READ(11)
SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                    J=1, NUMYCELL)
                    READ(12)
SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                    J=1, NUMYCELL)
     &
                 ENDDO
c If the specie is none of these things, read it into a dummy
array.
            else
                 DO Z = 1, NUMZCELL
                    READ(11)
SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                    J=1, NUMYCELL)
                    READ(12)
SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                    J=1, NUMYCELL)
     &
                 ENDDO
            endif
```

```
c Loop through all of the Layers
12
            CONTINUE
            if (diff.gt.0) then
                  do k=1,diff
                   DO Z = 1, NUMZCELL
                    READ(11)
SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                      J=1, NUMYCELL)
                   ENDDO
                  enddo
            endif
c Loop through all of the Hours
            write(*,'(a,2I)') 'Done reading Hour # ',H
9
           CONTINUE
         write(*,'(a)') 'done reading files'
c Now, we wish to find the difference in ozone and the differences
in
c nitric acid or NOz for the two runs. These values, when
combined,
c can give us an estimate for OPE.
                write(13, "(6(',',a))")'CELL','O3','HNO3','molO3',
                                        'max03','cellmax'
     &
                \max 03=0.
             DO H=18,18
              gridmax=0
              hrmass=0.
              DO Z=1, NUMZCELL
               layo3(z)=0.
               count(z)=0
               DO J=1, NUMYCELL
                DO I=1, NUMXCELL
                 lprint=.false.
                 GRIDCELL=I*100+J
c If we're not in the "plume," set all values = 0. Note, also,
that the
c flag for printing the values to the output files defaults to
.false.
С
                  if ((1000.*(delna(i,j,z,h))).le.THRESH) then
                    delo3(i,j,z,h)=0.
                    delna(i,j,z,h)=0.
```

С

```
c If we are in the "plume," meaning there is at least THRESH delta
HNO3
c between the two runs being processed, then store the following
c values:
С
                  else
                    lprint=.true.
С
c The number of grid cells in the current layer
                    count(z) = count(z) + 1
                    layo3(z) = layo3(z) + delo3(i,j,z,h)
                    if (delo3(i,j,z,h).gt.maxo3) then
                      \max 03 = delo3(i,j,z,h)
                      gridmax=i*100+j
                    endif
                  endif
С
c Then print the data for this cell, this layer.
                 if (lprint) then
                   write(13,"(',',i5,2(',',f6.3),',')")
                                  gridcell,
     &
                                  (1000.*delo3(i,j,z,h)),
     &
                                  (1000.*delna(i,j,z,h))
                 endif
c Now go back and check the next cell.
                ENDDO
               ENDDO
                  if(count(z).gt.0) then
                    masso3=layo3(z)*(16000.**2)*height(z)
     &
                                               /(1.E6*.0224)
                    kount(h)=kount(h)+count(z)
                    hrmass=hrmass+masso3
                  else
                    masso3=0.
                  endif
C This is the end of the layer loop...go back and start a new
layer.
                write(13, "(a,i2,4(','),F12.3,',',F6.3,',',i5)")
                           'LAYER ',Z,masso3,(maxo3*1000.),gridmax
     &
              print*,'finished writing layer',z
              ENDDO
```

 $\ensuremath{\text{C}}$ This is the end of the hourly loop...go back and start a new hour.

hr=h-1

WRITE(*,'(A)')' COMPLETE '

END

7. Aircraft Data Comparison Code (6 pages)

c234567890123456789012345678901234567890123456789012345678901234567

```
PROGRAM aircomp
c This program reads a UAM format .AVRG file
c and writes an ASCII format file for one hour,
c which reports the utm coordinates (centroid of a
c grid cell) and ozone values for each grid cell,
c which is useful for analyzing point source data.
c Dyron Hamlin, November 2001.
c Define Variables
       integer SEG, NUMSPE, BEGD, ENDD, ZONE, NUMXCELL, NUMYCELL, M
       integer NUMZCELL, SD, DT, SEGX, SEGY, SCELLX,
SCELLY, I, J, L, Z, H
       integer NUMCELLS, kount(24), SPECMOD,
GRIDCELL, k, count(9), hr, X, Y
       real BEGT, ENDT, REFORX, REFORY, XLOC, YLOC, XSIZE, YSIZE
       real SHGT, MINSD, MINDT, THRESH
       real hropenoz(24), hravope
       real O3(82,106,9,24),NOZ(82,106,9,24)
       real DUMM(82,106,9,24)
       real dx,utmx
       dimension MFILETYPE(10), MFILENAME(60)
       dimension MDUMMY(10), MSPECIES(10,30), MSPECIE2(10,30)
       integer SPECIE(10)
       character*100 IPATH
890123456789012345678901234567890
                                     4 5
        1
                 2
                  9
c Open files and make new output file
     WRITE(*,'(A)')' Enter the .avrg file to extract from:'
     READ (*,'(20x,A)') IPATH
     open (unit=11, file=IPATH, status='old',FORM='UNFORMATTED')
     WRITE(*,'(A)')' Enter the O3 OUTPUT file to be created: '
     READ (*,'(20x,A)') IPATH
```

```
open (unit=13, file=IPATH, status='unknown',FORM='FORMATTED')
      WRITE(*,'(A)')' Enter the NOz OUTPUT file to be created: '
      READ (*,'(20x,A)') IPATH
      open (unit=14, file=IPATH, status='unknown',FORM='FORMATTED')
      WRITE(*,'(A)')' Enter the grid resolution of the .avrg file:
      READ (*,'(20x,f3.1)') dx
      print*, 'dx = ', dx
        DO H=1,24
         DO Z=1, NUMZCELL
          DO I=1, NUMXCELL
          DO J=1, NUMYCELL
           O3(I,J,Z,H)=0.
           NOZ(I,J,Z,H)=0.
           DUMM(I,J,Z,H)=0.
           ENDDO
          ENDDO
         ENDDO
        ENDDO
        READ(11) MFILETYPE, MFILENAME, SEG, NUMSPE, BEGD, BEGT
       , ENDD, ENDT
        READ(11) REFORX, REFORY, ZONE, XLOC, YLOC, XSIZE
       , YSIZE, NUMXCELL, NUMYCELL, NUMZCELL, SD, DT, SHGT, MINSD
          , MINDT
        READ(11) SEGX, SEGY, SCELLX, SCELLY
        READ(11) ((MSPECIES(M,L),M=1,10),L=1,NUMSPE)
c Put the species list into a dummy array that can be changed for
reading.
        do L=1,NUMSPE
        do M=1,10
        MSPECIE2(M,L)=MSPECIES(M,L)
        enddo
        enddo
C Bswap the name and number of species to allow the flag index to
read the
\ensuremath{\mathtt{C}} "integer" MSPECIE2 as characters when converted to big endian
```

```
call bswap(MSPECIE2, 10, 30)
          do l=1, numspe
          WRITE(*,'(I5,A,10A1)') L,' ',(MSPECIE2(M,L),M=1,10)
          enddo
C Flag indices of O3, HNO3, PAN, and NXOY.
C - These will be used later to ensure that correct data is read.
        iflag=0
        do i=1,NUMSPE
           IF(MSPECIE2(1,i).EQ.'O'.AND.MSPECIE2(2,i).EQ.'3') then
           IFLAG=i
           write(*,'(a,i1)') 'found some O3. Species = ',iflag
           ENDIF
        end do
        jflag=0
        do j=1,NUMSPE
           IF(MSPECIE2(1,j).EQ.'H'.AND.MSPECIE2(2,j).EQ.'N'
            .AND.MSPECIE2(3,j).EQ.'O'.AND.MSPECIE2(4,j).EQ.'3')
then
           JFLAG=j
           write(*,'(a,i2)') 'found some HNO3. Species = ',jflag
           ENDIF
        end do
c Currently, for some reason, I can't recognize PAN using this same
c bswap technique. Thus, one should make sure that PAN is indeed
c species #4.
        iiflag=4
         do ii=1,NUMSPE
С
            IF((MSPECIE2(1,ii).EQ.'P')) then
С
С
            IIFLAG=ii
           write(*,'(a,i2)') 'found some PAN. Species = ',iiflag
            ENDIF
С
         end do
С
        jjflag=0
        do jj=1,NUMSPE
           IF((MSPECIE2(1,jj).EQ.'N'.AND.MSPECIE2(2,jj).EQ.'X'.AND.
     $
               MSPECIE2(3,jj).EQ.'O')) then
           JJFLAG=jj
           write(*,'(a,i2)') 'found some NXOY. Species = ',jjflag
           ENDIF
        end do
        kkflaq=0
        do kk=1,NUMSPE
           IF((MSPECIE2(1,kk).EQ.'H'.AND.MSPECIE2(2,kk).EQ.'O'.AND.
     $
               MSPECIE2(3,kk).EQ.'N')) then
```

```
KKFLAG=kk
           write(*,'(a,i2)') 'found some HONO. Species = ',kkflag
        end do
        llflag=0
        do ll=1, NUMSPE
           IF((MSPECIE2(1,11).EQ.'N'.AND.MSPECIE2(2,11).EQ.'T'.AND.
               MSPECIE2(3,11).EQ.'R')) then
           LLFLAG=11
           write(*,'(a,i2)') 'found some NTR. Species = ',llflag
           ENDIF
        end do
        iiiflag=0
        do iii=1,NUMSPE
IF((MSPECIE2(1,iii).EQ.'N'.AND.MSPECIE2(2,iii).EQ.'O'.AND.
              MSPECIE2(3,iii).NE.'2')) then
           IIIFLAG=iii
           write(*,'(a,i2)') 'found some NO. Species = ',iiiflag
          ENDIF
        end do
        jjjflag=0
        do jjj=1,NUMSPE
IF((MSPECIE2(1,jjj).EQ.'N'.AND.MSPECIE2(2,jjj).EQ.'O'.AND.
               MSPECIE2(3,jjj).EQ.'2')) then
           JJJFLAG=jjj
          write(*,'(a,i2)') 'found some NO2. Species = ',jjjflag
          ENDIF
        end do
c Read hourly stuff.
          DO 9 H = 1,24
            READ(11) BEGD, BEGT, ENDD, ENDT
c Read the two files, checking to see what the specie is.
           DO 12 S=1, NUMSPE
c If the specie is Ozone, read it into O3 array.
            if (S.EQ.IFLAG) then
             DO Z = 1, NUMZCELL
              READ(11) SEG,SPECIE,((O3(I,J,Z,H),I=1,NUMXCELL),
                                   J=1, NUMYCELL)
     &
             ENDDO
```

```
c If the specie is Nitric Acid, read it into an NOz array.
            elseif (S.EQ.JFLAG) then
             DO Z = 1, NUMZCELL
              READ(11) SEG, SPECIE, ((NOZ(I,J,Z,H),I=1,NUMXCELL),
     ď
                                    J=1, NUMYCELL)
             ENDDO
c If the specie is PAN, read it into a dummy array.
            elseif (S.EQ.IIFLAG) then
             DO Z = 1, NUMZCELL
              READ(11) SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                    J=1, NUMYCELL)
     &
             DO I=1, NUMXCELL
              DO J=1, NUMYCELL
              NOZ(I,J,Z,H) = NOZ(I,J,Z,H) + DUMM(I,J,Z,H)
              ENDDO
             ENDDO
             ENDDO
c If the specie is NTR, read it into a dummy array.
            elseif (S.EQ.LLFLAG) then
             DO Z = 1, NUMZCELL
              READ(11) SEG,SPECIE,((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                    J=1, NUMYCELL)
     &
             DO I=1, NUMXCELL
              DO J=1, NUMYCELL
              NOZ(I,J,Z,H) = NOZ(I,J,Z,H) + DUMM(I,J,Z,H)
              ENDDO
             ENDDO
             ENDDO
c If the specie is part of NOz, read it into a dummy array
            elseif ((S.EQ.JJFLAG).OR.(S.EQ.KKFLAG)) then
                 DO Z = 1, NUMZCELL
                     READ(11)
SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                    J=1, NUMYCELL)
             DO I=1, NUMXCELL
              DO J=1, NUMYCELL
              NOZ(I,J,Z,H) = NOZ(I,J,Z,H) + DUMM(I,J,Z,H)
              ENDDO
             ENDDO
                 ENDDO
```

c If the specie is NOx (NO or NO2), read it into a dummy array.

```
elseif ((S.EQ.IIIFLAG).OR.(S.EQ.JJJFLAG)) then
                 DO Z = 1, NUMZCELL
                    READ(11)
SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                    J=1, NUMYCELL)
     &
                 ENDDO
c If the specie is none of these things, read it into a dummy
array.
            else
                 DO Z = 1, NUMZCELL
                    READ(11)
SEG, SPECIE, ((DUMM(I,J,Z,H),I=1,NUMXCELL),
                                   J=1, NUMYCELL)
     &
                 ENDDO
            endif
c Loop through all of the Layers
12
            CONTINUE
c Loop through all of the Hours
            write(*,'(a,2I)') 'Done reading Hour # ',H
           CONTINUE
9
         write(*,'(a)') 'done with all the reading stuff'
c We wish to print only the ozone or NOz values for each gridcell,
and
c report the corresponding lat/lon coordinates.
                write(13, "(4(a,','))")'UTMx','UTMy','03','GRIDCELL'
write(14, "(4(a,','))")'UTMx','UTMy','NOz','GRIDCELL'
             DO H=15,15
              DO Z=1, NUMZCELL
               DO J=54,80
                DO I=57,83
                 GRIDCELL=J*100+I
c Define the UTM coordinate as the centroid of the current
c grid cell. Base the formula upon the grid resolution.
                 if (dx.eq.4) then
                   utmx=(i-1)*dx-2.-140.
                   utmy=(j-1)*dx-2.+3048.
                 elseif (dx.eq.16) then
```

```
utmx=(i-1)*dx-8.-204.
                 utmy=(j-1)*dx-8.+2952.
               elseif (dx.eq.32) then
                 utmx=(i)*dx-16.-300.
                 utmy=(j)*dx-16.+2824.
               endif
                 write(13,"(2(f12.3,','),f6.2,',',i5)")
    &
                              utmx, utmy,
    &
                              (1000.*o3(i,j,z,h)),
                              gridcell
    &
                 write(14,"(2(f12.3,','),f6.2,',',i5)")
                              utmx, utmy,
    &
                              (1000.*noz(i,j,z,h)),
    &
                              gridcell
    &
c Now go back and check the next cell.
              ENDDO
             ENDDO
c This is the end of the layer loop...go back and start a new
layer.
            print*, 'finished writing layer', z
            ENDDO
c This is the end of the hourly loop...go back and start a new
hour.
С
            print*,'finished writing hour',h
            ENDDO
         WRITE(*,'(A)')' COMPLETE '
89012
```

END

APPENDIX B: Aircraft Data Comparison

Aircraft Data from 09/10/2000; DOE G1 flight

- Table B-1. Locations and Distances of G-1 Transects From FPP
- Figure B-1. NOz/NOy relationship
- Figure B-2. NOx/NOy relationship
- Figure B-3. Loss of NOx in FPP plume
- Figure B-4. NOz/NOy_{corrected} relationship
- Figure B-5. Wind Speed and Trajectory from FPP flight data
- Figure B-6. Temperature Comparison
- Figure B-7. Modeled O₃ concentrations

Date	Time	Time	Lat	Long	Alt	Static P	P altitude
GPS	GPS	GPS	(de e)	(al a a)	()	(l- \	()
yyyy-mm-dd		hh:mm:ss.s		(deg)	(m)	(mb)	(m)
***Selected Da		***Selected		***Selected		***Selected	
FPP Only		***FPP Only		***FPP On	,	***FPP On	•
9/10/2000				-96.50635	863.7		825
9/10/2000				-96.51554	873.6		828
9/10/2000				-96.52497	867		824
9/10/2000				-96.53527	867.2		821
9/10/2000				-96.54475	864.8		826
9/10/2000				-96.55502	874.9		827 824
9/10/2000				-96.56522	867.5		
9/10/2000				-96.57519	864.7		820 831
9/10/2000 9/10/2000			29.88433	-96.583	867 878.3		833
9/10/2000				-96.59365 -96.60441	878.3 874.5		834
9/10/2000				-96.61224			819
9/10/2000				-96.62226	859.2		819
9/10/2000				-96.63276	868		834
9/10/2000				-96.64054	878.1	916.82	836
9/10/2000				-96.65176 -96.66227	871.4		819
9/10/2000 9/10/2000				-96.6622 <i>1</i> -96.67335	848.4 817.4		795
							772 764
9/10/2000 9/10/2000				-96.68257 -96.69489	806.3 812.6		764 780
9/10/2000					825.3		774
9/10/2000				-96.70466 -96.71542	625.3 788.3		774
9/10/2000					768.3		737 725
9/10/2000				-96.72584 -96.73583	754.2		705
9/10/2000				-96.74652	734.2		679
9/10/2000				-96.75686	700.5		665
9/10/2000				-96.76633	690.3		660
					686.8		658
9/10/2000 9/10/2000			29.88771	-96.7773 -96.78705	702.7		679
9/10/2000				-96.79657	702.7		691
9/10/2000				-96.79657 -96.80597	720.2		665
				-96.8059 <i>1</i>	678.8		648
9/10/2000 9/10/2000				-96.81885		937.76	668
9/10/2000							660
			29.90575	-96.818	677		
9/10/2000 9/10/2000				-96.81222 -96.80234			631 615
9/10/2000				-96.80234 -96.79186	635.3		614
9/10/2000				-96.79180 -96.78181	625.3		591
9/10/2000				-96.78181 -96.77143	592.1	944.28	559
9/10/2000	J.U I P W	∠∪.∪1.10	Z3.3ZZ34	-30.11 143	39Z. I	541.03	559

Date GPS	Time GPS	T amb	Theta	Dew Pt	RH	H2O MR	Wind Spee	Wind Dir
yyyy-mm-dd	hh:mm:ss.:	: (C)	(C)	(C)	(%)	(g/kg)	(m/s)	(deg)
Selected Da		***Selected		***Selected		***Selected	(III/5) I Data	***Selectec
***FPP Only**		***FPP Onl		***FPP Onl		***FPP Onl		***FPP Onl
9/10/2000			31.7	17.4	65	13.72	y 3.9	157.06
9/10/2000			31.7	17.3	64.7	13.65	4.6	
9/10/2000			32	17.1	63.1	13.5	4.7	
9/10/2000			31.9	17.1	63.1	13.46	4.2	
9/10/2000			31.9	17	63.2	13.42	3.5	
9/10/2000			31.8	17	63.1	13.36	3.4	
9/10/2000			31.9	16.9	62.4	13.31	3.6	138.89
9/10/2000			31.9	17.1	63.4	13.5	4.3	
9/10/2000			31.9	17.2	63.9	13.58	4.9	138.48
9/10/2000			31.8	17.2	64.4	13.56	3.4	
9/10/2000			31.8	17.1	64.2	13.52	4.3	163.74
9/10/2000	2:56 PM	24.5	31.8	17.1	63.3	13.46	3.6	128.06
9/10/2000	2:56 PM	24.5	31.8	17.5	65.2	13.84	4.1	153.69
9/10/2000	2:57 PM	24.5	32	17.4	64.6	13.79	4.9	140.41
9/10/2000	2:57 PM	24.3	31.8	17.4	65.4	13.78	4.5	143.44
9/10/2000	2:57 PM	24.4	31.7	17.5	65.4	13.85	4.1	146.38
9/10/2000	2:57 PM	24.7	31.8	17.7	64.9	13.95	4.2	137.7
9/10/2000	2:57 PM	25.1	32	17.8	63.7	14	4.1	134.31
9/10/2000	2:57 PM		31.8	17.6	63.3	13.83	4.3	
9/10/2000			31.9	17.5	63.2	13.74	3.3	
9/10/2000			31.7	17.6	64	13.81	3.5	143.52
9/10/2000			31.8	17.5	62	13.71	3.4	
9/10/2000			31.8	17.5	61.3	13.65	2.8	144.45
9/10/2000			31.7	17.5	61.1	13.66	3	
9/10/2000			31.7	17.7	60.9	13.76	2.9	154.06
9/10/2000			31.7	17.6	59.8	13.64	3.1	149.57
9/10/2000			31.8	17.4	58.8	13.49	3	
9/10/2000			31.9	17.5	58.6	13.54	4.4	
9/10/2000			31.8	17.5	59.5	13.58	2.6	116.67
9/10/2000			31.7	17.5	60.2	13.57	3.7	
9/10/2000			31.7	17.1	58	13.19	3.3	
9/10/2000			32	17.5	58	13.53	5.3	136.35
9/10/2000			32	17.4	58.2	13.46	5	154.82
9/10/2000			31.8	17.3	58.2	13.39	5	183.04
9/10/2000			31.7	17.4	58.1	13.42	4.5	
9/10/2000			31.8	17.5	57.6	13.49	3.6	210.73
9/10/2000			32.1	17.7	57	13.62	2	
9/10/2000			32	17.7	56.9	13.65	3.4	
9/10/2000	3:01 PM	27.3	31.9	17.6	55.7	13.5	3.6	201.35

Date GPS	Time GPS	UV sky	UV gnd	PCASP tot	FSSP total	bap	O3	CO
yyyy-mm-dd ***Selected Da ***FPP Only***	hh:mm:ss. ita***	: (W/m^2)	(W/m^2) ***Selected ***FPP Onl		(cm^-3) ***Selected ***FPP Only		(ppbv) ***Selected ***FPP On	
9/10/2000		20.2				2.19E-06		•
9/10/2000				304		1.84E-06		
9/10/2000			2.4			1.78E-06		130
9/10/2000						2.14E-06		
9/10/2000						2.17E-06		154
9/10/2000			_			1.93E-06		
9/10/2000						1.71E-06		
9/10/2000						1.96E-06		
9/10/2000						2.22E-06		
9/10/2000						2.24E-06		
9/10/2000						1.78E-06		147
9/10/2000				318.7		1.81E-06		
9/10/2000						2.76E-06		
9/10/2000				295		2.41E-06		
9/10/2000				312.1	0.524	2.19E-06		
9/10/2000				328.2		2.46E-06		
9/10/2000				334.7		2.99E-06		
9/10/2000	2:57 PM	44.5	2.8	330	0.519	2.66E-06		
9/10/2000	2:57 PM	44.1	2.7			2.02E-06		127
9/10/2000						1.68E-06		
9/10/2000	2:58 PM	30.7	2.1	351.4		2.38E-06		
9/10/2000			1.6			2.52E-06		
9/10/2000	2:58 PM	18.1	1.5	367.5	0.488	1.89E-06	46.4	160
9/10/2000	2:58 PM	18.5	1.4	394.6	0.481	2.20E-06	46.5	153
9/10/2000	2:58 PM	37.6	1.9	404.7	0.449	2.74E-06	47.3	149
9/10/2000	2:59 PM	42.1	2.2	400.5	0.54	2.11E-06		
9/10/2000	2:59 PM	42.7	2.3	395.4	0.534	1.61E-06	47	140
9/10/2000	2:59 PM	42.7	2.2	393.6	0.502	1.69E-06	46.8	127
9/10/2000	2:59 PM	29.9	2.2	355	0.525	2.58E-06	46.5	120
9/10/2000	2:59 PM			384.3	0.487	1.69E-06	47.2	123
9/10/2000	2:59 PM			403.9	0.464	1.35E-06	47.6	
9/10/2000	3:00 PM			431	0.555	2.52E-06	47.5	
9/10/2000	3:00 PM			383.6	0.454	2.49E-06	47.6	
9/10/2000	3:00 PM			431.1	0.494	1.97E-06	48.6	
9/10/2000	3:00 PM			428.7	0.428	2.32E-06	48.2	
9/10/2000	3:00 PM	41.8	2.3	399.1	0.469	2.93E-06		
9/10/2000	3:00 PM	28.8	1.9	355.1	0.448	3.39E-06	48.1	
9/10/2000	3:01 PM	21.3	1.5	399.9	0.476	2.55E-06	47.6	
9/10/2000	3:01 PM	39.4	1.7	383.5	0.455	2.34E-06	47.1	

Date	Time	SO2	NO	NO2	NOy	DelO3	NOz	DelO3
GPS	GPS					constant		bg by
yyyy-mm-dd	hh:mm:ss.		(ppbv)	(ppbv)	(ppbv)	bg		transect
Selected Da	ıta	***Selected	Data***	***Selected	Data***	***Selected	Data***	***Selectec
FPP Only	•	***FPP On	y***	***FPP Onl	y***	***FPP Onl	y***	***FPP Onl
9/10/2000	2:54 PM	0.31	0.07	0.277	1.586	-0.3	1.239	0.7
9/10/2000	2:55 PM		0.071	0.301	1.611	-0.6	1.239	0.4
9/10/2000	2:55 PM		0.063	0.266	1.507	0.1	1.178	1.1
9/10/2000			0.058		1.475		1.168	0
9/10/2000			0.056		1.533		1.208	0.1
9/10/2000			0.051		1.479		1.094	1.5
9/10/2000			0.047		1.438		1.05	0.9
9/10/2000			0.056		1.494		1.136	1.3
9/10/2000			0.086		1.5		1.165	1
9/10/2000			0.063		1.477		1.047	-2
9/10/2000			0.082		1.436		1.159	-0.1
9/10/2000			0.057		1.408		1.061	0
9/10/2000			0.05		1.463		1.113	-0.8
9/10/2000			0.075		1.464		1.092	-1.3
9/10/2000			0.063		1.458		1.011	-1.4
9/10/2000					1.485		1.139	-1.3
9/10/2000			0.118		1.59	-2.4	1.201	-1.4
9/10/2000			0.093		1.48	-1.1	1.062	-0.1
9/10/2000			0.075		1.507		1.172	0.1
9/10/2000			0.074		1.468			-2
9/10/2000			0.083		1.479		1.105	-0.7
9/10/2000					1.483			-0.2
9/10/2000			0.056		1.483		1.086	-0.6
9/10/2000			0.081		1.613		1.19	-0.5
9/10/2000			0.075		1.568		1.14	0.3
9/10/2000			0.071		1.536		1.222	0.2
9/10/2000			0.064		1.546		1.2	0
9/10/2000			0.078		1.573		1.23	-0.2
9/10/2000			0.064		1.625		1.229	-0.5
9/10/2000			0.087	0.139	1.636		1.41	0.2
9/10/2000					1.617			0.6
9/10/2000						-0.5		0.5
9/10/2000						-0.4		0.6
9/10/2000						0.6		1.6
9/10/2000			0.073		1.651	0.2		1.2
9/10/2000			0.36		2.516		0.813	-0.4
9/10/2000			0.08		1.817		1.187	1.1
9/10/2000			0.088		1.777		1.311	0.6
9/10/2000	3:01 PM	0.64	0.207	0.669	2.242	-0.9	1.366	0.1

Date	Time	OPE	%OX	%OX	NOy	NOz	%OX
GPS	GPS	(inst)	no bg cor	norm by	*1.3(byNOx)	by N	oy change
yyyy-mm-dd	hh:mm:ss.	ss		76%			
Selected Da	ta		***Selected D	ata***			
FPP Only			***FPP Only**	**			
9/10/2000	2:54 PM	0.56	78%	1.03	2.06	171%	0.8317
9/10/2000	2:55 PM	0.32	77%	1.01	2.09	172%	0.822375
9/10/2000	2:55 PM	0.93	78%	1.03	1.96	163%	0.832066
9/10/2000	2:55 PM	0.00	79%	1.04	1.92	161%	0.839896
9/10/2000	2:55 PM	0.08	79%	1.04	1.99	167%	0.836921
9/10/2000	2:55 PM	1.37	74%	0.97	1.92	154%	0.799761
9/10/2000	2:55 PM	0.86	73%	0.96	1.87	148%	0.792447
9/10/2000	2:56 PM	1.14	76%	1.00	1.94	158%	0.815673
9/10/2000	2:56 PM	0.86	78%	1.02	1.95	162%	0.828205
9/10/2000	2:56 PM	-1.91	71%	0.93	1.92	149%	0.776053
9/10/2000	2:56 PM	-0.09	81%	1.06	1.87	159%	0.851618
9/10/2000	2:56 PM	0.00	75%	0.99	1.83	148%	0.810424
9/10/2000	2:56 PM	-0.72	76%	1.00	1.90	155%	0.815974
9/10/2000	2:57 PM	-1.19	75%	0.98	1.90	153%	0.80454
9/10/2000	2:57 PM	-1.38	69%	0.91	1.90	145%	0.764166
9/10/2000	2:57 PM	-1.14	77%	1.01	1.93	158%	0.820772
9/10/2000	2:57 PM	-1.17	76%	0.99	2.07	168%	0.811805
9/10/2000	2:57 PM	-0.09	72%	0.94	1.92	151%	0.782744
9/10/2000	2:57 PM	0.09	78%	1.02	1.96	162%	0.829003
9/10/2000	2:58 PM	-1.80	76%	1.00	1.91	155%	0.81398
9/10/2000	2:58 PM	-0.63	75%	0.98	1.92	155%	0.805482
9/10/2000	2:58 PM	-0.18	76%	1.00	1.93	157%	0.814306
9/10/2000	2:58 PM	-0.55	73%	0.96	1.93		0.794076
9/10/2000	2:58 PM	-0.42	74%	0.97	2.10	167%	0.798274
9/10/2000	2:58 PM	0.26	73%	0.96	2.04	161%	0.790031
9/10/2000	2:59 PM	0.16	80%	1.05	2.00	168%	0.842748
9/10/2000	2:59 PM	0.00	78%	1.02	2.01	166%	0.827844
9/10/2000	2:59 PM	-0.16	78%	1.03	2.04	170%	0.832266
9/10/2000	2:59 PM	-0.41	76%	1.00	2.11	172%	
9/10/2000	2:59 PM	0.14	86%	1.13	2.13	190%	0.893737
9/10/2000	2:59 PM	#DIV/0!		#VALUE!	2.10	210%	1
9/10/2000	3:00 PM	#DIV/0!	#VALUE!	#VALUE!	#VALUE!	#VALUE!	#VALUE!
9/10/2000	3:00 PM	#DIV/0!	#VALUE!	#VALUE!	#VALUE!	#VALUE!	#VALUE!
9/10/2000	3:00 PM	#DIV/0!	#VALUE!	#VALUE!	#VALUE!	#VALUE!	#VALUE!
9/10/2000	3:00 PM	#DIV/0!		#VALUE!	2.15		0.965988
9/10/2000	3:00 PM	-0.49	32%	0.43	3.27	157%	0.479332
9/10/2000	3:00 PM	0.93	65%	0.86	2.36	173%	0.733288
9/10/2000	3:01 PM	0.46	74%	0.97	2.31	184%	0.798277
9/10/2000	3:01 PM	0.07	61%	0.80	2.91	204%	0.699444

```
GPS
             GPS
                        bg correct bg correct
yyyy-mm-dd
             hh:mm:ss.ss
***Selected Data***
***FPP Only***
    9/10/2000
                2:54 PM 0.008892 -0.338108
    9/10/2000
                2:55 PM 0.033892 -0.338108
    9/10/2000
                2:55 PM -0.070108 -0.399108
    9/10/2000
                2:55 PM -0.102108 -0.409108
    9/10/2000
                2:55 PM -0.044108 -0.369108
    9/10/2000
                2:55 PM -0.098108 -0.483108
    9/10/2000
                2:55 PM -0.139108 -0.527108
    9/10/2000
                2:56 PM -0.083108 -0.441108
    9/10/2000
                2:56 PM -0.077108 -0.412108
    9/10/2000
                2:56 PM -0.100108 -0.530108
    9/10/2000
                2:56 PM -0.141108 -0.418108
    9/10/2000
                2:56 PM -0.169108 -0.516108
    9/10/2000
                2:56 PM -0.114108 -0.464108
    9/10/2000
                2:57 PM -0.113108 -0.485108
    9/10/2000
                2:57 PM -0.119108 -0.566108
                2:57 PM -0.092108 -0.438108
    9/10/2000
    9/10/2000
                2:57 PM 0.012892 -0.376108
    9/10/2000
                2:57 PM -0.097108 -0.515108
    9/10/2000
                2:57 PM -0.070108 -0.405108
                2:58 PM -0.109108 -0.464108
    9/10/2000
    9/10/2000
                2:58 PM -0.098108 -0.472108
    9/10/2000
                2:58 PM -0.094108 -0.452108
                2:58 PM -0.094108 -0.491108
    9/10/2000
    9/10/2000
                2:58 PM 0.035892 -0.387108
    9/10/2000
                2:58 PM -0.009108 -0.437108
    9/10/2000
                2:59 PM -0.041108 -0.355108
    9/10/2000
                2:59 PM -0.031108 -0.377108
    9/10/2000
               2:59 PM -0.004108 -0.347108
    9/10/2000
                2:59 PM 0.047892 -0.348108
                2:59 PM 0.058892 -0.167108
    9/10/2000
    9/10/2000
                2:59 PM 0.039892 #VALUE!
                                             #VALUE!
    9/10/2000
                3:00 PM #VALUE!
                                  #VALUE!
                                             #VALUE!
    9/10/2000
                3:00 PM #VALUE!
                                  #VALUE!
                                             #VALUE!
    9/10/2000
                3:00 PM #VALUE!
                                  #VALUE!
                                             #VALUE!
                        0.073892 #VALUE!
    9/10/2000
                3:00 PM
                                             #VALUE!
    9/10/2000
                3:00 PM
                         0.938892 -0.764108
    9/10/2000
                3:00 PM
                         0.239892 -0.390108
    9/10/2000
                3:01 PM
                         0.199892 -0.266108
    9/10/2000
                3:01 PM 0.664892 -0.211108
```

Date

Time

NOy

NOz

%OX

Date GPS	Time GPS	Time GPS	Lat	Long	Alt	Static P	P altitude
yyyy-mm-dd ***Selected Da ***FPP Only***	hh:mm:ss.: ta***	hh:mm:ss.ss ***Selected ***FPP Only	Data***	(deg) ***Selected ***FPP On		(mb) ***Selecte ***FPP Or	
FIRST TRANS	ECT		FIRST TRA	ANSECT	FIRST TRA	ANSECT	FIRST TR/
9/10/2000	3:01 PM	20:01:20	29.92485	-96.76179	574.2	949.07	549
9/10/2000	3:01 PM	20:01:30	29.92685	-96.74985	575.7	948.32	555
9/10/2000	3:01 PM	20:01:40	29.92803	-96.74147	584.5	947.05	566
9/10/2000	3:01 PM	20:01:50	29.92885	-96.72825	596.5	946.19	574
	########						
	########						
	########						
9/10/2000				-96.71838			
9/10/2000				-96.70873			
9/10/2000				-96.70004			
9/10/2000			29.93821				
9/10/2000				-96.68948			
9/10/2000				-96.69144			
9/10/2000			29.96217				
9/10/2000				-96.70625			
9/10/2000				-96.71565			
9/10/2000	3:03 PM	20:03:30	29.97045	-96.72554	591.9	946.31	573
SECOND TRA	NSECT		SECOND	TRANSECT	SECOND	TRANSEC	SECOND 1
9/10/2000	3:03 PM	20:03:40	29.97201	-96.73549	609.3	944.65	587
9/10/2000	3:03 PM	20:03:50	29.97359	-96.74563	607.8	945.9	576
9/10/2000	3:04 PM	20:04:00	29.97511	-96.75522	598	946.69	569
9/10/2000	3:04 PM	20:04:10	29.97666	-96.76549	597.7	946.01	575
9/10/2000	3:04 PM	20:04:20	29.97781	-96.77303	599.5	946.06	575
9/10/2000	3:04 PM	20:04:30	29.97966	-96.78468	595.2	946.66	570
9/10/2000	3:04 PM	20:04:40	29.98107	-96.79336	602.3	945.15	583
9/10/2000				-96.80343			
9/10/2000	3:05 PM	20:05:00	29.98436	-96.81303	587.4	947.09	
9/10/2000				-96.82331	597.4		
9/10/2000				-96.83231	612.9		
9/10/2000			29.98961				
9/10/2000	3:05 PM	20:05:40	29.99138	-96.8516	593.5	945.99	576

Date GPS	Time GPS	T amb	Theta	Dew Pt	RH	H2O MR	Wind Spee	Wind Dir
yyyy-mm-dd ***Selected Da ***FPP Only**	hh:mm:ss. ata***	***Selecte		(C) ***Selected ***FPP On		(g/kg) ***Selected ***FPP On		(deg) ***Selectec ***FPP Onl
FIRST TRANS	SECT		FIRST TRA	ANSECT	FIRST TRANSECT		FIRST TRANSECT	
9/10/2000	3:01 PM					13.85	1.5	240.56
9/10/2000						13.73		217.83
9/10/2000						13.53		
9/10/2000			31.9	17.7	56.2	13.55	3.5	220.83
	#######							
	########							
0/40/0000	#######		20	47.7	50.0	40.50	0.0	004.45
9/10/2000 9/10/2000								201.15 216.53
9/10/2000								210.55
9/10/2000						13.86		
9/10/2000								
9/10/2000								160.42
9/10/2000						13.75		
9/10/2000								145.25
9/10/2000								
9/10/2000						13.5		144.99
SECOND TRA	ANSECT		SECOND	TRANSECT	SECOND	TRANSECT	SECOND	TRANSECT
9/10/2000	3:03 PM	1 27	31.9	17.7	56.8	13.6	4.4	158.41
9/10/2000						13.2		140.04
9/10/2000	3:04 PM	1 27.1	31.8	17.2	54.6	13.12		
9/10/2000	3:04 PM						3	
9/10/2000								132.12
9/10/2000								
9/10/2000								148.03
9/10/2000						13.42		129.64
9/10/2000							4.5	118.17
9/10/2000								
9/10/2000						13.52		145
9/10/2000								
9/10/2000	3:05 PM	1 27.3	32.1	17.8	56	13.67	5.2	132.36

Date GPS	Time GPS	UV sky	UV gnd	PCASP to	FSSP total	bap	О3	СО
yyyy-mm-dd ***Selected D ***FPP Only**	hh:mm:ss. ata***	: (W/m^2)	(W/m^2) ***Selected ***FPP On		(cm^-3) ***Selected ***FPP On		(ppbv) ***Selected ***FPP On	
FIRST TRAN	SECT	FIRST TR.	ANSECT	FIRST TR	ANSECT	FIRST TRAN	ISECT	
9/10/200	3:01 PM	41.8	1.9	357.4	0.574	3.04E-06	27.9	
9/10/200	3:01 PM	24.1	1.7	387.3	0.637	2.44E-06	31.7	
9/10/200	3:01 PM			358.2	0.502	1.59E-06	45.5	
9/10/200	3:01 PM	43.3	2	359.9	0.455	1.71E-06	46.3	
	########	ŧ						
	######## #########							
9/10/200	3:02 PM	42.9	2.2	333.7	0.478	2.36E-06	45.7	
9/10/200	3:02 PM			364.1	0.469	2.24E-06	47.2	
9/10/200	3:02 PM			344	0.473	2.35E-06	46.7	
9/10/200	3:02 PM			322.6	0.512	2.76E-06	45.3	126
9/10/200	3:02 PM			350.9	0.547	2.09E-06	45.5	139
9/10/200	3:02 PM			353.7	0.559	2.10E-06	45.1	157
9/10/200	3:03 PM			308.5	0.438	1.91E-06	46.5	127
9/10/200				333		2.03E-06		
9/10/200	3:03 PM	42.5	2.1	356	0.495	1.95E-06	47.2	122
9/10/200	3:03 PM	41.6	2.3	350.1	0.216	1.66E-06	46.8	132
SECOND TR	ANSECT	SECOND	TRANSECT	SECOND	TRANSECT	SECOND TR	ANSECT	
9/10/200	3:03 PM	41.1	2.4	351.6	0.274	1.48E-06	42.1	141
9/10/200								130
9/10/200				436.7	0.66	2.19E-06	33.8	127
9/10/200	3:04 PM	39.2	1.9	443.1	0.557	3.00E-06	44.1	121
9/10/200	3:04 PM	39	1.9	461.7	0.622	3.80E-06	42.6	145
9/10/200	3:04 PM	39.1	2	447.7	0.587	3.23E-06	43.2	141
9/10/200	3:04 PM	38.8	2	458.5	0.496	2.01E-06	50.2	153
9/10/200	3:04 PM	35.4	1.8	544.6	0.553	1.46E-06	51.5	137
9/10/200	3:05 PM							
9/10/200								
9/10/200								148
9/10/200								145
9/10/200	3:05 PM	40.1	2.2	543.4	0.606	3.17E-06	53.9	114

Date GPS	Time GPS	SO2	NO	NO2	NOy	DelO3 constant	NOz	DelO3 bg by
yyyy-mm-dd ***Selected Da	hh:mm:ss.sta***	***Selected		(ppbv) ***Selected		bg ***Selected		transect ***Selectec
FPP Only		***FPP On	ly***	***FPP On	ly***	***FPP On	y***	***FPP Onl
FIRST TRANS	ECT							
9/10/2000	3:01 PM	25.68			41.846			-19.1
9/10/2000	3:01 PM							-15.3
9/10/2000	3:01 PM				1.841		0.215	-1.5
9/10/2000	3:01 PM	2.99	0.08	0.328	1.707	' -1.7	1.299	-0.7
	########							
	########							
0/40/0000	########	2.24	0.070	0.440	4.04=			
9/10/2000	3:02 PM	0.61	0.079		1.647		1.15	-1.3
9/10/2000	3:02 PM	0.1	0.094		1.68		1.341 1.212	0.2
9/10/2000 9/10/2000	3:02 PM 3:02 PM	0.16 -0.02			1.618 1.537		1.212	-0.3 -1.7
9/10/2000 9/10/2000	3:02 PM 3:02 PM				1.53 1.498		1.067 1.128	-1.5 -4.9
9/10/2000	3:03 PM	0.12					1.120	-4.9 -3.5
9/10/2000	3:03 PM	0.09			1.577		1.121	-3.3
9/10/2000	3:03 PM	0.19			1.558		1.17	-3.3 -2.8
9/10/2000	3:03 PM	0.27			1.587		1.095	-3.2
0/ 10/2000	0.00	0.00	0.0.	00				0
SECOND TRA	NSECT							
9/10/2000	3:03 PM	5.07	1.576	3.741	7.697	,	2.38	
9/10/2000	3:03 PM	44.11	31.981		54.951		6.181	
9/10/2000	3:04 PM	50.14	14.664	15.138	28.996		-0.806	
9/10/2000	3:04 PM	23.27		7.311	11.701	-3.9	0.749	-5.9
9/10/2000	3:04 PM	17.97	4.336	8.204	13.414	-5.4	0.874	-7.4
9/10/2000	3:04 PM	18.17	4.201	7.654	12.891	-4.8	1.036	-6.8
9/10/2000	3:04 PM	9.01	0.934	2.894	4.816	2.2	0.988	0.2
9/10/2000	3:04 PM	4.9	0.567	1.967	4.072	3.5	1.538	1.5
9/10/2000	3:05 PM	4.68	0.683	2.549	5.075	4.8	1.843	2.8
9/10/2000	3:05 PM	5.49	0.756	2.511	4.735	5.7	1.468	3.7
9/10/2000	3:05 PM				3.441		1.847	5.1
9/10/2000	3:05 PM	2.25			3.031		1.759	6.1
9/10/2000	3:05 PM	1.07	0.163	0.787	2.474	5.9	1.524	3.9

Date GPS yyyy-mm-dd ***Selected Da ***FPP Only***		OPE (inst) ss	%OX no bg cor ***Selected D ***FPP Only**		NOy *1.3(byNOx)	NOz		%OX oy change
FIRST TRANS			- ,					
9/10/2000	3:01 PM	#DIV/0!		#VALUE!	54.40		148%	0.027239
9/10/2000		#DIV/0!		#VALUE!	96.31			-0.016951
9/10/2000		-6.98	12%	0.15	2.39		77%	0.320603
9/10/2000		-0.54	76%	1.00	2.22			0.816142
5, 75, 255	########		44%	0.58			, .	0.286758
	########							
	########							
9/10/2000	3:02 PM	-1.13	70%	0.92	2.14		164%	0.767876
9/10/2000	3:02 PM	0.15	80%	1.05	2.18		185%	0.84478
9/10/2000	3:02 PM	-0.25	75%	0.99	2.10		170%	0.806979
9/10/2000	3:02 PM	-1.45	76%	1.01	2.00		164%	0.818828
9/10/2000	3:02 PM	-1.41	70%	0.92	1.99		153%	0.76722
9/10/2000	3:02 PM	-4.34	75%	0.99	1.95		158%	0.810003
9/10/2000	3:03 PM	-3.12	76%	1.00	1.91		156%	0.816974
9/10/2000	3:03 PM	-2.82	74%	0.98	2.05		164%	0.801473
9/10/2000	3:03 PM	-2.37	76%	1.00	2.03		165%	0.814851
9/10/2000	3:03 PM	-2.92	69%	0.91	2.06		157%	0.761524
SECOND TRA	NSECT							
9/10/2000	3:03 PM	0.00	31%	0.41	10.01		4609/	0.468624
9/10/2000		0.00		0.41	71.44		2267%	0.400024
9/10/2000		0.00		#VALUE!	71. 44 37.69		789%	0.317294
9/10/2000	3:04 PM	-7.88	6%	#VALUE!	15.21		426%	0.280009
9/10/2000		-7.66 -8.47	7%		17.44		490%	0.280889
9/10/2000		-6.47 -6.56	8%	0.09	16.76		490%	0.292589
9/10/2000		0.20		0.11	6.26		243%	0.292569
9/10/2000		0.20		0.50	5.29		276%	0.521309
9/10/2000	3:05 PM	1.52		0.48	6.60		337%	0.521309
9/10/2000		2.52		0.46	6.16		289%	0.469255
9/10/2000		2.76		0.71	4.47		288%	0.409255
9/10/2000	3:05 PM	3.47	58%	0.76	3.94		267%	0.677182
9/10/2000	3:05 PM	2.56	62%	0.81	3.22		227%	0.70462

```
Date
              Time
                        NOy
                                  NOz
                                             %OX
GPS
              GPS
                        bg correct bg correct
yyyy-mm-dd
              hh:mm:ss.ss
***Selected Data***
***FPP Only***
                                                      1
                        -1.577108 -1.577108
FIRST TRANSECT
                        -1.577108 -1.577108
                                                      1
                                                      1
                        -1.577108 -1.577108
                3:01 PM 40.26889 -12.64911
    9/10/2000
    9/10/2000
                3:01 PM 72.51089 -25.43611
    9/10/2000
                3:01 PM
                         0.263892 -1.362108
    9/10/2000
                3:01 PM 0.129892 -0.278108
              ####### -1.577108 -1.577108
                                                      1
              ####### -1.577108 -1.577108
                                                      1
                                                      1
              ########
                          -1.82393
                                   -1.82393
                3:02 PM
                          -0.17693
    9/10/2000
                                    -0.67393
    9/10/2000
                3:02 PM
                          -0.14393
                                    -0.48293
                3:02 PM
                          -0.20593
    9/10/2000
                                    -0.61193
    9/10/2000
                3:02 PM
                          -0.28693
                                    -0.64893
    9/10/2000
                3:02 PM
                          -0.29393
                                    -0.75693
                3:02 PM
                          -0.32593
    9/10/2000
                                    -0.69593
                                    -0.70293
    9/10/2000
                3:03 PM
                          -0.35293
    9/10/2000
                3:03 PM
                          -0.24693
                                    -0.65393
    9/10/2000
                3:03 PM
                          -0.26593
                                    -0.64093
    9/10/2000
                3:03 PM
                          -0.23693
                                    -0.72893
SECOND TRANSECT
                3:03 PM
    9/10/2000
                          5.87307
                                     0.55607
                                              0.094681
    9/10/2000
                3:03 PM
                         53.12707
                                     4.35707
                                              0.082012
    9/10/2000
                3:04 PM
                         27.17207
                                    -2.62993
                3:04 PM
    9/10/2000
                          9.87707
                                    -1.07493
    9/10/2000
                3:04 PM
                         11.59007
                                    -0.94993
    9/10/2000
                3:04 PM
                         11.06707
                                    -0.78793
    9/10/2000
                3:04 PM
                          2.99207
                                    -0.83593
    9/10/2000
                3:04 PM
                          2.24807
                                    -0.28593
    9/10/2000
                3:05 PM
                           3.25107
                                     0.01907
                                              0.005866
    9/10/2000
                3:05 PM
                          2.91107
                                    -0.35593
    9/10/2000
                3:05 PM
                           1.61707
                                     0.02307
                                              0.014267
    9/10/2000
                3:05 PM
                           1.20707
                                    -0.06493
                3:05 PM
    9/10/2000
                          0.65007
                                    -0.29993
```

Date	Time	Time	Lat	Long	Alt	Static P	P altitude
GPS	GPS	GPS	(al a a)	(-l)	()	(l-)	()
yyyy-mm-dd		hh:mm:ss.ss		(deg)	(m)	(mb)	(m)
***Selected Da		***Selected		***Selected		***Selected	
FPP Only		***FPP Only		***FPP On	•	***FPP On	•
9/10/2000 9/10/2000				-96.86081	610.7		
				-96.87074			
9/10/2000				-96.87982			
9/10/2000 9/10/2000				-96.89016 -96.89875			
9/10/2000				-96.90967			
9/10/2000				-96.90967 -96.91762			
9/10/2000			29.98663				
9/10/2000				-96.92787			562
9/10/2000				-96.93617			571
9/10/2000				-96.94575			
9/10/2000				-96.95412			582
9/10/2000				-96.95968			
9/10/2000				-96.96119			
9/10/2000				-96.95827			
9/10/2000				-96.95106			
9/10/2000				-96.94581			
9/10/2000				-96.93543			
9/10/2000				-96.92471			
9/10/2000				-96.91484			
9/10/2000				-96.90547			
9/10/2000				-96.89596			
9/10/2000				-96.88687			
9/10/2000				-96.87768			
9/10/2000				-96.86907			573
THIRD TRANS	SECT		THIRD TR	ANSECT	THIRD TR	ANSECT	THIRD TRA
9/10/2000	3:10 PM	20:10:00	29.99763	-96.85793	603.1	945.63	579
9/10/2000	3:10 PM	20:10:10	29.99624	-96.84898	593.7	947.23	565
9/10/2000	3:10 PM	20:10:20	29.99461	-96.83942	591.8	945.61	579
9/10/2000	3:10 PM	20:10:30	29.99289	-96.82995	612.2	944.43	589
9/10/2000	3:10 PM	20:10:40	29.99222	-96.81976	592.1	946.88	568
9/10/2000	3:10 PM	20:10:50	29.99296	-96.80952	585	946.89	568
9/10/2000	3:11 PM	20:11:00	29.99393	-96.80149	589.1	945.78	578
9/10/2000	3:11 PM	20:11:10	29.99539	-96.79043	598.1	945.75	578
9/10/2000		20:11:20	29.99667	-96.78137	591.6	946.87	568
9/10/2000	3:11 PM	20:11:30	29.99811	-96.77129	583.2	946.49	571
9/10/2000				-96.76089			574
9/10/2000			30.00074	-96.75175			580
9/10/2000			30.00206	-96.7418			578
9/10/2000	3:12 PM	20:12:10	30.00353	-96.73111	590.4	945.5	580

Date GPS	Time GPS	T amb	Theta	Dew Pt	RH	H2O MR	Wind Spee	Wind Dir
yyyy-mm-dd	hh:mm:ss.	ε(C)	(C)	(C)	(%)	(g/kg)	(m/s)	(deg)
***Selected Da		***Selected		***Selected		***Selected		***Selectec
***FPP Only**		***FPP On		***FPP Onl		***FPP On		***FPP Onl
9/10/2000								
9/10/2000	3:06 PM				57.1	13.71	4.4	155.16
9/10/2000						13.77		
9/10/2000	3:06 PM				57.9	13.92		
9/10/2000					58.3			
9/10/2000								
9/10/2000					57.9	13.85		
9/10/2000						13.84		
9/10/2000						13.36		
9/10/2000								
9/10/2000								
9/10/2000					56.9	13.66		
9/10/2000					57.6			
9/10/2000					57.9	13.87		
9/10/2000								
9/10/2000				17.7 17.8				
9/10/2000 9/10/2000					57.5			
9/10/2000					58.2			
9/10/2000					57.7			
9/10/2000					57.7 57.9			
9/10/2000								
9/10/2000					57.7			
9/10/2000						13.58		
9/10/2000				17.7				
THIRD TRANS	SECT		THIRD TRA	ANSECT	THIRD TR	ANSECT	THIRD TR	ANSECT
9/10/2000	3:10 PM	1 27.2	32.1	17.8	56.4	13.69	1.6	192.87
9/10/2000			32	17.6	55.6	13.51	1.9	200.04
9/10/2000					54.9			
9/10/2000	3:10 PM			17.3				
9/10/2000	3:10 PM	1 27.2	31.9	17.2	54.2	13.14	2.7	187.65
9/10/2000	3:10 PM	1 27.2	31.9	17.5	55.2	13.38	2.9	213.86
9/10/2000								
9/10/2000	3:11 PM	1 27.2	32	17.7				
9/10/2000								
9/10/2000				17.4		13.29		
9/10/2000					54.3			
9/10/2000						13.38		
9/10/2000				17.8				
9/10/2000	3:12 PM	1 27.5	32.4	17.7	54.9	13.57	3.7	226.87

Date GPS	Time GPS	UV sky	UV gnd	PCASP tot	FSSP total	bap	О3	CO
yyyy-mm-dd ***Selected Da	hh:mm:ss.	: (W/m^2)	(W/m^2)	(cm^-3)	(cm^-3)	(m^-1)	(ppbv)	(ppbv)
FPP Only								
9/10/2000		40.9	2.1	520	0.505	3.17E-06	52.1	86
9/10/2000	3:06 PM	40.3	2	538.9	0.532	2.82E-06	52.2	144
9/10/2000	3:06 PM	29.1	1.9		0.44	2.81E-06	51.4	166
9/10/2000	3:06 PM	21.3	1.8	523.7	0.566			140
9/10/2000				582.4		2.95E-06		
9/10/2000	3:06 PM			572.4	0.596	2.45E-06	51.4	124
9/10/2000	3:06 PM			547.4	0.545	2.39E-06	51.3	119
9/10/2000	3:07 PM	41.7	2.2	569.4	0.53	2.47E-06	50.5	159
9/10/2000	3:07 PM			596	0.555	1.77E-06	51.8	150
9/10/2000	3:07 PM			575.7	0.581	2.17E-06	51.4	135
9/10/2000	3:07 PM			520.1	0.597	3.29E-06	51.8	151
9/10/2000	3:07 PM			582.6	0.596	2.28E-06	51.7	142
9/10/2000	3:07 PM			535.4		2.49E-06	50.9	
9/10/2000	3:08 PM			532		3.21E-06	49.4	134
9/10/2000	3:08 PM			559	0.559	2.29E-06		
9/10/2000				603.8	0.588	2.46E-06		
9/10/2000				560.5		2.83E-06		
9/10/2000								
9/10/2000		_		_		3.43E-06	_	
9/10/2000					0.547	2.90E-06		
9/10/2000						2.78E-06		
9/10/2000								
9/10/2000		_	-					
9/10/2000					0.547			
9/10/2000	3:09 PM	40.5	2	585.6	0.513	2.32E-06	52.8	130
THIRD TRANS	SECT	THIRD TR	ANSECT	THIRD TR	ANSECT	THIRD TRAN	ISECT	
9/10/2000	3:10 PM	34.6			0.474	2.96E-06	55.4	156
9/10/2000			2.2			2.18E-06		
9/10/2000			2					
9/10/2000				607.6				
9/10/2000								
9/10/2000								_
9/10/2000								
9/10/2000								145
9/10/2000			2.1	476.2		1.53E-06		
9/10/2000			2.1	423.4		1.65E-06		
9/10/2000				403		1.92E-06		
9/10/2000		_		377.9		2.87E-06		
9/10/2000								
9/10/2000	3:12 PM	42	2.4	348	0.475	2.85E-06	49.5	151

Date GPS	Time GPS	SO2	NO	NO2	NOy	DelO3 constant	NOz	DelO3 bg by
yyyy-mm-dd	hh:mm:ss.s	(ppbv)	(ppbv)	(ppbv)	(ppbv)	bg		transect
***Selected Da		u	W 1 /	(11 /	(11 /	4.1	1.505	2.1
FPP Only						4.2		2.2
9/10/2000	3:05 PM	0.35	0.131	0.529	2.165	3.4	1.392	1.4
9/10/2000	3:06 PM		0.097	0.347	1.912			0.7
9/10/2000	3:06 PM	0.33	0.105	0.439	1.936	3.3	1.476	1.3
9/10/2000	3:06 PM	-0.02	0.202	0.849	2.473	3.4	1.421	1.4
9/10/2000	3:06 PM	0.2	0.125	0.323	1.924	3.3	1.519	1.3
9/10/2000	3:06 PM	0.23	0.079	0.447	1.947	2.5	1.539	0.5
9/10/2000	3:06 PM	0.34	0.095	0.383	1.997	3.8	1.497	1.8
9/10/2000	3:07 PM	-0.12	0.097	0.375	2.011	3.4	1.464	2.9
9/10/2000	3:07 PM	0.38	0.052	0.438	1.987	3.8	1.38	3.3
9/10/2000	3:07 PM	0.34	0.076	0.409	1.949	3.7	1.516	3.2
9/10/2000	3:07 PM	0.3	0.087	0.444	1.911	2.9	1.555	2.4
9/10/2000	3:07 PM	0.24	0.07	0.379	1.965	1.4	1.551	0.9
9/10/2000	3:07 PM	0.4	0.083	0.397	2.035	3.9	1.497	3.4
9/10/2000	3:08 PM	-0.03	0.082	0.33	1.963	3.2	1.633	2.7
9/10/2000	3:08 PM	0.03	0.068	0.409	1.974	2.4	1.644	1.9
9/10/2000	3:08 PM	-0.4	0.064	0.343	2.04	1.9	1.551	1.4
9/10/2000	3:08 PM	0.18	0.073	0.348	2.065	3.2	1.596	2.7
9/10/2000	3:08 PM	0.51	0.08	0.443	2.074	2.3	1.562	1.8
9/10/2000	3:08 PM	0.44	0.069	0.406	2.071	2.2	1.511	1.7
9/10/2000	3:09 PM	0.42	0.087	0.371	2.02	2.9	1.568	2.4
9/10/2000	3:09 PM	0.44	0.093	0.445	2.049	2.2	1.453	1.7
9/10/2000	3:09 PM	0.41	0.122	0.625	2.315	3.6	0.82	3.1
9/10/2000	3:09 PM	0.36	0.124	0.741	2.318	4.8		4.3
9/10/2000	3:09 PM	0.33	0.275	1.615	2.71			
9/10/2000	3:09 PM	0.45			2.128			
THIRD TRANS	ECT					7.4		6.9
						7.9		7.4
9/10/2000	3:10 PM					7.4		6.9
9/10/2000	3:10 PM	2.57				7.8	1.943	7.3
9/10/2000	3:10 PM		0.653	2.523	4.933			5.2
9/10/2000	3:10 PM		0.672		4.735			2.3
9/10/2000	3:10 PM	4.16	0.634	2.097	4.415	0.9	1.476	0.4
9/10/2000	3:10 PM		1.077		5.63	-0.9	1.341	-1.4
9/10/2000	3:11 PM		1.425		6.311	-1.1	1.494	-1.6
9/10/2000	3:11 PM	10.59	2.6	5.653	9.594	-0.4	1.074	-0.9
9/10/2000	3:11 PM		2.117	4.869	8.48	-0.3	1.533	-0.8
9/10/2000	3:11 PM		1.174		5.567			-0.3
9/10/2000	3:11 PM		1.129	2.767	5.429			-0.3
9/10/2000	3:11 PM		0.813		4.094			1
9/10/2000	3:12 PM		0.17		2.027			-0.3
9/10/2000	3:12 PM	1.67	0.297	1.093	2.609	1.5	1.219	1

Date	Time	OPE	%OX	%OX	NOy	NOz	%OX
GPS	GPS	(inst)	no bg cor	norm by	*1.3(byNOx)	by N	loy change
yyyy-mm-dd	hh:mm:ss.			76%			
***Selected Da		1.395349		0.914671205	2.8145		0.7655
FPP Only		1.498638		1.010240035	2.4856		
9/10/2000			72%	0.95			0.783853
9/10/2000			58%	0.76			0.673085
9/10/2000 9/10/2000			77% 73%	1.01 0.96	2.50 2.53		0.820886 0.792185
9/10/2000			75% 76%	1.00			0.792165
9/10/2000			70% 77%	1.00	2.61	214%	0.819455
9/10/2000			75%	0.99	2.58		0.810305
9/10/2000			75% 75%	0.99	2.53		0.80858
9/10/2000			72%	0.95			
9/10/2000			77%	1.02			0.824232
9/10/2000			76%	1.01	2.65		0.81856
9/10/2000			79%	1.04			
9/10/2000			76%	1.00			0.814122
9/10/2000		1.65	80%	1.05	2.65		0.846531
9/10/2000	3:08 PM	1.16	80%	1.05	2.68	226%	0.843174
9/10/2000		0.90	75%	0.98	2.70	217%	0.806023
9/10/2000	3:08 PM	1.69	77%	1.01	2.69	222%	0.823571
9/10/2000	3:08 PM	1.15	77%	1.02	2.63	217%	0.82559
9/10/2000	3:08 PM		74%	0.97		213%	0.798025
9/10/2000			68%	0.89	3.01	226%	0.751786
9/10/2000	3:09 PM	1.17	63%	0.82	3.01	215%	0.712949
9/10/2000			30%	0.40			0.463525
9/10/2000				#VALUE!	2.77	277%	1
9/10/2000							
9/10/2000	3:09 PM						
THIRD TRANS	SECT		#VALUE!	#VALUE!	#VALUE!	#VALUE!	#VALUE!
			#VALUE!	#VALUE!	#VALUE!	#VALUE!	#VALUE!
9/10/2000	3:10 PM	3.93	36%	0.47	6.41	324%	0.504748
9/10/2000			41%	0.54			0.546422
9/10/2000	3:10 PM		38%	0.50			0.524175
9/10/2000			34%	0.45	7.32		0.49187
9/10/2000	3:10 PM		23%	0.31	8.20		0.410675
9/10/2000	3:10 PM		14%	0.18		422%	0.338288
9/10/2000			18%	0.23			0.366292
9/10/2000			19%	0.25	7.24		0.379171
9/10/2000			28%	0.37			0.447979
9/10/2000			25%	0.33			0.42148
9/10/2000			49%	0.64			0.605328
9/10/2000			47%	0.61	3.39		0.590176
9/10/2000			49%	0.18	-0.86		
9/10/2000	3:12 PM	0.82	47%	0.76	-0.63		

Date	Time	NOy	NOz	%OX
GPS	GPS	bg correct	bg correct	bg correct
yyyy-mm-dd	hh:mm:ss.			
***Selected Da		0.31822		
FPP Only		0.06522		
9/10/2000				
9/10/2000				
9/10/2000				
9/10/2000				
9/10/2000				
9/10/2000				
9/10/2000 9/10/2000				
9/10/2000				
9/10/2000				
9/10/2000				
9/10/2000				
9/10/2000				
9/10/2000				
9/10/2000				
9/10/2000				
9/10/2000				
9/10/2000				
9/10/2000				
9/10/2000				
9/10/2000				
9/10/2000				
9/10/2000				#VALUE!
9/10/2000	3:09 PM	-1.84678	-1.84678	1
9/10/2000	3:09 PM	-1.84678	-1.84678	1
		-1.84678	-1.84678	1
THIRD TRANS	SECT	#VALUE!	#VALUE!	#VALUE!
		#VALUE!	#VALUE!	#VALUE!
9/10/2000		3.08622	-0.08978	
9/10/2000				0.033315
9/10/2000		2.56822		
9/10/2000		000	0.00.==	0.016975
9/10/2000				
9/10/2000				
9/10/2000				
9/10/2000			-0.77278	
9/10/2000			-0.31378	
9/10/2000			-0.83178	
9/10/2000				
9/10/2000			-0.62778	
9/10/2000				
9/10/2000	3:12 PM			

Date GPS	Time GPS	Time GPS	Lat	Long	Long Alt		P altitude
yyyy-mm-dd ***Selected Da ***FPP Only***	hh:mm:ss.: ta***	hh:mm:ss.ss ***Selected ***FPP Only	Data***	(deg) ***Selected ***FPP On		(mb) ***Selected ***FPP On	
9/10/2000		•		-96.72082	617		
9/10/2000				-96.71185	610.5		579
9/10/2000				-96.70409	597		579 570
				-96.69968	602.6		
9/10/2000 9/10/2000				-96.69 776	619.4		
				-96.69359	635.2		
9/10/2000 9/10/2000				-96.68531	599.9		
9/10/2000				-96.67622	596.1		
9/10/2000				-96.66612			
9/10/2000				-96.65782	600.9		
9/10/2000				-96.65393	607.3		
9/10/2000				-96.65456	603.9		
9/10/2000			29.99891		590		
9/10/2000				-96.66645	580.5		
9/10/2000				-96.67284	598		
9/10/2000				-96.68533	608.2		582
9/10/2000			30.01228	-96.6957			
9/10/2000				-96.70556	602		
9/10/2000				-96.71474	607.8		
3/10/2000	3.13 T W	20.13.20	30.01000	-30.7 1474	007.0	344.04	300
FOURTH TRA	NSECT		FOURTH 1	RANSECT	FOURTH	TRANSECT	FOURTH T
9/10/2000	3:15 PM	20:15:30	30.01791	-96.72435	615	944.91	585
9/10/2000	3:15 PM	20:15:40	30.01989	-96.73455	595.7	946.88	568
9/10/2000	3:15 PM	20:15:50	30.02219	-96.74558	595.7	945.79	577
9/10/2000	3:16 PM	20:16:00	30.0243	-96.75552	592	946.57	571
9/10/2000	3:16 PM	20:16:10	30.02616	-96.7641	599.9	945.32	582
9/10/2000	3:16 PM	20:16:20	30.02914	-96.77523	604.8	945.28	582
9/10/2000	3:16 PM	20:16:30	30.03275	-96.78521	596.5	946.2	574
9/10/2000	3:16 PM	20:16:40	30.03475	-96.79035	597	944.71	587
9/10/2000	3:16 PM	20:16:50	30.03977	-96.80293	592.3	946.84	568
9/10/2000	3:17 PM	20:17:00	30.04363	-96.81256	585.3	946.09	575
9/10/2000	3:17 PM	20:17:10	30.04763	-96.82249	600.3	944.89	585
9/10/2000	3:17 PM	20:17:20	30.05128	-96.83154	594.2	946.22	574
9/10/2000	3:17 PM	20:17:30	30.05522	-96.84132	585.8	946.77	569
9/10/2000	3:17 PM	20:17:40	30.05842	-96.84935	591.6	946.28	573
9/10/2000		20:17:50	30.0616	-96.85755	591.2	945.45	580
9/10/2000	3:18 PM	20:18:00	30.06655	-96.86992	606.2	945.48	580
9/10/2000	3:18 PM		30.07029	-96.87885	589.9	947.31	564
9/10/2000	3:18 PM	20:18:20	30.07423	-96.88829	587.2	946.64	570

Date GPS	Time GPS	T amb	Theta	Dew Pt	RH	H2O MR	Wind Spee	Wind Dir
yyyy-mm-dd	hh:mm:ss.s	(C)	(C)	(C)	(%)	(g/kg)	(m/s)	(deg)
***Selected Da		***Selected		***Selected		***Selected		***Selectec
FPP Only		***FPP Onl	V***	***FPP Onl	V***	***FPP Onl		***FPP Onl
9/10/2000			32.2		56.8	13.85	•	186.25
9/10/2000			31.8		57.9	13.85		163.9
9/10/2000	3:12 PM		31.9	17.9	57			17.57
9/10/2000	3:12 PM		31.9		57.1	13.74		59.11
9/10/2000	3:13 PM		32.1	17.9	57.1	13.79	1.4	
9/10/2000	3:13 PM	27	31.9	17.9	57.7	13.81	0.5	228.37
9/10/2000	3:13 PM	27	31.9	17.9	57.4	13.78	3.2	228.05
9/10/2000	3:13 PM	27.2	32.1	17.8	56.4	13.68	3.3	230.8
9/10/2000	3:13 PM	27.1	32	17.8	56.9	13.7	3.7	200.51
9/10/2000	3:13 PM	27.1	32	17.8	56.8	13.66	4.2	174.07
9/10/2000	3:14 PM	27.1	32	17.6	56	13.52	4.4	184.04
9/10/2000	3:14 PM	27	31.8	17.8	57.1	13.65	4.1	182.77
9/10/2000	3:14 PM	26.9	31.7	17.6	56.9	13.52	4.6	167.19
9/10/2000	3:14 PM	27	31.9	17.2	55	13.17	4.6	158.33
9/10/2000	3:14 PM		31.8	17.5	56	13.42	4.2	150.49
9/10/2000	3:14 PM	27.1	31.9	17.8	57	13.72	3.9	145.72
9/10/2000	3:15 PM	27.1	32	17.8	56.6	13.66	3.5	139.57
9/10/2000	3:15 PM	27.1	31.9	18	57.4	13.83	4.8	117.18
9/10/2000	3:15 PM	27.2	32.1	18	57.1	13.83	3.4	124.83
FOURTH TRA	NSECT		FOURTH 1	TRANSECT	FOURTH 1	RANSECT	FOURTH 1	RANSECT
9/10/2000	3:15 PM	27.1	32	17.7	56.4	13.57	3.9	149.88
9/10/2000	3:15 PM	27.4	32.1	17.7	55.5	13.56	3.7	158.46
9/10/2000	3:15 PM	27.3	32.1	17.7	55.6	13.56	4.8	133.6
9/10/2000	3:16 PM	27.4	32.1	17.6	55.1	13.47	6.5	149.23
9/10/2000	3:16 PM	27.2	32.1	17.3		13.28	6.1	144.96
9/10/2000	3:16 PM	27.3	32.2	17.3	54.4	13.25	3.9	158.39
9/10/2000	3:16 PM	27.6	32.4		52.6	13.04	4.6	153.66
9/10/2000	3:16 PM	27.4	32.3		53.4		4.9	147.96
9/10/2000	3:16 PM	27.5	32.2		53.2	13.1	4.5	142.83
9/10/2000	3:17 PM	27.5	32.3	17.3	53.9	13.26		159.41
9/10/2000	3:17 PM	27.2	32.1	17.2	54.6	13.19	3.1	164.28
9/10/2000	3:17 PM	27.2	32	17.5	55.1	13.37	4.5	143.28
9/10/2000	3:17 PM		32	17.5	55.2	13.42		134.33
9/10/2000	3:17 PM		31.9		57	13.71	4.3	140.31
9/10/2000	3:17 PM		32.2		56.9	13.88		163.16
9/10/2000	3:18 PM	27.2		18	57	13.86		156.07
9/10/2000	3:18 PM		31.9		56.6	13.73		146.04
9/10/2000	3:18 PM	27.1	31.8	18	57.7	13.87	6	144.7

Date GPS	Time GPS	UV sky	UV gnd	PCASP tot	FSSP total	bap	О3	CO
yyyy-mm-dd ***Selected Da	hh:mm:ss.	: (W/m^2)	(W/m^2)	(cm^-3)	(cm^-3)	(m^-1)	(ppbv)	(ppbv)
FPP Only	•							
9/10/2000	3:12 PM			319.1	0.512	2.86E-06	47.1	124
9/10/2000	3:12 PM			332.8	0.487	2.33E-06	46	
9/10/2000	3:12 PM			348.6	0.488	1.92E-06	46.8	133
9/10/2000			1.2			2.10E-06		
9/10/2000	3:13 PM			312.2	0.504	2.26E-06	45.1	123
9/10/2000				320.7		2.41E-06		132
9/10/2000				335.7		1.86E-06		
9/10/2000				359.9	0.57	1.83E-06	46.1	120
9/10/2000	3:13 PM			311.2	0.561	2.66E-06	45.9	135
9/10/2000	3:13 PM			299.4	0.465	2.25E-06	45.3	131
9/10/2000	3:14 PM			320.8	0.487	1.84E-06	46	154
9/10/2000	3:14 PM			309.2	0.52	1.79E-06	45.4	138
9/10/2000	3:14 PM			334.9	0.472	1.46E-06	46.1	129
9/10/2000	3:14 PM			341.3	0.417	1.30E-06	46.1	155
9/10/2000	3:14 PM	37.8	1.4	332.3	0.529	2.11E-06	46.3	177
9/10/2000	3:14 PM	20.3	1.2	341.3	0.495	3.09E-06	46.1	
9/10/2000	3:15 PM	28.4	1.2	358.9	0.547	2.42E-06	46.3	
9/10/2000	3:15 PM	17	1.1	346.1	0.529	2.39E-06	45.7	
9/10/2000	3:15 PM	17.9	1.5	334.5	0.488	2.15E-06	48.4	
FOURTH TRA	NSECT	FOURTH 7	TRANSECT	FOURTH	TRANSECT	FOURTH TR	ANSECT	
9/10/2000	3:15 PM	35.5	2.1	373.4	0.473	1.86E-06	49.2	
9/10/2000	3:15 PM	38.8	2.1	365.8	0.493	1.99E-06	49.5	
9/10/2000	3:15 PM	38.9	2.2	398	0.492	2.16E-06	48.5	
9/10/2000	3:16 PM	38	2.2	392.9	0.516	1.87E-06	48.5	
9/10/2000	3:16 PM	37.6			0.52	1.88E-06	49.1	
9/10/2000						2.01E-06		
9/10/2000	3:16 PM	37.9			0.479	2.17E-06		
9/10/2000					0.462	2.35E-06		
9/10/2000	3:16 PM				0.476	2.88E-06		
9/10/2000						3.03E-06		
9/10/2000	3:17 PM				0.536	3.23E-06	59.2	131
9/10/2000	3:17 PM				0.619	3.12E-06		
9/10/2000					0.645	2.88E-06		144
9/10/2000	3:17 PM					3.36E-06		
9/10/2000								
9/10/2000						2.65E-06		
9/10/2000					0.537	2.43E-06		
9/10/2000	3:18 PM	24.6	1.6	567.8	0.513	2.69E-06	53.9	153

Date GPS	Time GPS	SO2	NO	NO2	NOy	DelO3 constant	NOz	DelO3 bg by
yyyy-mm-dd	hh:mm:ss.	(vdqq)	(ppbv)	(ppbv)	(ppbv)	bg		transect
***Selected Da		- (1-1)	(1-1-1)	(FF)	(1-1)	4.1	1.505	2.1
FPP Only						4.2		2.2
9/10/2000		0.35	0.117	0.653	1.865			1.4
9/10/2000			0.057		1.555			0.7
9/10/2000			0.031	0.409	1.504			1.3
9/10/2000			0.031	0.419	1.468			1.4
9/10/2000					1.497			1.3
9/10/2000					1.461	2.5		0.5
9/10/2000	3:13 PM					3.8		1.8
9/10/2000						3.4		2.9
9/10/2000	3:13 PM	0.02				3.8		
9/10/2000	3:13 PM	-0.06				3.7	1.516	3.2
9/10/2000			0.028		1.578	2.9	1.555	2.4
9/10/2000	3:14 PM	-0.05				1.4	1.551	0.9
9/10/2000	3:14 PM	-0.12	-0.004		1.48	3.9	1.497	3.4
9/10/2000	3:14 PM	-0.18	0.028	0.37	1.573	3.2	1.633	2.7
9/10/2000	3:14 PM	-0.38	0.052		1.558	2.4	1.644	1.9
9/10/2000	3:14 PM	-0.06	0.073	0.322	1.616	1.9	1.551	1.4
9/10/2000	3:15 PM	-0.09	0.076	0.465	1.726	3.2	1.596	2.7
9/10/2000	3:15 PM	0.01	0.056	0.39	1.727	2.3	1.562	1.8
9/10/2000	3:15 PM	0.13	0.101	0.726	2.016	2.2	1.511	1.7
						2.9		2.4
FOURTH TRA	NSECT					2.2		
						3.6	0.82	3.1
9/10/2000	3:15 PM		0.199	1.006	2.502	4.8		4.3
9/10/2000			0.228					
9/10/2000			0.351	1.403				
9/10/2000			0.6					
9/10/2000			1.222		5.86	7.4		6.9
9/10/2000			1.336		6.441	7.9		7.4
9/10/2000			1.192		6.193			6.9
9/10/2000			1.18		6.301	7.8		7.3
9/10/2000			1.246					5.2
9/10/2000			1.179		6.583			2.3
9/10/2000			0.706		5.465			0.4
9/10/2000			0.658			-0.9		-1.4
9/10/2000			0.754		6.027			-1.6
9/10/2000			0.687		4.823			-0.9
9/10/2000			0.453					-0.8
9/10/2000			0.207		2.561	0.2		-0.3
9/10/2000			0.218	0.85	2.735			-0.3
9/10/2000	3:18 PM	0.99			2.306	1.5	1.219	1

Date	Time	OPE	%OX	%OX			%OX
GPS	GPS	(inst)	no bg cor	norm by	*1.3(byNOx)	by N	oy change
yyyy-mm-dd	hh:mm:ss.s			76%			
***Selected Da		1.395349		0.914671205	2.8145		0.7655
FPP Only	•	1.498638		1.010240035	2.4856		0.821371
9/10/2000			72%	0.95	2.52		0.783853
9/10/2000				0.76	3.21		0.673085
9/10/2000				1.01	2.50		0.820886
9/10/2000				0.96	2.53		0.792185
9/10/2000		0.86		1.00	2.60		0.815878
9/10/2000				1.01	2.61		0.819455
9/10/2000				0.99	2.58		0.810305
9/10/2000		1.98		0.99	2.53		0.80858
9/10/2000				0.95	2.48		0.786258
9/10/2000		2.11	77%	1.02	2.55		0.824232
9/10/2000		1.54		1.01	2.65		0.81856
9/10/2000				1.04	2.55		0.838552
9/10/2000		2.27		1.00	2.57		0.814122
9/10/2000		1.65		1.05	2.65		0.846531
9/10/2000		1.16		1.05	2.68		0.843174
9/10/2000	3:14 PM	0.90		0.98	2.70		0.806023
9/10/2000				1.01	2.69		0.823571
9/10/2000		1.15		1.02	2.63		0.82559
9/10/2000	3:15 PM	1.13		0.97	2.66		0.798025
		1.53		0.89	3.01	226%	0.751786
FOURTH TRA	NSECT	1.17		0.82			0.712949
		3.78	30%	0.40	3.52		0.463525
9/10/2000				#VALUE!	2.77	277%	1
9/10/2000							
9/10/2000							
9/10/2000							
9/10/2000			#VALUE!	#VALUE!	#VALUE!	#VALUE!	#VALUE!
9/10/2000			#VALUE!	#VALUE!	#VALUE!	#VALUE!	#VALUE!
9/10/2000		3.93		0.47			0.504748
9/10/2000	3:16 PM	3.76		0.54	6.16		0.546422
9/10/2000				0.50	5.74		0.524175
9/10/2000	3:17 PM	1.20	34%	0.45	7.32	360%	0.49187
9/10/2000	3:17 PM			0.31	8.20		0.410675
9/10/2000	3:17 PM	-1.04	14%	0.18	12.47	422%	0.338288
9/10/2000				0.23			0.366292
9/10/2000			19%	0.25	7.24		0.379171
9/10/2000		-0.52		0.37	7.06		0.447979
9/10/2000				0.33	5.32		0.42148
9/10/2000		-0.30		0.64	2.64		0.605328
9/10/2000	3:18 PM	0.82	47%	0.61	3.39	200%	0.590176

Date	Time	NOy	NOz	%OX
GPS	GPS	bg correct	bg correct	bg correct
yyyy-mm-dd	hh:mm:ss.s	SS		
Selected Da	ta	0.31822	-0.34178	
FPP Only		0.06522	-0.37878	
9/10/2000	3:12 PM	0.08922	-0.45478	
9/10/2000	3:12 PM	0.62622	-0.42478	
9/10/2000	3:12 PM	0.07722	-0.37078	
9/10/2000	3:12 PM	0.10022	-0.42578	
9/10/2000	3:13 PM	0.15022	-0.32778	
9/10/2000	3:13 PM	0.16422	-0.30778	
9/10/2000	3:13 PM	0.14022	-0.34978	
9/10/2000	3:13 PM	0.10222	-0.38278	
9/10/2000	3:13 PM	0.06422	-0.46678	
9/10/2000	3:13 PM	0.11822	-0.33078	
9/10/2000	3:14 PM	0.18822	-0.29178	
9/10/2000	3:14 PM	0.11622	-0.29578	
9/10/2000	3:14 PM	0.12722	-0.34978	
9/10/2000	3:14 PM	0.19322	-0.21378	
9/10/2000	3:14 PM	0.21822	-0.20278	
9/10/2000	3:14 PM	0.22722	-0.29578	
9/10/2000	3:15 PM	0.22422	-0.25078	
9/10/2000	3:15 PM	0.17322	-0.28478	
9/10/2000	3:15 PM	0.20222	-0.33578	
		0.46822	-0.27878	
FOURTH TRA	NSECT	0.47122	-0.39378	
		0.86322	-1.02678	
9/10/2000	3:15 PM	0.28122	#VALUE!	#VALUE!
9/10/2000	3:15 PM	-1.84678	-1.84678	1
9/10/2000	3:15 PM	-1.84678	-1.84678	1
9/10/2000	3:16 PM	-1.84678	-1.84678	1
9/10/2000	3:16 PM	#VALUE!	#VALUE!	#VALUE!
9/10/2000	3:16 PM	#VALUE!	#VALUE!	#VALUE!
9/10/2000	3:16 PM	3.08622	-0.08978	
9/10/2000	3:16 PM	2.88822	0.09622	0.033315
9/10/2000	3:16 PM	2.56822	-0.16278	
9/10/2000	3:17 PM	3.78322	0.06422	0.016975
9/10/2000	3:17 PM	4.46422	-0.37078	
9/10/2000	3:17 PM	7.74722	-0.50578	
9/10/2000	3:17 PM	6.63322	-0.35278	
9/10/2000	3:17 PM	3.72022	-0.77278	
9/10/2000	3:17 PM	3.58222	-0.31378	
9/10/2000	3:18 PM	2.24722	-0.83178	
9/10/2000	3:18 PM	0.18022	-0.85978	
9/10/2000	3:18 PM	0.76222	-0.62778	
2 0, 2000	2		21320	

Date GPS	Time GPS	Time GPS	Lat	Long	Alt	Static P	P altitude
yyyy-mm-dd ***Selected Da ***FPP Only***	ta***	***Selected Data***		(deg) ***Selected ***FPP On		(mb) ***Selected ***FPP On	
9/10/2000		,		-96.89791	•		•
9/10/2000				-96.90652	590.7 588.6		
9/10/2000				-96.91132			
9/10/2000				-96.91318		945.92	
9/10/2000				-96.90779			
9/10/2000				-96.90028			
9/10/2000				-96.88985			
9/10/2000				-96.88035			
9/10/2000	3:19 PM	20:19:50	30.10754	-96.87239	603.7	944.91	585
FIFTH TRANS	ECT		FIFTH TRA	ANSECT	FIFTH TRA	ANSECT	FIFTH TR/
9/10/2000	3:20 PM	20:20:00	30.10344	-96.86023	605.2	944.54	588
9/10/2000				-96.85112			
9/10/2000			30.0971	-96.84133	596	944.53	589
9/10/2000				-96.83216			581
9/10/2000				-96.82126			561
9/10/2000				-96.81254			
9/10/2000				-96.80189			
9/10/2000				-96.79082		946.17	
9/10/2000				-96.78011	591.3		
9/10/2000				-96.77131	580.6		
9/10/2000				-96.75979			
9/10/2000				-96.74938			
9/10/2000				-96.73833		946.46	
	########					: Hi/Lo UTM	
	########			-96.96119			DELTAX
	########		30.11278	-96.50635	740353	3334195	-43336.95
9/10/2000				-96.72833			575
9/10/2000				-96.71825			572
9/10/2000	3:22 PM	20:22:30	30.09957	-96.70805	596.7	944.41	590
9/10/2000	3:22 PM	20:22:40	30.10057	-96.69875	603.1	946.77	569
9/10/2000	3:22 PM		30.10145	-96.69048	567.7	948.81	551
9/10/2000	3:23 PM	20:23:00	30.0997	-96.67889	591.3	944.04	593
9/10/2000	3:23 PM	20:23:10	30.09424	-96.67102	610.8	945.23	582
9/10/2000	3:23 PM	20:23:20	30.09092	-96.6681	601.4	947.42	563
9/10/2000	3:23 PM	20:23:30	30.0776	-96.66655	585.9	945.4	581
9/10/2000	3:23 PM	20:23:40	30.0702	-96.67134	611.5	943.94	594
9/10/2000	3:23 PM		30.06529	-96.67856		945.05	584
9/10/2000				-96.69008		946.41	572
9/10/2000			30.06189	-96.6999		943.22	
9/10/2000				-96.70964		945.28	
9/10/2000			30.06839	-96.7209		946.64	

Date GPS	Time GPS	T amb	Theta	Dew Pt	RH	H2O MR	Wind Spee	Wind Dir
yyyy-mm-dd	hh:mm:ss.s		(C)	(C)	(%)	(g/kg)	(m/s)	(deg)
Selected Da	ta	***Selected	Data***	***Selected	Data***	***Selected		***Selectec
FPP Only		***FPP Onl	y***	***FPP Onl	y***	***FPP Onl	y***	***FPP Onl
9/10/2000	3:18 PM	27.1	31.9	18	57.5	13.87	6.8	
9/10/2000	3:18 PM	27.3	32	18.1	57.3	13.96	5.9	148.18
9/10/2000					57.2		6.9	
9/10/2000					56.2		7.3	
9/10/2000					56.3		4.9	
9/10/2000					56.9		3.5	
9/10/2000					57.3		3.5	
9/10/2000			32.1		57.6		3	
9/10/2000					56.2		1.2	
FIFTH TRANS			FIFTH TRA		FIFTH TRA		FIFTH TRA	
TII III IIIANO	LOT		111 111 110	ANOLOT	111 111 110	NOLOT	111 111 110	ANOLOT
9/10/2000					56.1	13.66	0.9	
9/10/2000					56		2.7	
9/10/2000	3:20 PM				56.1	13.78	2.2	
9/10/2000	3:20 PM	27.3	32.1	17.6			1.1	172.93
9/10/2000	3:20 PM				53.8		2.6	217.79
9/10/2000	3:20 PM	27.4	32.4	17.7	55.5	13.65	0.9	208.59
9/10/2000	3:21 PM	27.5	32.3	17.5	54.6	13.45	2.4	195.02
9/10/2000	3:21 PM	27.7	32.5	17.5	53.9	13.41	2.1	213.38
9/10/2000	3:21 PM	27.6	32.3	17.4	53.8	13.34	3.3	216.22
9/10/2000	3:21 PM	27.6	32.3	17.6	54.5	13.45	2.4	222.06
9/10/2000	3:21 PM	27.4	32.3	17.7	55.3	13.56	3.9	200.91
9/10/2000	3:21 PM	27.5	32.3	17.7	55.2	13.62	5.2	204.53
9/10/2000	3:22 PM	27.7	32.4	17.5	53.9	13.39	3.3	199.48
	########							
	########							
		-29001.72	52.15	km across	the stinkin i	olume		
9/10/2000					54.3		3	
9/10/2000					54.6		2.7	
9/10/2000	3:22 PM			17.7	54.8	13.65	4.1	199.27
9/10/2000					55			
9/10/2000	3:22 PM	27.9			53.5		2.4	228.19
9/10/2000	3:23 PM	27.7	32.7	17.6	54.3	13.53	1.6	221.82
9/10/2000			32.3		54.9	13.52	0.4	201.23
9/10/2000	3:23 PM	27.5	32.2	17.7	55.2	13.58	1.4	18.65
9/10/2000	3:23 PM	27.6	32.5	17.7	54.6	13.57	2	51.92
9/10/2000	3:23 PM	27.4	32.3	17.5	54.9	13.44	2.3	135.98
9/10/2000	3:23 PM	27.4	32.3	17.3	53.9	13.26	4.5	140.7
9/10/2000	3:24 PM	27.6	32.3	17.5	54.1	13.38	3.5	134.7
9/10/2000	3:24 PM	27.7	32.7	17.6	54.2	13.5	4	149.13
9/10/2000	3:24 PM	27.4			54.3	13.27	4.2	155.14
9/10/2000	3:24 PM	27.5	32.3	17.3	53.5	13.19	4.8	142.88

Date GPS	Time GPS	UV sky	UV gnd	PCASP tot	FSSP total	bap	O3	CO
yyyy-mm-dd ***Selected Da	hh:mm:ss.	: (W/m^2)	(W/m^2)	(cm^-3)	(cm^-3)	(m^-1)	(ppbv)	(ppbv)
FPP Only								
9/10/2000	3:18 PM	22.1	1.5	565.3	0.558	2.65E-06	53	128
9/10/2000	3:18 PM		1.0	568.7	0.55	2.54E-06	52.8	
9/10/2000				567.2	0.586	2.70E-06	52.6	
9/10/2000	3:19 PM			573.6	0.487	2.46E-06	53.7	
9/10/2000				518.7	0.594	2.79E-06	53.2	
9/10/2000	3:19 PM			571.4	0.516	2.86E-06	52.1	
9/10/2000				491.8	0.527	3.12E-06	53.2	
9/10/2000			1.6	541.1	0.533	3.00E-06		
9/10/2000			1.1	605.3	0.529	2.22E-06	55.1	
3/10/2000	J. 13 1 W	10.5	1.1	000.5	0.323	2.22L-00	55.1	
FIFTH TRANS	ECT	FIFTH TRA	ANSECT	FIFTH TRA	ANSECT	FIFTH TRAN	SECT	
9/10/2000	3:20 PM	16	1.1	607.6	0.502	2.14E-06	56.3	
9/10/2000	3:20 PM		1.2		0.518	2.60E-06	58.1	
9/10/2000	3:20 PM			559	0.510	2.00E-00 2.94E-06	59.2	
9/10/2000	3:20 PM		1.4		0.577	1.99E-06	60.4	
9/10/2000	3:20 PM		1.4	751.7	0.506	2.39E-06	59.4	
9/10/2000	3:20 PM		1.7		0.541	2.84E-06	58.3	
9/10/2000			2		0.341	2.04E-06	56.3	
9/10/2000	3:21 PM		1.9	529		2.04E-06 2.33E-06	56.2	
9/10/2000						2.74E-06		
9/10/2000	3:21 PM		1.9		0.507	2.74L-00 2.33E-06		
9/10/2000			1.8		0.553	2.33E-06 2.83E-06		
9/10/2000	3:21 PM		1.0	_	0.533	2.63E-06 2.44E-06		
9/10/2000					0.524	2.44L-06 2.00E-06	49.3	
9/10/2000	J.ZZ FIVI	33.2	1.7	390.9	0.513	2.00E-00	49	
	########							
	########							
	########							
	""""""""							
9/10/2000	3:22 PM	39.6	1.9	391.2	0.458	1.98E-06	48.1	
9/10/2000			1.9	393.6	0.538	2.62E-06	49.1	
9/10/2000	3:22 PM		1.9		0.468	2.56E-06	47	126
9/10/2000	3:22 PM		2.2		0.559	2.51E-06	47.1	151
9/10/2000	3:22 PM			400.3	0.475	1.91E-06	47.3	
9/10/2000				317	0.537	2.20E-06	46.3	
9/10/2000	3:23 PM			388.6	0.484	2.17E-06	46.5	
9/10/2000				374	0.497	2.09E-06	46.4	_
9/10/2000	3:23 PM			323.8	0.539	2.00E-06	48	
9/10/2000	3:23 PM			347.1	0.412	2.08E-06	48.5	
9/10/2000	3:23 PM			359.3	0.472	2.13E-06	47.9	
9/10/2000	3:24 PM			379.5	0.47	1.96E-06	47.8	
9/10/2000	3:24 PM			307.7	0.499	2.56E-06	48.3	
9/10/2000	3:24 PM		1.8		0.436	2.00E-06	48.3	
9/10/2000	3:24 PM	38.2			0.430	1.92E-06	49.3	
S, 13, 2000	O.L IVI	55.Z	1.0	000.1	0.112		.0.0	.50

Date GPS	Time GPS	SO2	NO	NO2	NOy	DelO3 constant	NOz	DelO3 bg by
yyyy-mm-dd ***Selected Da	hh:mm:ss.	(ppbv)	(ppbv)	(ppbv)	(ppbv)	bg		transect
FPP Only								
9/10/2000	3:18 PM	0.5				5		3
9/10/2000	3:18 PM			0.719	2.225			2.8
9/10/2000	3:18 PM				2.159			2.6
9/10/2000	3:19 PM				2.24			2.7
9/10/2000	3:19 PM				2.191			2.2
9/10/2000	3:19 PM				2.118		1.448	1.1
9/10/2000	3:19 PM				2.314		_	2.2
9/10/2000	3:19 PM				2.378			3.2
9/10/2000	3:19 PM			0.700	2.712		1.170	4.1
		0.7			2.7.12	• • • • • • • • • • • • • • • • • • • •		
FIFTH TRANS	ECI							
9/10/2000	3:20 PM	1.15				8.3		5.3
9/10/2000	3:20 PM	2.14				10.1		7.1
9/10/2000	3:20 PM	3.34				11.2		8.2
9/10/2000	3:20 PM	4.45	0.33		4.98	12.4		9.4
9/10/2000	3:20 PM	5.58	0.497	2.48	5.482	11.4	2.505	8.4
9/10/2000	3:20 PM	6.17	0.743	2.908	5.995	10.3	2.344	7.3
9/10/2000	3:21 PM	6.3	0.797	2.724	5.753	8.3	2.232	5.3
9/10/2000	3:21 PM	4.96	0.653	2.186	4.921	8.2	2.082	5.2
9/10/2000	3:21 PM	4.85	0.737	2.316	4.869	5.5	1.816	2.5
9/10/2000	3:21 PM	4.21	0.629	2.139	4.595	5.2	1.827	2.2
9/10/2000	3:21 PM	3.27	0.359	1.605	3.48	4.6	1.516	1.6
9/10/2000	3:21 PM	2.41	0.225	1.038	2.738	1.5	1.475	-1.5
9/10/2000	3:22 PM	0.96	0.084	0.595	1.856	1	1.177	-2
	########							
	########							
	########							
9/10/2000	3:22 PM	0.38	0.079	0.48	1.673	0.1	1.114	-2.9
9/10/2000	3:22 PM	0.19	0.106	0.442	1.717		1.169	-1.9
9/10/2000	3:22 PM	0.15			1.848	-1		-4
9/10/2000	3:22 PM					-0.9		-3.9
9/10/2000	3:22 PM	0.56	0.062		1.587	-0.7	1.09	-3.7
9/10/2000	3:23 PM	0.07	0.073	0.399	1.53	-1.7	1.058	-4.7
9/10/2000	3:23 PM	-0.01	0.054	0.478	1.561	-1.5	1.029	-5.5
9/10/2000	3:23 PM	0.29	0.056	0.436	1.499	-1.6	1.007	-5.6
9/10/2000	3:23 PM	0.18	0.086	0.444	1.538	0	1.008	-4
9/10/2000	3:23 PM			0.425	1.497	0.5		-3.5
9/10/2000	3:23 PM	0.29	0.066	0.501	1.47	-0.1	0.903	-4.1
9/10/2000	3:24 PM	0.47			1.513	-0.2	0.923	-4.2
9/10/2000	3:24 PM				1.628			-3.7
9/10/2000	3:24 PM				1.512			-3.7
9/10/2000	3:24 PM	0.11	0.1	0.519	1.745	1.3	1.126	-2.7

Date GPS	Time GPS	OPE (inst)	%OX no bg cor	%OX norm by	NOy *1.3(byNOx)	NOz	%OX loy change
yyyy-mm-dd	hh:mm:ss.s		no by cor	76%	1.5(by140x)	Dy I	oy change
Selected Data							
***FPP Only**							
9/10/2000		#DIV/0!	#VALUE!	#VALUE!	#VALUE!	#VALUE!	
9/10/2000		1.98	64%				
9/10/2000		1.94	62%				
9/10/2000		1.90	63%				
9/10/2000		1.57	64%				
9/10/2000 9/10/2000		0.76 1.50	68% 63%				
9/10/2000		2.17	62%				
9/10/2000		#DIV/0!	02 /6	0.28		#VALUE!	
3/10/2000) 3.131 W	#DIV/0:	#DIV/0!	-2.66			
FIFTH TRANS	SECT		#DIV/0!	-2.66			
111 111 110/1140	DEOT		#DIV/0!	-2.66			
9/10/2000	3:20 PM	#DIV/0!	#VALUE!	#VALUE!	#VALUE!	#VALUE!	
9/10/2000		#DIV/0!	#VALUE!	#VALUE!	#VALUE!	#VALUE!	
9/10/2000		#DIV/0!	#VALUE!	#VALUE!	#VALUE!	#VALUE!	
9/10/2000		#DIV/0!		2.98	_	#VALUE!	
9/10/2000		3.35	46%		_		
9/10/2000		3.11	39%				
9/10/2000		2.37	39%				
9/10/2000		2.50	42%				
9/10/2000		1.38	37%				
9/10/2000	3:21 PM	1.20	40%				
9/10/2000	3:21 PM	1.06	44%	1.48	-0.48		
9/10/2000	3:21 PM	-1.02	54%	0.74	-0.53		
9/10/2000	3:22 PM	-1.70	63%	-0.14	-0.82		
			45%	-2.66	-2.66	100%	
	########		#DIV/0!	-2.66			
	########		#DIV/0!	-2.66			
	########		#DIV/0!	-2.66			
_ , ,			#DIV/0!	-2.66			
9/10/2000		-2.60	67%				
9/10/2000		-1.63	68%				
9/10/2000		#DIV/0!	#\ /A	-0.81		#VALUE!	
9/10/2000		#DIV/0!	#VALUE!	#VALUE!	#VALUE!	#VALUE!	
9/10/2000		-3.39	69%				
9/10/2000		-4.44	69%				
9/10/2000		-5.34 5.56	66%				
9/10/2000 9/10/2000		-5.56 -3.97	67% 66%				
9/10/2000		-3.52	66%				
9/10/2000		-3.52 -4.54	61%				
9/10/2000		-4.55	61%				
9/10/2000		-3.63	63%				
9/10/2000		-3.95	62%				
9/10/2000		-2.40	65%				
2, . 3, 2300	2.2		2370	5.02			

```
Date
                       NOy
                                  NOz
                                            %OX
             Time
GPS
             GPS
                       bg correct bg correct
             hh:mm:ss.ss
yyyy-mm-dd
***Selected Data***
***FPP Only***
    9/10/2000
               3:18 PM
    9/10/2000
               3:18 PM
    9/10/2000
               3:18 PM
               3:19 PM
    9/10/2000
    9/10/2000
               3:19 PM
    9/10/2000
               3:19 PM
    9/10/2000
               3:19 PM
    9/10/2000
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    9/10/2000
               3:19 PM
FIFTH TRANSECT
    9/10/2000
               3:20 PM
    9/10/2000
               3:21 PM
    9/10/2000
               3:21 PM
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               3:21 PM
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               3:21 PM
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               3:21 PM
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               3:22 PM
              ########
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    9/10/2000
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               3:23 PM
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    9/10/2000
               3:24 PM
    9/10/2000
               3:24 PM
    9/10/2000
               3:24 PM
```

Table B-1. Locations and Distances of G-1 Transects From FPP (based on flight

data taken 9/10/2000 during TEXAQS).

Item	Latitude Latitude	Longitude	UTMx (m)	UTMy (m)	Distance
	(degrees)	(degrees)		-	from FPP
					(m)
FPP	N 29.9122	W 96.759026	3315000	137000	-
Transect 1	N 29.928033	W 96.741468	3316401	137933.2	1,680
Transect 2	N 29.979657	W 96.784684	3322370	134670.4	7,700
Transect 3	N 29.995393	W 96.790433	3324134	134262.6	9,540
Transect 4	N 30.039766	W 96.802925	3329096	133220.3	14,590
Transect 5	N 30.090113	W 96.801886	3334677	133506.4	19,980
Transect 6	N 30.216853	W 96.848711	3350153	129054.9	36,040

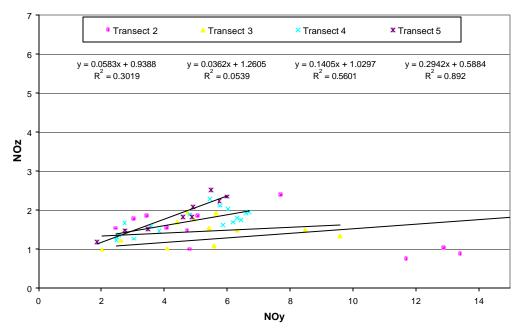


Figure B-1. Correlation of NOz and NOy for FPP G-1 Data 09/10/2000.

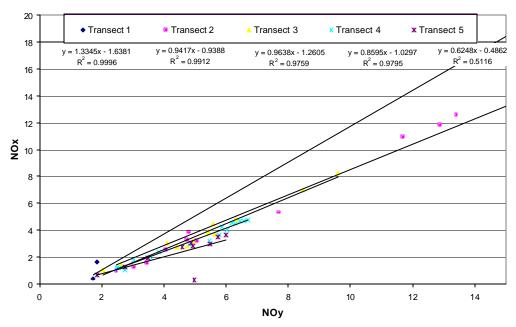


Figure B-2. Correlation of NOx and NOy for FPP G-1 Data 09/10/2000.

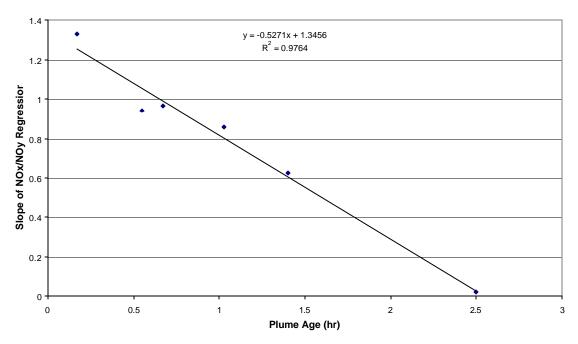


Figure B-3. Cumulative Loss of NOx in FPP Plume (G-1 Data 09/10/2000).

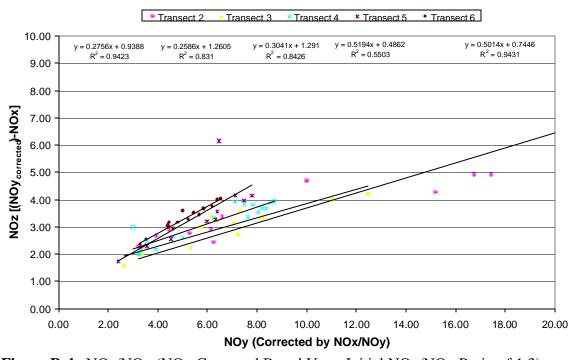


Figure B-4. NOz/NOy (NOy Corrected Based Upon Initial NOx/NOy Ratio of 1.3)

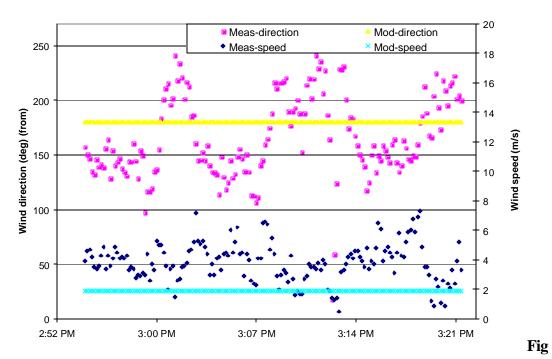


Figure B-5. Wind Speed and Trajectory Comparison for July 9, 1995 (Mod) and FPP G-1 Data 09/10/2000 (Meas).

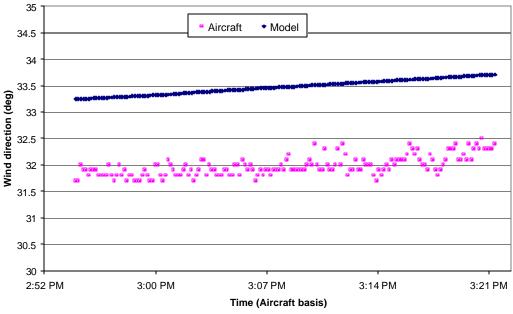
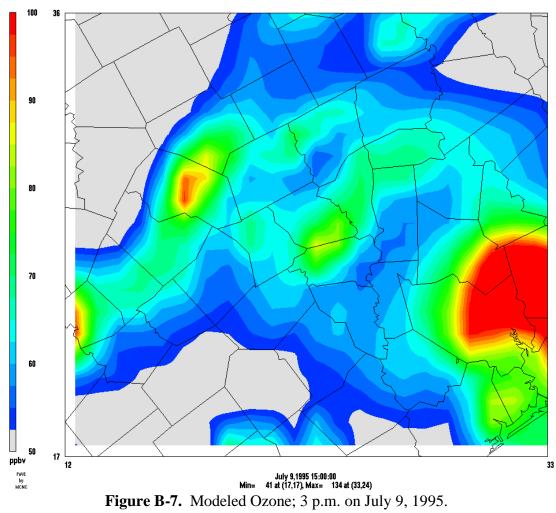


Figure B-6. Temperature Comparison near FPP (July 9, 1995, and FPP G-1 Data 09/10/2000).



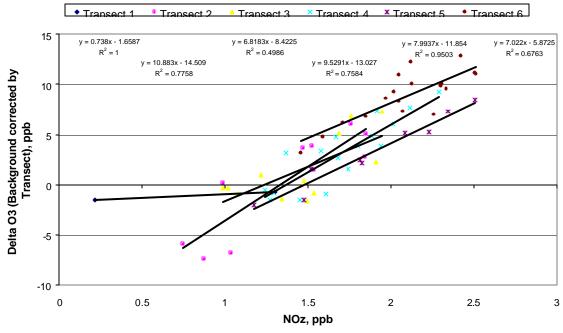


Figure B-8. OPE by Transect for FPP Data Collected 09/10/2000.

APPENDIX C: Diurnal Sensitivity Figures and Spreadsheet Data

Methods for Temporal Sensitivity Modeling

- 1. Find the time-resolved emission rate for the source of interest.
 - use ptsumpig.f, reference a CAMx-ready point source emission file to print out data
- 2. Determine how you wish to normalize the emissions, and create a spreadsheet which will calculate factors to change the emission rates in the CAMx-ready point source file to the normalized value. The spreadsheet "factor.generator.xls" is available on disk; the only requirement for the factor file is that it be text tab delimited.
- 3. Compile and run ptmodpig.f to create a new emissions file, using the factor file you have created. Save the file under a name in your directory.
- 4. Change a CAMx runscript to reference the new point source file.
- 5. Rename the runscript so that it reflects the goal of the run (i.e., cpssafull implies full, normalized emissions for the <u>City Public Service plant in San Antonio.</u>)
- 6. Run CAMx. (at the prompt, nohup ./[runscript name])
- 7. You will need to create the following runs:
 - Normalized, full emissions case.
 - Half of the above emissions rate.
 - Emissions increase back to full for 2-hr periods

- 8. The data from these runs can be analyzed by compiling and running psettemp.f (C-shell runscripts for various timeslots are available on disk)
- 9. The output of psettemp.f should be compiled into a spreadsheet, such as the ones included on disk (psettemp.xls, psettemp3pm.xls, and psettemp5pm.xls). This spreadsheet allows generation of impact assessments.
 - Bar charts, as in Chapter IV
 - Spatial analysis, as in Figure 4-7. Generated using Arcview.
- 10. Additional comparison of modeled output to aircraft data: use the On-Off CAMx runs; process the data using pset.f, and send the output to a file such as pset_all3good.xls, included on disk.
- 11. Plot the O₃ vs the NOz that is reported in the output of pset.f, the slope is the OPE of the source. Other analysis can be done to correlate OPE with Plume Chemical Age.
- 12. If wishing to compare the data to aircraft data from the base case, simply run aircomp.f. This program assigns O₃ and NOz to UTM coordinates. These concentrations can then be compared to aircraft data taken at similar points in space using Golden Surfer software.

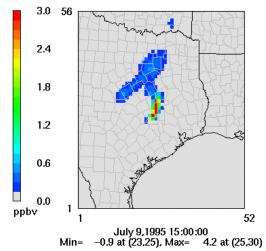


Figure C-1. 24-hour Ozone Puff at 3pm on Day 3 due to 100% Emissions Increase from Base Case (Base Case = 50% Reduction per SB7).

Layer 1 (O3h-O3b)*1000

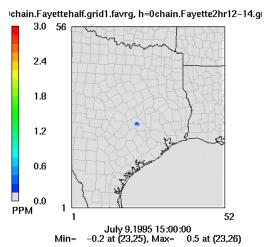


Figure C-2. Noon-2pm Ozone Puff at 3pm on Day 3 due to 100% Emissions Increase from Base Case (Base Case = 50% Reduction per SB7).

Layer 1 (O3f-O3b)*1000

-0chain.Fayettehalf.grid1.favrg, f=0chain.Fayette2hr2-4.grid1.favrg, f=0chain.Fayette2hr2-4.grid1.favr

Figure C-3. 2am-4am Ozone Puff at 3pm on Day 3 due to 100% Emissions Increase from Base Case (Base Case = 50% Reduction per SB7).

Layer 1 (O3i-O3b)*1000

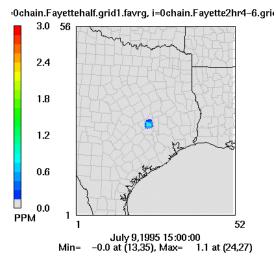


Figure C-4. 4am-6am Ozone Puff at 3pm on Day 3 due to 100% Emissions Increase from Base Case (Base Case = 50% Reduction per SB7).

Layer 1 (O3j-O3b)*1000

0.chain.Fayettehalf.grid1.favrg, j=0chain.Fayette2hr8-10.gri
3.0 56
2.4
1.8
1.2
0.6
PPM
0.0
1
1
52
July 9,1995 15:00:00
Min= -0.0 at (23,25), Max= 0.6 at (24,27)

Figure C-5. 8am-10am Ozone Puff at 3pm on Day 3 due to 100% Emissions Increase from Base Case (Base Case = 50% Reduction per SB7).

psettemp	2nm						
	les Ozone in Plur	me			Fraction of	Total	
TOTAL IVIO	Day 3		Day 5	Day 6	1 raction of		Day 4
12-14	-22125.854	-31688.8	-10698.1	-31898.44	12-14	-1%	-1%
16-18	0	0	8181.991	59024.797	16-18	0%	0%
19-21	127723.547	_	117896.21	363930.81	19-21	4%	0%
22-24	456987.156			388757.78	22-24	16%	1%
0-2		228319.16		339160.88	0-2	8%	7%
2-4		275073.94		180931	2-4	5%	8%
4-6		228481.89			4-6	4%	7%
8-10		114911.58		161807.88	8-10	2%	3%
24hr	2861797.521			4517669.8	24hr	100%	100%
Moles O3	3 formed per Mol		IOx emitted		Emission F	Rate (tons/hr)
	Day 3	Day 4	Day 5	Day 6	Day 2	Day 3	Day 4
12-14	-0.93808716	-0.844957	-0.263731	-0.779334	1.603669	0.839542	1.334924
16-18	0		0.2181664	1.4550853	1.603669	0.839542	1.334924
19-21	2.834925755	0.2283088	3.1436109	8.9716591	1.603669	0.839542	1.334924
22-24	10.14319355	2.1729851	3.0214667	9.5836961	1.603669	0.839542	1.334924
0-2	9.713544061	6.0879529	6.8020478	8.2862836	1.603669	0.839542	1.334924
2-4	6.486982005				1.603669	0.839542	1.334924
4-6	4.410457862	6.0922921	3.9235926	6.5894243	1.603669	0.839542	1.334924
8-10	2.363130188		4.9583148		1.603669	0.839542	1.334924
24hr	7.330971175	9.0979421	7.9546962	9.2322592	1.603669	0.839542	1.334924
					**Emission	Rate is 85.5	5%NO, 14.5
OPE in Plume				Emission F	Rate (moles/l	or)	
OI L III I	Day 3	Day 4	Day 5	Day 6	Day 2		Day 4
12-14	-5	-3.9	-4.21	0.262	45053.58		37503.44
16-18	0	0.0	0	1.27	45053.58		37503.44
19-21	2.32	4.12	19	6.96	45053.58		37503.44
22-24	7.24	4.12	6.7	8.39	45053.58		37503.44
0-2	8.76	6.91	12.87	4.53	45053.58		37503.44
2-4	2.58	8.25	7.54	3.31	45053.58		
4-6	2.514	7.5	4.91	3.28	45053.58		
8-10	2.28	2.53	1.95	1.86	45053.58		37503.44
24hr	2.17	3.54	3.49	3.2	10000.00	20000.14	07000.11
		0.01	0.10	0.2			
OPE in P	lume						
	Day 3	Day 4	Day 5	Day 6			
12-14	-0.11062927	-0.123586	-0.045039	-0.008357			
16-18	0	0	0	0.0749615			
19-21	0.296318629	0.0221859	2.240028	2.5329585			
22-24	3.308587009	0.2111596	0.7592131	3.2616778			
0-2	2.0069598	1.5776854	3.5511113	1.5363988			
2-4	0.394747376	2.26936	2.3712412	0.5988816			
4-6	0.261520539						
8-10	0.127080627	0.2907263	0.3922065	0.3009626			
24hr	6.210100621	12.253198	13.08886	14.456543			
**OPEs a	are the slopes of	the o3/hno3	plots for the	ir respective days.			
***		ODE -1-4- /					

**Slopes were taken from OPE plots (contained in this worksheet)

For Sinusoid Graph

Day 5	Da	ay 6		Day 3	Day 4	Day 5	Day 6
	0%	-1%	12-14	-0.938087	-0.844957	-0.263731	-0.779334
	0%	1%	16-18	0	0	0.218166	1.455085
	3%	8%	19-21	2.834926	0.228309	3.143611	8.971659
	3%	9%	22-24	10.14319	2.172985	3.021467	9.583696
	7%	8%	0-2	9.713544	6.087953	6.802048	8.286284
	8%	4%	2-4	6.486982	7.334633	7.752795	4.420456
	4%	6%	4-6	4.410458	6.092292	3.923593	6.589424
	5%	4%	8-10	2.36313	3.064028	4.958315	3.953245
10	00%	100%	24hr	7.330971	9.097942	7.954696	9.232259

Day 5	Day 6
1.443882	1.456906
1.443882	1.456906
1.443882	1.456906
1.443882	1.456906
1.443882	1.456906
1.443882	1.456906
1.443882	1.456906
1.443882	1.456906
1.443882	1.456906
%NO2 for a	ll days

Day 5	Day 6
40564.49	40930.4
40564.49	40930.4
40564.49	40930.4
40564.49	40930.4
40564.49	40930.4
40564.49	40930.4
40564.49	40930.4
40564.49	40930.4

Puff posit	tion (defined by max	O3)					
MaxO3 Gridcell		Data For	Surfer				
	Day	3		T			
12-14			12-14	X Y		O3(mol)	OPE
Day 3	0.213	1532	Day 3	15	32	-22125.85	-5
Day 4	0	0	Day 4	0	0	-31688.8	
Day 5	0.213	2327	Day 5	23	27	-10698.1	-4.21
Day 6	0.156	1827	Day 6	18	27	-31898.44	0.262
16-18			16-18				
Day 3	0 n/a		Day 3	0	0	0	
Day 4	0 n/a		Day 4	0	0	0	
Day 5	0.223	2226	Day 5	22	26	8181.991	0
Day 6	0.617	1726	Day 6	17	26	59024.8	1.27
19-21			22-24				
Day 3	0.899	2333	Day 3	23	33	127723.5	
Day 4	0.656	3231	Day 4	32	31	5384.922	4.12
Day 5	0.986	3028	Day 5	30	28	117896.2	
Day 6	3.456	1826	Day 6	18	26	363930.8	6.96
22-24			22-24				
Day 3	3.735	2530	Day 3	25	30	456987.2	7.24
Day 4	0.648	3330	Day 4	33	30	51252.33	4.12
Day 5	1.038	3228	Day 5	32	28	113315.4	6.7
Day 6	1.424	2628	Day 6	26	28	388757.8	8.39
0-2			0-2				
Day 3	2.167	2528	Day 3	25	28	229105	8.76
Day 4	1.171	3129	Day 4	31	29	228319.2	6.91
Day 5	1.72	3027	Day 5	30	27	275921.6	12.87
Day 6	1.518	2627	Day 6	26	27	339160.9	4.53
2-4			2-4				
Day 3	1.676	2427	Day 3	24	27	153002.9	2.58
Day 4	1.721	3028	Day 4	30	28	275073.9	8.25
Day 5	1.652	3027	Day 5	30	27	314488.2	7.54
Day 6	1.022	2526	Day 6	25	26	180931	3.31
4-6			4-6				
Day 3	1.39	2427	Day 3	24	27	104025.7	2.514
Day 4	1.57	2827	Day 4	28	27	228481.9	7.5
Day 5	0.864	2826	Day 5	28	26	159158.5	4.91
Day 6	2.207	2526	Day 6	25	26	269707.8	3.28
8-10			4-6				
Day 3	0.885	2326	Day 3	23	26	Day 3	0
Day 4	1.418	2526	Day 4	25	26	Day 4	0
Day 5	1.823	2525	Day 5	25	25	Day 5	0
Day 6	1.438	2326	Day 6	23	26	Day 6	0
24hr			24hr				
Day 3	4.145	2529	Day 3	25	29	238483.1	2.17
Day 4	2.695	2827	Day 4	28	27	288446.3	
Day 5	4.171	3027	Day 5	30	27	312532.5	
Day 6	4.393	1826	Day 6	18	26		

In UTM (for Arcview):							
12-14	Х	,	Υ		MAXO3	OPE	
Day 3		44		3472	-22125.85		-5
Day 4		0		0	0		0
Day 5		172		3392	-10698.1		-4.21
Day 6		92		3392	-31898.44		0.262
16-18	Χ	,	Υ		MAXO3	OPE	
Day 3		0		0	0		0
Day 4		0		0	0		0
Day 5		156		3376	8181.991		0
Day 6		76		3376	59024.8		1.27
22-24	X	,	Υ		MAXO3	OPE	
Day 3		172		3488	127723.5		2.32
Day 4		316		3456	5384.922		4.12
Day 5		284		3408	117896.2		19
Day 6		92		3376	363930.8		6.96
22-24	Χ	,	Υ		MAXO3	OPE	
Day 3		204		3440	456987.2		7.24
Day 4		332		3440	51252.33		4.12
Day 5		316		3408	113315.4		6.7
Day 6		220		3408	388757.8		8.39
0-2	Χ		Y		MAXO3	-	
Day 3		204		3408			8.76
Day 4		300		3424	228319.2		6.91
Day 5		284			275921.6		12.87
Day 6		220		3392			4.53
2-4	Χ		Y		MAXO3	OPE	
Day 3		188		3392			2.58
Day 4		284		3408			8.25
Day 5		284		3392			7.54
Day 6	.,	204	. ,	3376	180931		3.31
4-6	X		Y	0000	MAXO3		
Day 3		188		3392			2.514
Day 4		252		3392			7.5
Day 5		252		3376			4.91
Day 6	V	204	.,	3376			3.28
4-6 D0	Х		Y	0070	MAXO3	OPE	0
-					-		0
-					-		0 0
-					-		
	V		~	33/6	•	ODE	0
	^		I	3/12/		OPE	
-							
Day 3 Day 4 Day 5 Day 6 24hr Day 3 Day 4 Day 5 Day 6	х	172 204 204 172	Y	3376 3360	Day 3 Day 4 Day 5 Day 6 MAXO3 238483.1 288446.3 312532.5	OPE	(

APPENDIX D: Episode Base Case Tables and Figures.

- D1-D6. Fayette Power Project Emission Rates (Pre- and Post-Normalized)
- **D7-D12.** Maximum Ozone Concentration by Day (Spatial Plots).
- D13-D18. Maximum Ozone Contribution of Fayette Power Project by
 Day

Figure D-1. Actual (top) and Normalized (bottom) Emission Rate for the Fayette Power Project (July 7, 1995).

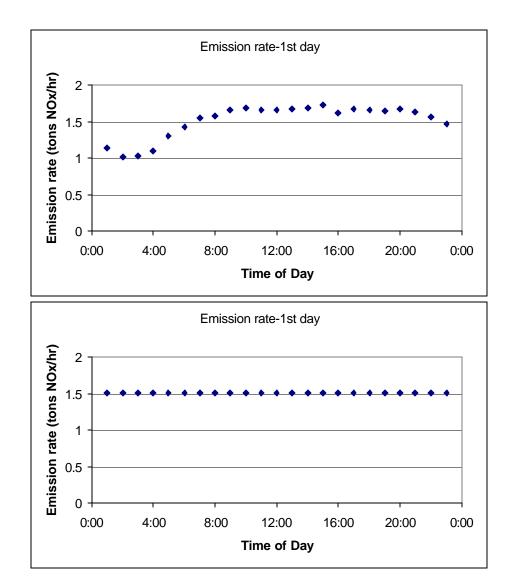


Figure D-2. Actual (top) and Normalized (bottom) Emission Rate for the Fayette Power Project (July 8, 1995).

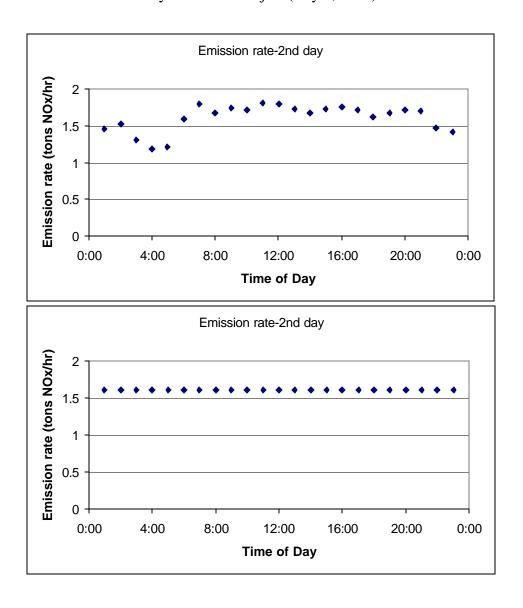


Figure D-3. Actual (top) and Normalized (bottom) Emission Rate for the Fayette Power Project (July 9, 1995).

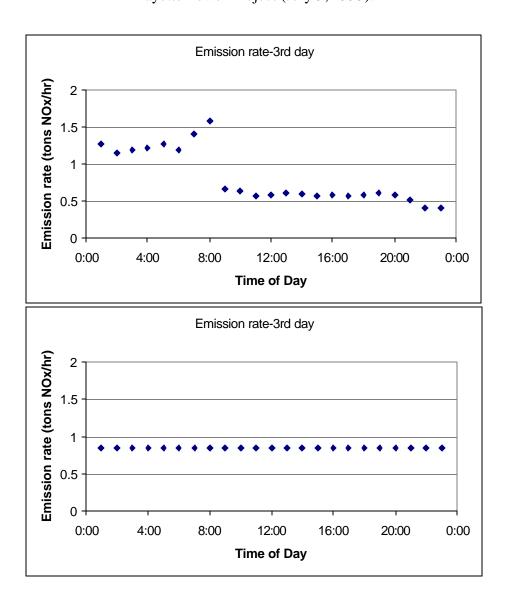


Figure D-4. Actual (top) and Normalized (bottom) Emission Rate for the Fayette Power Project (July 10, 1995).

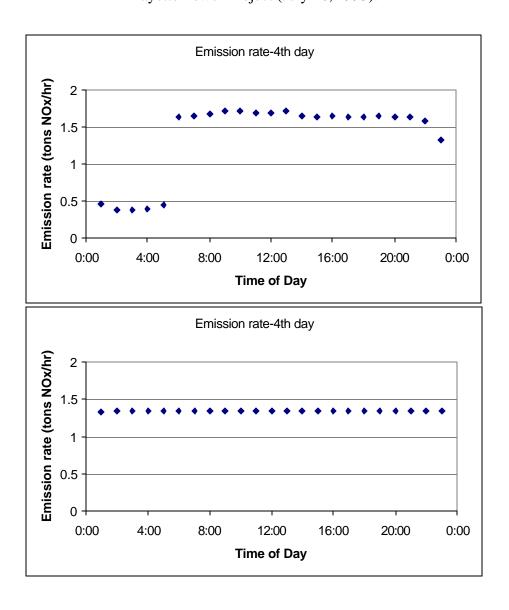


Figure D-5. Actual (top) and Normalized (bottom) Emission Rate for the Fayette Power Project (July 11, 1995).

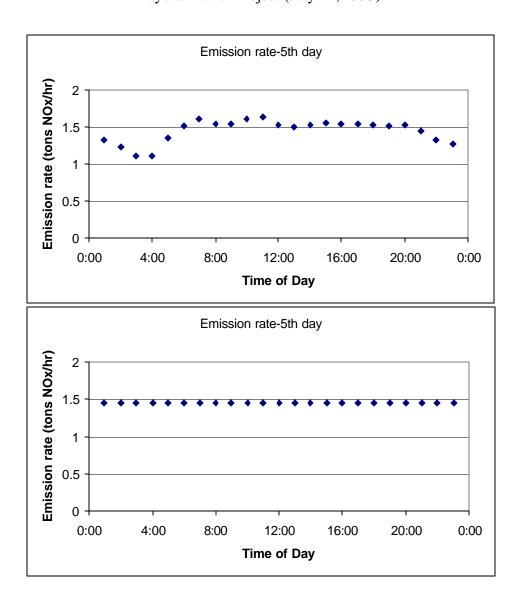
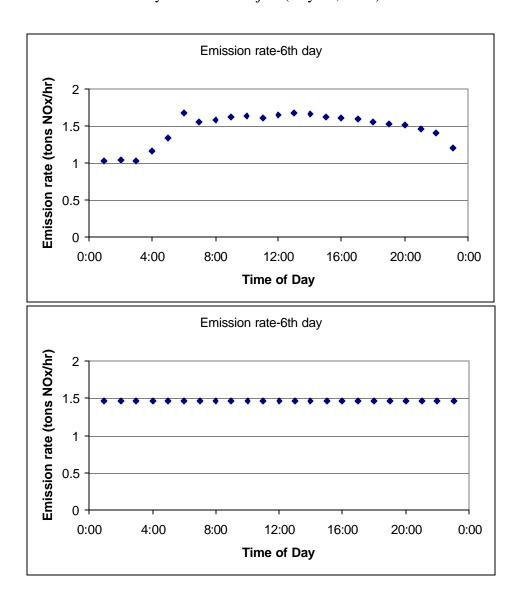
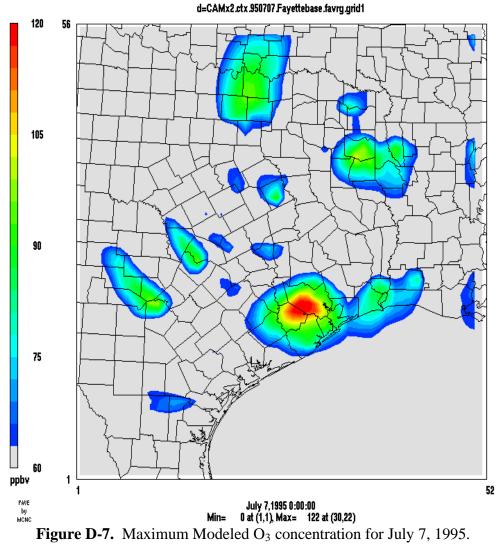
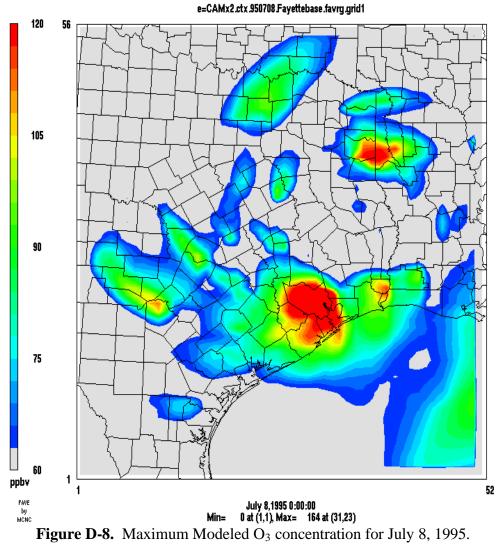
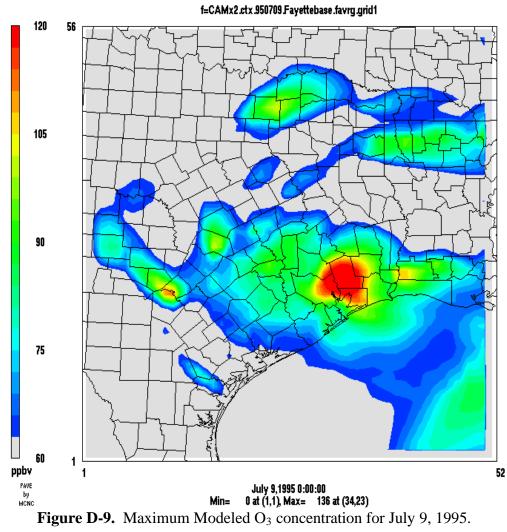


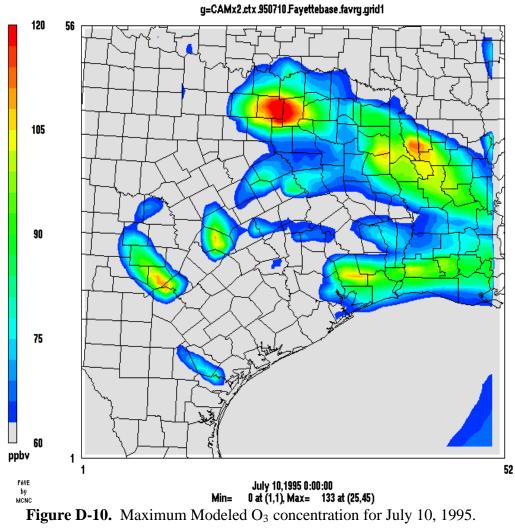
Figure D-6. Actual (top) and Normalized (bottom) Emission Rate for the Fayette Power Project (July 12, 1995).

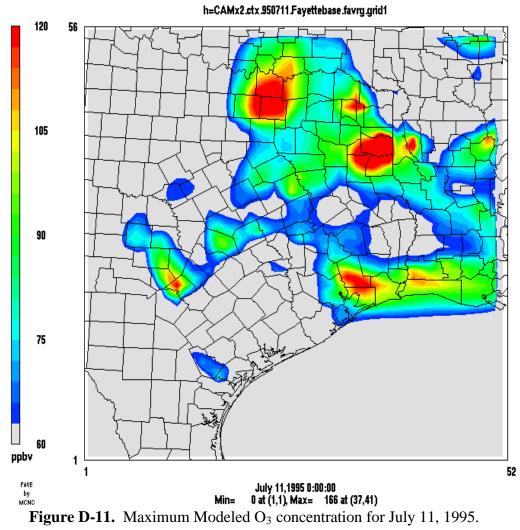


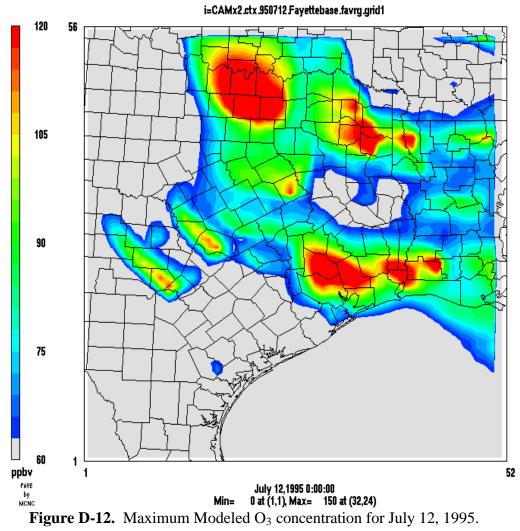












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VITA

Dyron Thomas Hamlin was born in Richmond, Virginia on August 31, 1976, the son of Thomas Richard Hamlin and Cheryl Jeanne Stanton Hamlin. He attended Ruby F. Carver Elementary, Harry F. Byrd Middle, and Mills E. Godwin High Schools, living all the while at 11603 Lothbury Lane, 23233. On June 30, 1994, shortly after graduating from high school with the fourth-highest grade point average in a class of 347, Dyron packed his new Saturn SL sedan with all of his earthly belongings and bid farewell to his parents and sisters, Carmen Leah Hamlin and Shannon Hamlin. The destination, North Little Rock, Arkansas, was reached late that 30th day of June, 1994. His life would change drastically over the next year, for exactly one year later came the eve of his marriage to Marria Lane Fitzgerald, of North Little Rock, Arkansas. By July 1, 1995, at 6:30 p.m., Dyron had achieved marital status, and sophomore status at the University of Arkansas in Fayetteville. After one year in the freshman dorm, Yocum Hall, Dyron ventured into the off-campus world with his new bride, choosing Leverett Gardens, at 2100 N. Leverett, Apartment #5 in Fayetteville as his new dwelling place. It was a cozy one-bedroom apartment which suited the newlyweds just fine for the next year. September of 1996 witnessed another major event in the life of Dyron: purchase of his and Marria's first home. A cute bungalow in need of repair, the house was ideally located for the couple's activities. At 216 Conner, 72701 in Fayetteville, the house was just steps from downtown Fayetteville, and a mere 6minute bike ride for Dyron to class at the University of Arkansas. participated in the cooperative education program by accepting a position at Molex, Inc., in Maumelle, Arkansas for the spring and summer sessions of 1997. He graduated in December, 1998, with a 3.78 grade point average and magna cum laude honors. He accepted continuing, full-time employment with Bio-Tech Pharmacal, Inc. as a quality control and research and development chemist. In May of 1999, he discovered a local job more suited to his training as a chemical engineer, and joined Bioengineering Resources, Inc. As a pilot plant engineer, he supervised and maintained a novel biotechnological process and performed process changes and analysis. During his employment, he and Marria celebrated the birth of their first child, a beautiful son, Asher Dyron Hamlin, on October 6, 1999. In his desire for continued education, Dyron chose The University of Texas at Austin over Cornell University, and entered The Graduate School in August of 2000.

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