Abstract

PAGANO, LARA ELIZABETH. A Comparative Study Between FLEXPART-WRF and HYSPLIT in an Operational Setting: Analysis of Fire Emissions Across Complex Geography Using WRF. (Under the direction of Ryan P. Boyles).

Transport and dispersion models are frequently used by the meteorological community to understand and predict the trajectories of anthropogenic, natural and accidental chemical releases of hazardous materials. There are several reputable dispersion models that can handle a wide range of applications under the direction of global, synoptic or mesoscale forecasts. One such application is the forecast of smoke emissions from wildfires which is important to operational air quality and meteorology communities.

Fire emissions have direct impacts to property and respiratory health. Operational meteorologists are responsible for providing meteorological support to emergency management agencies within their county warning area in the event of incidents involving harmful chemical releases, radiation and smoke emissions. A comparative study between two dispersion models during recent wildfire events across complex geography is presented to identify the sensitivities of each dispersion model and the operational benefits of utilizing each model for smoke emission forecasts.

FLEXPART-WRF is a Lagrangian dispersion model that predicts the transport and dispersion of trace gases forward or backward from a point, line or area source. Similar to FLEXPART-WRF, the HYbrid Single Particle Integrated Trajectory (HYSPLIT) model simulates the dispersive nature of the environment. Model configuration differences include the prerequisite meteorological data, density correction, dispersion algorithms and removal calculations.

Mesoscale meteorological models are needed to provide the ambient environment as well as simulate the small scale flux exchanges and boundary layer processes that can affect dispersion
simulations on a local and regional scale. Therefore, both dispersion models are using meteorological input from the WRF ARW mesoscale atmospheric model using both a 12 km and 4 km grid-resolution domain.

Two fire events, one along the coast of the Mid-Atlantic (Evans Road Case) and the other within the Appalachians (South Mountain Case), are investigated for this analysis. Simulations are analyzed to identify the relative performance of each dispersion model given identical meteorological input. The dispersion models are evaluated for accurate dispersive simulations and also on their ability to support operational forecast needs. Satellite observations provided by the National Environmental Satellite, Data and Information Service along with other remote sensing tools are used for evaluation of dispersion model performance.

The spatial analysis, based on both case studies and resolutions, indicates that HYSPLIT disperses particles 10-20 degrees to the right of FLEXPART-WRF for at least a portion of the simulations. FLEXPART-WRF better replicates the observed plume and also yields a higher air concentration throughout most of the simulations, especially downwind. These differences in plume compositions and concentrations are likely linked to the differing diffusion equations. While the air concentration differences are small compared to the amount being released, the spatial differences are statistically significant. To account for the air concentration differences, dry deposition is analyzed. HYSPLIT sporadically deposited significantly more mass to the ground compared to FLEXPART-WRF. These deposition differences impact the diffusion process and account for only part of the concentration variations. This study suggests that FLEXPART-WRF performs better compared to HYSPLIT and may serve as an improved operational tool.
A Comparative Study Between FLEXPART-WRF and HYSPLIT in an Operational Setting: Analysis of Fire Emissions Across Complex Geography Using WRF

by
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Lara Pagano was born in Queen, NY on March 26, 1986. She is the daughter of Anthony and Ruth Pagano of Charlotte, NC. She has one sister, Leslie Pagano. Lara attended Weddington High School, graduating in May, 2004. Following high school, Lara enrolled in the Marine, Earth and Atmospheric Science (MEAS) Department at North Carolina State University. While attending classes and working towards a Bachelor of Science in Meteorology, she worked part-time as a researcher and within several Intern positions. Lara received two fellowships under the Department of Energy (DOE) Global Climate Education Program (GCEP) allowing her to Intern at Brookhaven National Laboratory. As the Chief Broadcast Meteorologist at Carolina Week in UNC, Lara was exposed to the media side of Meteorology. This enabled her to gain an Internship position at CBS in Charlotte, NC working under the direction of Eric Thomas.

Lara spent 2 years working for the University as an undergraduate research assistant with topics ranging from hurricanes to radar analysis. After a Student Internship at the NWS, Lara finally found her place in the Meteorological Community. In May of 2005, she graduated from NCSU with a Bachelor of Science Degree in Meteorology.

Following graduation, Lara began her Master’s Degree at North Carolina State University under the guidance of Dr. Ryan Boyles. During this time, Lara also received the Student Career Experience Program (SCEP) Fellowship at the NWS in Raleigh, NC.
I would like to first thank my Advisor, Ryan Boyles, for taking me on as his first graduate student. Ryan has been very patient during my hectic schedule. Between the responsibilities of school, work and conducting graduate research, Ryan, who also has many responsibilities, made time to provide worthy and sound advice throughout my graduate career. I would also like to acknowledge my committee members, Sethu Raman, Helena Mitasova and Hugh Devine. Each member provided me with their specialized knowledge that allowed me to produce a detailed analysis. My thanks also go out to the staff and students at the State Climate Office, especially my lab mates (Heather, Adrienne and John). Without their relentless support, I would not be where I am today.

To my parents, Tony and Ruth Pagano, who have always supported my interest in Meteorology. Without their encouragement and constant love, an achievement such as this would be both far less attainable and far less joyful to celebrate. You both have motivated me in so many ways. I can never thank you enough. To my beautiful sister Leslie, you have always been such a blessing in my life with your moral support and positive outlook; thank you.

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Chapter 1

Introduction

Atmospheric transport and dispersion models are used by the Environmental Protection Agency (EPA) and operational forecasters such as the National Weather Service in collaboration with emergency managers and researchers in an effort to utilize and advance simulations of pollutant plumes. The typical responsibilities surrounding operational agencies during accidental or 'terrorist-caused' hazardous releases are to provide site specific meteorological conditions and atmospheric transport and dispersion information to emergency managers and the public. Since hazardous material entering the atmosphere can pose a threat to life and property, accurately forecasting the transport and dispersion of particles is of vital importance.

During a local pollution episode, operational forecasters rely on internal expertise, meteorological observations and forecast dispersion simulations to provide guidance to local, state, and national agencies. The first generation of dispersion models used available weather observing networks to provide an estimate of atmospheric flow and stability. Unfortunately, the spatial and temporal resolution of input data was much too coarse to provide meaningful results (Pack et al., 1978; Artz et al., 1985). Later, global scale meteorological models were used as input for dispersion simulations of long range transport. When using global scale models, mesoscale features tend to be neglected leading to inaccurate depictions of dispersion at smaller scales (Pielke, 2002). Therefore, use of a regional meteorological model to provide accurate atmospheric forcings is better suited for simulating
dispersion under complex terrain and meteorological conditions.

There are two types of dispersion models that describe the basic structure of flow and diffusion: Eulerian and Lagrangian. An Eulerian model is commonly used to describe flow at a given point either within a fixed or moving frame of reference (Arya, 1999). Since Eulerian models use discrete grids and equations, these are often times more diffusive than the original equations themselves. Therefore, in Eulerian simulations the tracer released will instantaneously mix within a grid box which is not realistic (Stohl et al., 2005). Lagrangian models are independent of a computational grid and have in principle, infinitesimally small resolution (Stohl et al., 2005). A Lagrangian dispersion model follows the flow which is transported by mean wind and turbulence (Arya, 1999). Hence, a Lagrangian dispersion model would best replicate the characteristics of the atmosphere during plume simulations.

1.1 Objectives

North Carolina (NC) has over one million acres of forests that are continually being monitored and protected by the Division of Forest Resources. Wildfires are not uncommon in this region, with over 26,000 acres burned per year on average (NCDENR, 2009). Fires within NC are typically initiated by human activity (60%). However, from a suppression perspective, lightning ignited wildfires can pose serious issues, especially in remote locations where longer response time occurs (Flannigan, 2000). No matter what the cause, fires emit many volatile chemicals into the atmosphere that can be harmful to health, reduce visibility and alter the local scale atmosphere (Spichtinger et al., 2001; Mott et al., 2002). Wildfire case studies observed across NC are used to evaluate dispersion models. Other hazardous release types could have also been used for this study, but smoke plumes are more visible via satellite.

NC has complex topography and weather that create dynamic weather. Within the state, the topography is defined by the mountains, foothills, piedmont, sandhills and coastal plain. These regions have different elevations and land use producing dynamic flow regimes. Figure 1.1 illustrates the complex terrain along the Appalachians with elevation in excess of 2000 meters across western
The topography transitions into rolling hills across central NC with the coastal plain abutting the complex shoreline along the Atlantic Ocean. The challenging terrain and coastline allows a robust evaluation of dispersion modeling tools and the meteorological data on which it relies.

The focus of this study is to compare two Lagrangian dispersion models that are used to forecast pollutant plumes: Hybrid Single Particle Lagrangian Integrated Trajectory (HYSPLIT) and Flexible Particle (FLEXPART-WRF). Little research has been conducted comparing the two models which are based on meteorology forecast provided by the Weather Research and Forecasting (WRF) Advanced Research model. Application of these two models is similar, but currently the HYSPLIT model is widely used in an operational setting while FLEXPART is used mostly for research applications. Another goal of this research is to determine if the FLEXPART-WRF model can be compatible, reliable and versatile as an operational tool. The objectives of this study are:

1. Identification of the physics, limitations and assumptions of each model in order to attain the most reliable and advanced dispersion simulations for smoke management and emergency response,
2. Identification of model applications and sensitivities,
3. Evaluation of existing dispersion models using past events with remote sensing technologies,
4. Identification of key parameters that influence the individual model performance,
5. Suggestions for future improvement of the model components.

1.2 The Planetary Boundary Layer

The planetary boundary layer (PBL) is the closest part of the atmosphere that interacts directly with the earth’s surface. The stress and friction posed by the rough surface creates turbulence within this layer that dictates the depth of dispersion. Usually the distribution and local maxima of ground-level particle concentration is proportional to the depth of the PBL, also called the mixing height (Arya, 1999). It is important to understand the physical properties embedded within the PBL that can affect transport and dispersion of pollutants (Stull, 1988; Arya, 1999). In this section the physics, characteristics and impacts of the PBL are reviewed.
1.2.1 Mechanically Forced PBL circulations

Mesoscale circulations can be thermally and/or mechanically induced. Mechanically forced flows interact with hills, valleys and mountains which can exist over all atmospheric scales (Arya, 1999). The PBL can often go through separation over complex topography, but the extent depends on the obstacle size and atmospheric stability. When the upstream boundary layer flow is deep and unstable, wakes on the lee side of large hills and valleys can form (Figure 1.2). Wake cavities can lead to pollutants being trapped and recirculating close to the land surface. Unfortunately, these features are not always accurately depicted by the dispersion models due to resolution constraints. Therefore, these factors need to be taken into account when analyzing dispersion model output.

1.2.2 Thermally Forced PBL Circulation

Due to differences in heat capacity of various land surfaces, air above each land surface heats and cools at different rates. These differences produce horizontal variations in atmospheric pressure and create circulations that are, due to differential heating, thermally induced. Sea and land breezes are examples of thermally induced circulations. During the night, the warmer water in contact with the cooler land creates horizontal density stratification inducing an offshore breeze, often referred to as a land breeze (Figure 1.3). During the day, the land gets warmer than the ocean creating the sea breeze. Mountains undergo similar mesoscale thermal circulations. Valley breezes form during the day as the slopes of the mountains warm allowing the air to rise (Figure 1.4). Conversely, mountain breezes form during the night as the slopes cool and air sinks. Under weak synoptic forcing, thermally induced mesoscale circulations will determine pollutant dispersion patterns.

1.2.3 Wind and Temperature Distribution

Wind and temperature fields explicitly dictate the diffusion, direction and speed of pollutant transport from a near ground release. The factors defining the wind field profile are the large scale pressure and temperature gradients, surface friction, earth’s rotation, horizontal and vertical advection and convective processes (Arya, 1999). The overall direction of wind in the PBL column is driven directly by the synoptic pattern and modified by the mesoscale flow. The vertical tempera-
ture profile helps determine the height of pollutant mixture (PBL height). There are many plume structures that can set up due to wind and temperature profiles which can affect the air and ground level concentration (referenced in section 1.2.4). Diurnal fluctuations of the PBL are linked to wind and temperature variations. As the heating of the day progresses the stability of the atmosphere generally decreases. Instability increases vertical mixing and turbulent flow forcing the PBL to grow vertically. Nocturnal surface cooling forces the PBL to contract in response to stability and decreasing turbulent motion (Figure 1.6). In summary, the height of the PBL is determined by the magnitude of turbulence which is forced by thermal and mechanical circulations.

1.2.4 Dispersion

Dispersion is influenced by the atmospheric turbulent processes found within the PBL. Unlike molecular diffusion, particles that release into the atmosphere will diffuse in different directions and at different speeds. Over time pollutants generally become normally distributed, also referred to as a Gaussian distribution (bell curve), and are then diluted within the atmosphere. However, the Gaussian dispersion model assumes a uniform flow with homogeneous turbulence, which is not always valid within the PBL. Like previously mentioned, particles are influenced heavily by the turbulence. There are three types of atmospheric turbulence: 1. Mechanical 2. Shear 3. Buoyant. Mechanical turbulence is very similar to the mechanical circulations that set up within the PBL. Shear turbulence is produced by horizontal wind shifts with height. Buoyant turbulence relates to the thermal circulations that are found within the PBL. Thermal circulations (turbulence) can be dictated by the stability (buoyancy) of the air. This process can occur during an explosion, fire or diurnal heating. Stability is the degree to which the atmosphere will support, tolerate or suppress turbulent motions (COMET, 2008). There are five classic plume types that are influenced by the stability of the atmosphere (Figure 1.6):

1. Fanning: plumes which typically occur during very calm and stable nocturnal conditions. The strong stability and low lapse rate limits the amount of vertical turbulence and dispersion. Normally winds are calm at night allowing little horizontal spread. Occasionally the winds can be variable leading a wider horizontal spread.
2. Fumigation: plumes that occur right after sunrise as the PBL height rises to the nocturnal lapse rate. Initially the plume is ‘Fanning’ but as the PBL height rises to the pollutant height the particles mix down to the surface. This process can lead to high concentrations away from the source.

3. Looping: plumes that occur primarily during the afternoon hours at the peak of convective eruptions. Updrafts and downdrafts within the PBL will lead the plume to loft and subside, respectively.

4. Lofting: plumes that occurs after sunset as the nocturnal stable layer forms under the daytime unstable layer. The plume which was initially within the unstable layer will get trapped aloft as the stable layer will prevent downward diffusion.

5. Conning: plumes that undergo neutral stability conditions commonly associated with cloudy, windy conditions. The plume is able to grow vertically and advect horizontally leading to a cone like shape.

Turbulent dispersion can be measured by the standard deviation of horizontal ($\sigma_u, \sigma_v$) and vertical ($\sigma_w$) wind fluctuations. A way to estimate turbulent diffusion is to calculate friction velocity following

$$\rho u_*^2 = \rho L_z^2 \left( \frac{D u}{D z} \right)^2 = \rho (u'w')$$

(1.1)

where $u_*$ is the friction velocity, $z$ is the reference height, $\rho$ is the air density, $u$ is the mean horizontal wind speed, $L_z$ is the mixing length, $w'$ is the vertical eddy velocity and $u'$ is the horizontal eddy velocity. Eq. 1.1 can be used to predict the wind profile within the PBL according to the log wind profile

$$u(z) = \frac{u_*}{k} \ln \left( \frac{z}{z_o} \right)$$

(1.2)

where $k$ is the Von Karman constant (0.40) and $z_o$ is the surface roughness parameter. The friction velocity relies on the horizontal shear with height and the mixing height.
Plume rise is an important factor when trying to determine the dispersion of air pollution. Since wind profiles deviate with height, sometimes significantly, it is critical to know the height at which the plume will start to disperse horizontally. Plume rise is proportional to the ejection velocity and buoyancy while inversely proportional to wind speed and stability. When the plume temperature ($T_p$) is warmer than the ambient air ($T_a$) it will continue to rise until it reaches the equilibrium level ($T_p = T_a$). Light winds will allow the plume to keep its form whereas strong winds will lead to high entrainment and mixing rates. Smoke plumes typically don’t have an ejection velocity, but do undergo thermal rise (COMET, 2008).

1.3 Mesoscale Meteorological Model

A mesoscale meteorological model is used in this analysis as the input for the dispersion models. The Numerical Weather Prediction (NWP) meteorological model used in this study is the WRF model. The WRF package includes initiation routines, data assimilation and physic schemes with numerical and dynamical options. There are two dynamic solvers within the WRF package: Advanced Research WRF (ARW) for research settings and Non-hydrostatic Mesoscale Model (NMM) for default operational mode. Within this study, the ARW solver developed by the National Center for Atmospheric Research (NCAR) is used (Skamarock et al., 2008). More detail regarding the WRF framework is presented in this section.

1.3.1 Governing Equations

Each dispersion model requires different meteorological inputs. Most dispersive models need the typical wind components, temperature ($T$), humidity ($q$), pressure ($P$) and height ($z$) variables in order to drive the simulation properly. Other important parameters may be required for 2D and 3D fields depending on the dispersion model. The required inputs for HYSPLIT is provided in Chapter 2 and for FLEXPART-WRF in Chapter 3. Initial conditions are used to aid in calculation of variables at later time steps. The governing equations used to calculate characteristics of the atmosphere can either be adapted to a hydrostatic or non-hydrostatic model of the atmosphere.
The non-hydrostatic approximation can resolve the mesoscale features that are typically important to dispersion models and is used within this study (Skamarock et al., 2008). When trying to solve for a turbulent atmosphere, the set of governing equations can not be solved due to a closure problem; the number of unknown variables within the set of equations is larger than the known (Kraichnan, 1961). In order to resolve this issue, the unknown terms must be parameterized based on the known quantities and parameters. Following the common practice across most mesoscale models, variables \( U \) are split into the mean state \( u \) and small scale perturbations \( u' \):

\[
U = u + u'.
\] (1.3)

The variable perturbations are then placed into the governing equations, linearized and solved. Both the explicit and parameterized variables are output by the WRF model and ingested into the dispersion models. The variable values can be altered based on the parametrization scheme chosen. A review of the different schemes used within this analysis is provided in the next section.

1.3.2 Model Physical Schemes

There are many physical options within the WRF that can be easily modified for specific application purposes. These physical options are categorized as microphysics, cumulus parametrization, planetary boundary layer, land surface model and radiation (Skamarock et al., 2008). The main focus will be on the physics that drive and impact the dispersion models.

1.3.2.1 Convective Scheme

Cumulus parametrization is typically used within NWP models to resolve convective clouds at a sub-grid scale as a function of the larger scale synoptic pattern. There are several cumulus parametrization schemes with different trigger mechanisms for precipitation development. Since convection was not widely present within this study, the default Kain-Fritsch (K-F) scheme was used. The K-F scheme (Kain and Fritsch, 1990; Kain, 2004) is a mass flux system dependent on the amount of convective available potential energy (CAPE) and downdrafts in the atmosphere.
Once the precipitation is initialized, a cloud model is introduced that replicates the thermodynamic processes of microphysics, detrainment and entrainment (Skamarock et al., 2008). This process will affect the precipitation production process.

1.3.2.2 PBL Scheme

Sources of air pollution are usually released within the PBL. The atmospheric flow within the PBL will dictate the dispersion rate and direction. Therefore, the choice of PBL scheme can dramatically affect the dispersion concentration and plume pattern (Peffers and Fuelburg, 2009; Challa et al., 2008). The Mellor-Yamada-Janic (MYJ) scheme (Janjic, 1990; Mellor and Yamada, 1982) uses the turbulent kinetic energy (TKE) to describe the flow based on the stability of the surrounding atmosphere. According to a sensitivity study conducted by Challa et al. (2008), the MYJ performed well across a coastal region. Hence, the MJY scheme was chosen for simulations conducted over the coastal plain in this study. A study conducted by Olson and Brown (2009) compared the newer Mellor-Yamada-Nakanishi-Niino (MYNN) scheme to the original MJY across complex terrain. The MYNN is also a TKE based scheme that is integrated into the WRF ARW version 3.1. This scheme may potentially reduce the common biases associated with the MJY scheme over complex terrain, such as shallow PBL height (Olson and Brown, 2009). The results reported by Olson and Brown (2009) indicated that the MYNN performed well compared to the MJY. The MYNN had larger TKE and mixing lengths affecting the overall PBL depth. MJY underpredicted these values which can lead to concentrations being altered at the surface and in the air (Olson and Brown, 2009). Similarly, a study by Peffers and Fuelburg (2009) suggests that MYJ also illustrated lower than observed PBL heights over complex terrain. Therefore, the MYNN PBL scheme is used for simulations conducted across the complex terrain of the Appalachians. Microscale motions and processes also occur in the PBL. To incorporate these processes, the PBL scheme relies on the calculations from the surface layer and land-surface schemes. While using these two (MYJ and MYNN) schemes, the surface Eta similarity theory and NOAH land-surface scheme are used and described in section of 1.3.2.3 and 1.3.2.4.
1.3.2.3 Surface Layer Scheme

The surface layer is the layer closest to the earth’s surface within the PBL. Turbulence flows are produced by the underlying rough surface and aid in the transformation of momentum, energy and heat exchange inside this layer. Within these schemes, friction velocities and exchange coefficients are calculated which are used by the land-surface and PBL schemes for further parametrization. The similarity theory scheme introduced by Paulson (1970) uses the Charnock relation to capture correlations within the surface layer (Dyer and Hicks, 1970; Webb, 1970; Beljaars, 1995). The Eta Similarity Theory (Janjic, 2002; Monin and Obukhov, 1954) is used within the WRF 3.1 configuration to parameterize the viscous sub-layer. Instead of using the explicit Charnock relation, the scheme uses the Obukhov length which is a measure of the length where shear effects are significant. The ratio between the surface layer height (z) and the Obukhov length (L) is a measure of the buoyancy verses shear effects. Surface fluxes can be calculated from these relations, but only the Mellor-Yamada PBL schemes use these relationships.

1.3.2.4 Land Surface Scheme

It has been illustrated by Fast and Easter (2006c) that land-surface models, when altered, can affect the dispersive nature of pollutants. This conclusion seems reasonable since the scheme integrates all the physic parameterization categories within the WRF in order to calculate surface fluxes over both land and sea. The schemes take into account the soil type and vegetation canopy effects in order to correctly approximate surface fluxes. The NOAH land-surface scheme (Chen and Dudhia, 2001) used within WRF 3.1 has a four layer soil temperature and moisture model with canopy and snow cover prediction. Like most models, the scheme provides sensible and latent heat fluxes.

1.3.2.5 Configuration WRF ARW 3.1

Other physic schemes within the WRF hold less of an impact on the dispersion simulations and are beyond the scope of this study. However, these should be noted since they are within the WRF framework (Skamarock et al., 2008). To ensure the atmospheric dynamics are accurately predicted, the schemes chosen for the WRF ARW configuration are:
1. WSM5 microphysic (Hong et al., 2004; Hong and Lim, 2006)
2. Rapid Radiative Transfer Model (RRTM) longwave radiation (Mlawer et al., 1997)
3. MM5 shortwave radiation (Dudhia, 1989)
4. K-F Convective scheme (Kain and Fritsch, 1990)
5. Eta similarity theory (Janjic, 2002)
6. NOAH Land-Surface (Chen and Dudhia, 2001)

More detailed information regarding the scheme features is provided by Skamarock et al. (2008).
Figure 1.1: 2D Elevation map of NC. The Appalachians along the west, foothills and piedmont in the central part of the state and the coastal plain along eastern NC.
Figure 1.2: Flow over an obstacle forming a wake cavity (a) and the mean velocity profile around the obstacle (b) (Arya, 1999).
Figure 1.3: Plumes being influenced by sea (left panel) and land (right panel) breezes (Arya, 1999).

Figure 1.4: Valley Breeze (a) and Mountain Breeze (b) (Arya, 1999).
Figure 1.5: Diurnal evolution of the planetary boundary layer over land (Wyngaard, 1992).
Figure 1.6: Schematic of the five classic plume types (Arya, 1999).
Chapter 2

HYSPLIT

2.1 Overview

The HYSPLIT model was introduced by the Air Resources Laboratory (ARL) of the U.S. National Oceanic and Atmospheric Administration (NOAA) and Australian Bureau of Meteorology in 1979 for trajectory and dispersion simulations using rawinsonde observations (Draxler and Taylor, 1982). HYSPLIT is maintained by NOAA’s ARL and is run routinely under experimental and operational mode by the National Weather Service’s (NWS) National Center for Environmental Prediction (NCEP). HYSPLIT has capabilities ranging from simple trajectory to complex dispersion and deposition calculations for both puffs and particles. HYSPLIT can simulate dispersion based on input variables (wind, temperature, pressure, etc.) from various meteorological models. These fields are then integrated both in space and time to the particles position in order to simulate the dispersive nature of the atmosphere.

Since its inception, HYSPLIT has transformed in many ways to simulate the dispersion within the atmosphere. As research and computer capacity have increased so too have the capabilities of HYSPLIT simulations. The first version of HYSPLIT had a uniform mixing height throughout the day with no mixing at night although, the mixing height has a known diurnal fluctuation (Stull, 1988). Therefore, this characteristic was adjusted in later versions. Also, within the first
version, only rawinsonde data was used as the meteorological input data, which is both spatially and temporally coarse. HYSPLIT version 2.0 introduced and demonstrated continuous vertical diffusivity and version 3.0 added the capabilities to support meteorological gridded fields. By the fourth version of HYSPLIT multiple gridded meteorological inputs were available with a combination particle-puff dispersion capability (Draxler and Hess, 1997, 1998). An ensemble capability was one of the first improvements made after the fourth version of HYSPLIT. This ensemble option was created to alleviate the dispersion sensitivity and create more representative results (Draxler, 2003). An ensemble option allowed HYSPLIT to generate multiple simulations from a single meteorological data base (Draxler, 2003). The newest revision of HYSPLIT (4.9) was introduced in February of 2009 with computation and graphical advancements. A new feature within this version is the advection algorithm. This feature includes temporal interpolation and an added option which considers puff dispersion in the horizontal and particle dispersion in the vertical. HYSPLIT also includes many processes for pollutant plume removal and alteration. The various equations that calculate vertical dispersion have been revised due to recent research. The initial horizontal dispersion was previously constant, but is now calculated based on the divergence of the wind field (Draxler, 2006). Additional detail regarding the applications, limitations and code are discussed in the following sections.

2.2 Sensitivity

Challa et al. (2008) documented the sensitivity of HYSPLIT to the input meteorological model. Mesoscale models are important over complex terrain and geography where local winds and heating patterns can create complex dispersion. Challa et al. (2008) used mesoscale data to simulate dispersion along the complex coast of Mississippi with an emphasis on the variability of the wind field and PBL height. Six different physics scheme combinations for the PBL and land surface processes were investigated to provide a comprehensive sensitivity of HYSPLIT to these factors. Using these different schemes created an ensemble of ground level air concentration patterns which aided in the sensitivity analysis. Challa’s results indicated that HYSPLIT is sensitive to the input meteorological fields which can lead to errors in plume pattern and concentration distribution. Among the combi-
nations tested, the MYJ PBL and NOAH Land Surface schemes were the best representation of the atmosphere and actual plume. Challa et al. (2008) also shows that the ensemble mean concentration could better produce a trend that replicates the observation.

2.3 Verification

The various HYSPLIT applications have aided in the validation of the dispersion model. Large field experiments have also been conducted to depict the accuracy of the dispersion models. HYSPLIT was evaluated based on several field experiments (e.g. CAPTEX, ANATEX, ETEX) and compared to 21 other transport models (Draxler, 1999). Draxler found that the HYSPLIT calculations were in the middle of the performance range. More information regarding HYSPLIT’s verification based on these field experiments is available at the Air Resources Laboratory website (cited 2009). Draxler (1999) did note that the largest difference found between HYSPLIT and the other transport models was that HYSPLIT substantial overestimated wet deposition.

2.4 Model Description

HYSPLIT is used to model the atmospheric transport and dispersion of pollutants plumes that may originate from various source types (nuclear power plants, dust storms, volcanic eruptions, chemical reactions, fire smoke, etc.). HYSPLIT provides tools to analyze and process the output of trajectories and dispersion concentrations for operational efficiency. However, the binary software that is commonly run on personal computers does not allow for software modification.

Meteorological data fields are used to better simulate particulates dispersing within the atmosphere. For flexibility, HYSPLIT can use different meteorological data for input. The horizontal grid system of a model input is linearly interpolated to HYSPLIT’s horizontal terrain coordinate system, which enables many meteorological source inputs to be used. There are three projections supported by HYSPLIT: Polar Stereographic, Mercator and Lambert Conformal Conic. Meteorological variables within the gridded fields are required at specific temporal intervals which may range from 1 hours to over 6 hours. Meteorological input must be provided on a pressure-sigma, terrain-sigma,
pressure-absolute or hybrid absolute pressure-sigma coordinate system. The model requires at a minimum horizontal and vertical wind components, temperature, height or pressure, and surface pressure. Moisture and vertical motion is optional but depends on the application. For example, moisture content is valuable for wet deposition calculations while vertical motion is needed to describe a convective atmosphere. Vertical motion is most typically available with meteorology data input, but during special circumstances may be calculated with the assumption that the pollutant parcel is transported along some other surface (isobaric, isosigma, isopycnic or isentropic).

An important parameter for dispersion calculations is the advection of a particle or puff. A puff model releases pollutant puffs at regular time intervals over the duration of the release time (Draxler and Hess, 1997). Each puff contains the appropriate amount of pollutant mass and is advected according to the trajectory of the center of the puff. A turbulent component is introduced to account for the dispersive nature of the puff in both space and time. The particle model continually releases particles over the duration of the release (Draxler and Hess, 1997). Advection and turbulence of the particles is added at each time step. HYSPLIT is a lagrangian particle dispersion model, allowing advection to be calculated following the particle or puff. The advection is computed using the average three-dimensional velocity vectors \( V \) for the initial position \( P(t) \) and the first guess position \( P' \) according to

\[
P'(t + \Delta t) = P(t) + V(P,t)\Delta t
\]

where \( t \) is time and \( \Delta t \) is the integrated time step. The velocity vectors are then integrated both in space and time until the final position \( P(t + \Delta t) \) is achieved following,

\[
P(t + \Delta t) = P(t) + 0.5[V(P,t) + V(P', t + \Delta t)]\Delta t
\]

which is based on Petterssen (1940). This technique is known as the integration method. The integration time step can vary throughout the simulation between 1 minute and an hour. The time step \( \Delta t \) is based on the requirement that the advection distance per time step is less than the grid spacing following
\[ V_{\text{max}} \Delta t < 0.75 \quad (2.3) \]

where \( V_{\text{max}} \) is the maximum transport velocity. When particle trajectory exceeds the model top (10000 m) then advection is terminated. If the trajectory intersects the ground, then advection continues horizontally along the surface.

In order to capture the turbulent nature of the atmosphere, stability and mixing coefficients are calculated. Atmospheric stability is estimated in two fashions: by heat and momentum flux or by the temperature and wind gradients. Heat and momentum flux are provided by the meteorological model and is most commonly used. When fluxes are not directly provided, temperature and wind gradients are calculated from the meteorological input data to estimate the fluxes. This method is not commonly used, but documented in the HYSPLIT manual. For both methods, fluxes are utilized in conjunction with the friction velocity and temperature to first calculate the Obukhov length \( (L) \) following

\[ L = z \left( Z^2 k g T^* \left( u^* T^2 \right)^{-1} \right) \quad (2.4) \]

where \( z \) is the reference height, \( u^* \) is the friction velocity, \( Z^2 \) indicates the height of the surface layer, \( T^* \) is the friction temperature, \( T \) is the temperature, \( k \) is the Von Karman’s constant (0.40) and \( g \) is gravity (9.8 m s\(^{-2}\)). This length scale represents the height above which convective turbulence dominates over mechanically driven turbulence, and is typically found at or just below the surface layer (0-200 m). The boundary layer depth \( (z) \) is also a good indication of the stability or turbulence within the lower atmosphere. If the PBL height is not available as a direct output from the input meteorological model, the depth is computed at each grid point and is assumed to equal the height at which the potential temperature first exceeds the value at the ground by 2K. This method may lead to overestimation during the night time hours (Draxler and Hess (1997)). Another option is to calculate the mixing height based on the TKE field, if available. The height is assumed where TKE drops by more than half its previous value. Both vertical and horizontal mixing coefficients are assumed following the coefficients for heat and velocity deformation, respectively. Further documentation of
the explicit calculations used for mixing is provided in the HYSPLIT manual.

Puff and particle dispersion rates are heavily influenced by turbulent velocity components. For both methods of dispersion, a random motion is added to better replicate dispersion within the atmosphere. Using the puff dispersion technique, turbulence is used to help expand the cloud both in space and time. For particle dispersion, a turbulent component is added to the mean particle position \( Z_{\text{mean}} \) to obtain the final position \( Z_{\text{final}} \) from which diffusion is computed following

\[
Z_{\text{final}}(t + \Delta t) = Z_{\text{mean}}(t + \Delta t) + W'(t + \Delta t)\Delta tZ_{\text{top}}^{-1}
\]  

(2.5)

where \( W' \) is the vertical turbulent component, \( t \) is time and \( Z_{\text{top}} \) is the required unit conversion factor. The incremental time step \( \Delta t \) in this case follows

\[
\Delta t = \frac{(\Delta z)^2}{8\sigma^2_w T_{L_w}}
\]  

(2.6)

where \( \Delta z \) is the vertical grid spacing, \( \sigma^2_w \) is the vertical velocity variance and \( T_{L_w} \) is the Lagrangian time step. If a the particle intersects the ground or model top (10000 m), the particle is fully reflected. The vertical turbulent component \( W' \) is computed following

\[
\frac{W'(t + \Delta t)}{\sigma_w} = R(\Delta t)\left( \frac{W'(t)}{\sigma_w(t)} \right) + \frac{W''}{\sigma_w(t)}(1 + R(\Delta t)) * 0.5 + T_{L_w}(1 - R(\Delta t))\left( \frac{\partial \sigma_w(t)}{\partial z} \right)
\]  

(2.7)

where \( \sigma_w \) is the vertical turbulent standard deviation, \( R(\Delta t) \) is the autocorrelation factor and \( W'' \) is the Gaussian random component.

Methods for estimating turbulent velocity variances affect the individual velocity components. There are typically two ways to estimate the turbulent variances: by calculating a diffusion coefficient or obtaining stability functions. Using the diffusion coefficient requires assumptions about the turbulent scales and averaging of the vertical velocity variances across a boundary layer. HYSPLIT uses stability functions in conjunction with the TKE fields to estimate turbulence variances. Following this method, there are no turbulent scale assumptions and the velocities are not averaged which is a better representation of the atmosphere since turbulence varies with height (Draxler and
Hess, 1997). In puff simulations, there are two domains used to calculate dispersion. HYSPLIT assumes that the meteorological model is capable of resolving turbulence when the puff is larger than the meteorological grid. However, for puffs smaller than the meteorological grid, the puffs’ rate of vertical growth has to be modified. In the vertical direction, a puff distribution utilizes the “top-hat” approach where everything inside the puff is one value while outside the puff the value is zero.

Air concentration calculations can be computed for the vertical and horizontal directions. The particle concentration calculates the sum within a grid-cell using either a top-hat (vertical) or Gaussian puff distribution (horizontal). Dry and wet depositions are two mechanisms for particle removal within the atmosphere. Dry deposition is defined as deposition velocity (flux) or it may be equal to the gravitational settling velocity with the option of using a resistance method and information about the surface. The deposition velocity \( V_d \) following the resistance method

\[
V_d = \left[ R_a + R_b + R_a R_b V_g \right]^{-1} + V_g
\]  

is computed from the sum of different constraints within the atmosphere such as the atmospheric layer \( R_a \)

\[
R_a = \frac{1}{k u_*} Pr \left( ln \left( \frac{z}{z_o} \right) - \Psi_h \right),
\]  

and the quasi-laminar sublayer \( R_b \)

\[
R_b = Pr \left( \frac{d_1}{k u_*} \right) Sc^{d_2}
\]

where \( z \) is the reference height, \( z_o \) is the surface roughness height, \( k \) is Von Karman’s constant (0.40), \( u_* \) is friction velocity, \( \Psi_h \) is the surface correction factor based on heat, the constants \( d_1 = 2 \) and \( d_2 = 2/3 \), \( Pr \) is Prandtl number and \( Sc \) is the Schmidt number. HYSPLIT uses land use inventory to modify the atmospheric layer (Wesely and Hicks, 1977) and computes the settling velocity \( V_g \) based on Hoven (1968),
\[ V_g = \frac{d_p^2 g (\rho_g - \rho)(18\mu)^{-1}}{d_p^2 g (\rho_g - \rho)(18\mu)^{-1}} \] (2.11)

where \( V_g \) is calculated from a spherical particle based on the particle diameter \( (d_p) \), air density \( (\rho) \), particle density \( (\rho_g) \), gravity \( (g) \) and the dynamic viscosity \( (\mu) \) of air \((0.000018 \text{ kgm}^{-1}\text{s}^{-2})\). Gravitational velocity is important for deposition of particle to the ground and is estimated based on particle size and density. If the molecular weight is known, it can aid in the computation of the settling velocity. The velocity is then adjusted to replicate a gradual sinking motion depending on the vertical position. Wet removal is computed using the scavenging ratio within the cloud and below the cloud base. Deposition also accounts for deposited radioactive pollutants which can decay. Also, there are certain occasions when the wind is strong near the surface allowing for resuspension of the particulates into the atmosphere. This mechanism is automatically enabled when deposition is being calculated.

Draxler and Hess (1997) provides a more detailed description of HYSPLIT model physics. The description of the graphical interface was updated in 2009 but explanation of the command line edition of HYSPLIT is not well documented. A detailed description of the graphical interface is available online:


2.5 Applications

HYSPLIT has been widely used for many different applications. As HYSPLIT increases in popularity, the versatility and validation becomes better documented. Applications of the HYSPLIT dispersion model include uses for emergency response, urban dispersion, fire weather, and pathogen transport.

2.5.1 Emergency Response

Two Greek agencies, the Institute of Nuclear Technology and Radiation Protection and the Hellenic National Meteorological Service (EMY) assist the Greek Atomic Energy Commission in
response to nuclear emergencies (Housiadas, 1999). In order to protect the public from the threat of radioactive material, a Customized Meteorological (Cm)-HYSPLIT model was developed. Similar to the standard HYSPLIT model, the modified version predicts plume trajectory, dispersion and deposition after a radioactive release in Europe. However, a customized atmospheric meteorological grid from the EMY is used as input for the model (Housiadas, 1999).

Likewise, the US has a nuclear response plan that activates the HYSPLIT model. The action plan documented and maintained by NOAA has explicit instructions to effectively simulate a plume for immediate response (Draxler, 1999). In the event of a nuclear emergency, the appropriate personnel will be notified and perform the initial default simulations. NCEP and ARL then collaborate to produce a more appropriate simulation accounting for the specific situation. For smaller scale emergency response, NWS forecast offices run HYSPLIT using either the online ARL interface or the PC version (Ruminski et al., 2006).

2.5.2 Urban Dispersion

Urban areas have very dynamic boundary layers that can influence dispersion in complex ways. One experiment designed to investigate this complexity was the Metropolitan Tracer Experiment (METREX). METREX was implemented throughout Washington D.C. from 1983 to 1984 (Draxler, 1985). Hundreds of tracer particles were released and air samples were collected to document dispersion patterns. However, at the time of the experiment, no meteorological models had sufficient resolution to resolve atmospheric dynamics at the local scale. Today, there are many meteorological inputs that could represent dispersion at local scales. Draxler (2006) used data from the METREX experiment in combination with higher resolution input data. The simulation was run with the PSU/NCAR mesoscale meteorological model (MM5) using a 4 km domain. HYSPLIT has been shown to be effective for longer distance transport simulations, but this study elevated HYSPLIT performance at high resolutions and shorter distances (Draxler, 2006). The model predicted air concentrations were compared with tracer measurements up to 75 km from the source release. After the simulations were complete, intensive analysis of over 500 tracer releases were conducted. Draxler’s results suggested that HYSPLIT can be valid under short ranges as compared to the longer
range experiments that had been previously conducted.

2.5.3 Fire Weather

The spring of 1998 was one of the worst smoke episodes within Central America leading to health hazards and low visibility. In response to this event, daily fire and smoke products were produced operationally by the National Environmental Satellite and Data Information Service (NESDIS). In 2001, NESDIS created the Hazard Map System (HMS). This program uses satellite tools and capabilities to identify fire and smoke emissions from natural and prescribed burns across North America. There are both geostationary and polar orbiting satellites that continue to monitor the earth below and the subsequent smoke within its atmosphere. Unfortunately, satellites, which are suspended miles above the earth’s surface, have disadvantages with regards to identifying the pollutant, weather interaction and night time visibility (Ruminski et al., 2006). Therefore, different automated aerosol and smoke products are input into HMS for quality control purposes. NESDIS also monitors for missed hot spots. Once the fire sources have been correctly identified they are placed within HYSPLIT for simulations. Initially, NESDIS was using a constant emission rate, but has recently improved this feature based on the Blue Skies framework (Ruminski et al., 2006). The Blue Skies framework calculates the amount of smoke emissions from a fire based on the number of points an expert adds to a particular fire location. In most cases, the number of points set by the analyst is proportional to the hot spots detected by satellites. The rate of burn depends on the burn area, vegetation, and fuel moisture and consumption.

HYSPLIT is run operationally at NCEP once daily at 06 UTC using the North American Model (NAM) as the meteorological input. Air concentration is output with a 12 km spatial resolution every hour. Since, fire duration can last from a couple of hours for prescribed burns to over 24 hours for wildfires, NESDIS determines the duration based on fire origin. The Geostationary Operational Environmental Satellite (GOES) Aerosol and Smoke Product (GASP) was implemented in 2006 to assist in determining the smoke concentration beyond the scope of HYSPLIT (Ruminski et al., 2006).
2.5.4 NWS Operational Applications

HYSPLIT is run operationally at the NWS in Melbourne, FL and in Houston, TX at the NWS Spaceflight Meteorology Group (SMG). Like most NWS offices, NWS-Melbourne is responsible for providing meteorological insight to emergency managers at the state and county level in the event of an accidental chemical release or smoke episode from wildfires. SMG is also concerned about Space Shuttle landings and hopes to gain more confidence in cumulus cloud development, smoke visibility and anvil trajectories from thunderstorms (Dreher, 2009). As previously noted, most weather offices use either the online or PC-based HYSPLIT tool to gain confidence regarding dispersion within the atmosphere. However, both Melbourne and SMG were interested in obtaining a more useful tool that would automate HYSPLIT. Therefore, the Applied Meteorology Unit (AMU), a team that bridges the gap between research and operational efforts at NASA, the 45th Weather Squadron and the NWS-Melbourne, was commissioned to configure HYSPLIT on Linux. AMU configured HYSPLIT with the most current NCEP and locally run WRF model products (Dreher, 2009). It was hypothesized that the local models provided a more accurate representation of the mesoscale environment than the NCEP products (Dreher, 2009). Therefore, the HYSPLIT simulations should also be more accurate. Since this is a newer development, no further analysis has been conducted on the NCEP versus the local WRF models.

2.5.5 Pathogen Transport

HYSPLIT has been used to predict the dispersion of vegetation diseases. The North American Plant Disease Forecast Center (NAPDFC) at North Carolina State University in Raleigh, NC provides forecasts across North America for tobacco and cucurbit diseases. Diseases are first confirmed by farmers and placed into a centralized database where specific information (time, location, species, etc) is then input into HYSPLIT. Trajectories from HYSPLIT assist disease analyst in deciding where the risk for tobacco blue mold or cucurbit downy mildew may reside up to 72 hours in advance (Main et al., 2001). A similar procedure was done for soybean rust across much of Asia, where HYSPLIT was used to help understand and predict the season of increased risk for soybean plants (Pan et al., 2006). Pasken and Pietrowicz (2005) also used HYSPLIT to calculate the forward
trajectory of air parcels from oak tree sources to predict the movement of tree pollen for respiratory and allergy applications. If the trajectories move over a particular region, then they identify that location as a risk area (Levetin, 1998). Such a forecast can predict the influx of pollen but perhaps not have the sophistication to quantify the concentration. Pasken and Pietrowicz (2005) emphasized the need for a quality mesoscale meteorological model since trajectories rely heavily on smaller scale boundary layer dynamics.

2.5.6 Comparison of Dispersion Models

There are several dispersion models that are used for various dispersion purposes. An intercomparison of dispersion models (AERMOD, HPDM, PCCOSYMA and HYSPLIT) is provided by Caputo (2003) with a focus on model applications, advantages and limitations. HYSPLIT is the only model within the group to use Lagrangian trajectories to calculate dispersion, which provides several advantages. In HYSPLIT, meteorological data available for the whole domain is used to advect and disperse the plume in accordance to the local atmospheric conditions at each time step. In contrast, the other models use insitu meteorological data at the source location. This method ignores the meteorological conditions that may change spatially and temporally. While overall results suggest the models compare similarly with each other, Caputo’s results show that HYSPLIT performed best.
Chapter 3

FLEXPART

3.1 Overview

In 1995, Andrea Stohl (University of Munich) introduced FLEXPART, an open source lagrangian dispersion model, for Austria’s emergency response system. Quick validation of this transport model (Stohl, 1998) led to an increase in popularity. Over 30 groups within 17 countries utilize this dispersion model for air quality, fire emission, emergency response, ozone and stratospheric exchanges.

FLEXPART first evolved from the simple trajectory model FLEXTRA (Stohl et al., 2005) and uses the European Center for Medium Range Forecasts (ECMWF) model. FLEXPART (version 2.0) was initially introduced by Stohl (1998) while he was in military service. By version 3.0 improvements were made to projection options, uncertainty statistics, density correction and inverse modeling capabilities. Throughout the next couple of versions, FLEXPART development focused on enhancing the accuracy of the model, including the addition of several new features such as age spectra of trace gases, introducing mass flux in both the horizontal and vertical, addition of a convective algorithm, and a particle position to re-initialize a simulation. Computational efficiency has increased in response to alterations of the memory storage organization and simulation code. The most recent version (8.0) of FLEXPART handles global attributes and reads both the Global Forecast System (GFS) and ECMWF for meteorological inputs.
Most particle dispersion models do not account for the differential density with height in an atmospheric column (Stohl, 1998). The atmospheric density decreases with height and the density at the top of the planetary boundary layer can be 20% lower than the density at the ground level (Stohl, 1998). This can lead to an underestimation of ground level concentration and an overestimation of concentration near the PBL top (Stohl, 1998). A density correction scheme was introduced into FLEXPART by Stohl in 1998 with only a small increase in computational requirements. Demonstration of this correction using the Langevin equation showed an 8% time-averaged ground concentration correction (Stohl, 1998). Depending on the depth of the PBL and the atmospheric conditions, the correction could vary. Stohl (1998) suggests that the density correction would show larger differences within a convective atmosphere. Results were also found to be negligible if there were other large sources of errors.

Convection parameterization is necessary in any model that tries to reproduce atmospheric dynamics. Many convective schemes exist but with closure limitations (Seibert et al., 2001). The Emanuel scheme, which accounts for the effects of updrafts and downdrafts with entrainment and consequential subsidence, seemed to address many of the key features currently missing within the FLEXPART model (Seibert et al., 2001). Limited observational data prevented more robust verification of this scheme, but the Emanuel scheme produces reasonable simulations (Seibert et al., 2001). This new feature was implemented into FLEXPART (version 4.0) and is called every time step.

An adapted version of FLEXPART was unveiled by Fast and Easter (2006c) who integrated the WRF into the dispersion model, now referred to as FLEXPART-WRF. An earlier version of FLEXPART used the PSU/NCAR mesoscale model (MM5), which is similar to the mesoscale model WRF, but is no longer under development. FLEXPART, until this point, was designed to calculate dispersion based on meteorological input from the ECMWF model. Therefore, changes were made to the code in order to ingest the WRF data. Some of these changes included the alteration of the particle position computations using the native WRF grid, the ability to read netCDF output files from WRF and adjustments to allow for mesoscale rather than global attributes (Fast and Easter, 2006c). The output created by the ECMWF is defined on a latitude-longitude grid, while
WRF is defined either by a Lambert Conformal or polar stereographic grid. One of the key benefits of FLEXPART-WRF is the ability to ignore parameterization of mesoscale features once used by the ECMWF. Variables such as frictional velocity and PBL height can be computed directly from WRF instead of parameterized within FLEXPART. FLEXPART-WRF uses internal calculations for meteorological variables if they are not provided by the input mesoscale model.

3.2 Verification

Stohl (1998) applied FLEXPART (version 2.0) to past long range dispersion experiments to gage the accuracy in comparison to three large scale observation campaigns (CAPTEX, ANATEX and ETEX) that were dynamically different based on terrain, synoptic weather patterns and the spatial and temporal sampling and releases conducted. CAPTEX was conducted in 1983 in northeastern North America (U.S. and Canada) and was a small scale experiment compared to ANATEX and ETEX. There were seven 3 hourly releases of a tracer gas from two different locations. During this experiment, a sampling network took measurements every 3 hours at distances of up to 1000 km until 48 hours after the release. Stohl (1998) showed that FLEXPART performed well during CAPTEX since the weather pattern was homogeneous. ANATEX was a larger scale experiment with 33 releases of a tracer gas from two sites in the eastern U.S. between January 5 and March 29, 1987. The releases had durations of 3 hours every 2.5 days which was alternated between day and night. A network of 77 monitoring sites across the U.S. collected concentration every 24 hours at distances of up to 3000 km from the source which led to smaller spatial and temporal resolution of data compared to both CAPTEX and ETEX. The results were relatively poor compared to the other experiments. The reasoning was due to the meteorological conditions that prevailed at that time. The most recent field experiment was ETEX conducted in 1994. Two sites within western France released trace gases into the atmosphere for twelve hours. A network of 168 sites were scattered across 17 European countries to collect data up to 72 hours after the release. Three aircraft were used for upper air observations. The first ETEX release was dominated by westerly flow with little vertical mixing due a cold frontal passage prior to the release. FLEXPART performed well.
However, during the second release the tracers were released ahead of a cold front which introduced both horizontal and vertical shearing. Stohl (1998) shows that FLEXPART performed poorly and overestimated ground level concentrations. It is evident that FLEXPART has limitations. One limitation is the numerical and spatial variability of the planetary boundary layer estimation which is based on interpolation of the input meteorological fields (Stohl, 1998). Another limitation is the poor model performance during frontal passages. These limitations affect concentration estimations depending on atmospheric conditions. A solution to both these issues is to ingest higher resolution meteorological data increasing the variability of vertical motion. Another solution is to incorporate a convective scheme which could correctly disperse the particles out of the planetary boundary layer. These solutions were implemented into FLEXPART in later versions subsequent to Stohl (1998).

### 3.3 Sensitivity

Peffers and Fuelburg (2009) conducted a study using FLEXPART-WRF to simulate CO plumes from Iranian fires and anthropogenic activity. The study identified the sensitivity of FLEXPART based on differing WRF parameters and schemes. Several WRF configuration options were modified including horizontal and vertical resolution, the planetary boundary layer schemes and land surface schemes. Verification of the WRF analysis was conducted based on available observations from the area of interest. Results indicated that changing the horizontal resolution from 8 km to 2.67 km altered the plume structure while increasing the resolution to 1.6 km added little value. Peffers and Fuelburg (2009) show that increasing the number of vertical levels and packing the levels within the PBL or mid troposphere had little impact on the plume composition. However, changing the PBL schemes and land surface models did alter the plumes. Peffers and Fuelburg (2009) noted that the ACM2 PBL and Xie Land Surface scheme appear to better replicate the CO structure as compared to the other scheme combinations.
3.4 Model Description

FLEXPART is a Lagrangian model that simulates forward transport and dispersion of air particles within the atmosphere over short or long distances. FLEXPART can also be used backward with time to determine the potential source of the pollutant (Stohl et al., 2005). Particles can either release from a line, point or area source undergoing diffusion, deposition and/or radioactive decay. There is no graphical user interface for FLEXPART. Most FLEXPART simulations are run on a Linux machine through the FORTRAN executable allowing code automation and alteration (Stohl, 1998). The documentation for the source code (version 6.2) is provided by Stohl et al. (2005). FLEXPART has the ability to produce simulations using either the MM5, GFS, ECWF or the WRF meteorological fields. Version 6.2 incorporates the large scale ECMWF meteorological model and is very well documented. For this analysis WRF version 3.1 is used with FLEXPART-WRF and subsequent changes made to the code are discussed within this overview.

FLEXPART is designed to read gridded binary meteorological data from NWP models. Extensive modifications were made to version 6.2 in order to adapt to the mesoscale meteorological data from WRF (Fast and Easter, 2006c). FLEXPART-WRF is modified to ingest WRF netCDF format data files instead of the GRIB formation output by ECMWF. The output produced by FLEXPART-WRF is defined on a lambert conformal conic or polar stereographic grid. Within FLEXPART-WRF, the concentration output is reprojected to a latitude-longitude grid using post processing techniques. Meteorological data are placed on a terrain-following Cartesian vertical coordinate system in which grid resolution does not vary in the horizontal. FLEXPART-WRF requires at a minimum the wind components (horizontal and vertical), temperature and humidity in three directions. The two dimensional requirements include: surface pressure, total cloud cover, 10 meter horizontal wind, 2 meter temperatures and dew point temperature, convective parameters, sensible heat flux, solar radiation, surface stress, topography and land-use inventory. Variables that are missing are calculated or parameterized within FLEXPART-WRF.

Particle transport and diffusion is one of the most important calculations embedded within the FLEXPART code. Trajectories (advection) can be calculated using the “zero acceleration” scheme where the initial position \(X(t_j)\) and first guess position \(X(t_{j+1})\) follow...
\[ X(t + \Delta t) = X(t) + v(X, t)\Delta t \]  

(3.1)

which is accurate to the first order to calculate the final position \( \frac{dX}{dt} \),

\[ \frac{dX}{dt} = v[X(t)] \]

(3.2)

with \( t \) being time, \( \Delta t \) the time step, \( X \) is the position of the vector, \( v \) is the velocity vectors.

Particle transport and diffusion by turbulence is based on wind fluctuations within the planetary boundary layer. In FLEXPART 6.2, the wind field from the operational ECMWF is too coarse to illustrate the turbulent eddies within the PBL, so parameterization was used. This feature is turned off in FLEXPART-WRF due to higher spatial resolution within the WRF configuration (Fast and Easter, 2006c). Gaussian turbulence is estimated by FLEXPART-WRF which is assumed to be valid for stable and neutral conditions. Under unstable convective patterns this assumption is breached. The error can be quite small if the layer is well mixed and transported over long distances (Stohl et al., 2005).

Stohl and Thomson (1999) added a density correction to the turbulence scheme that would better represent the atmospheric distribution of particles. The Langevin equation was implemented to calculated turbulent fluctuations

\[ d\left( \frac{w'}{\sigma_w} \right) = -\frac{w'}{\sigma_w} \frac{\Delta t}{\tau_{L_w}} + \frac{\partial \sigma_w}{\partial z} \Delta t + \frac{\sigma_w}{\rho} \frac{\partial \rho}{\partial z} \Delta t + \left( \frac{2}{\tau_{L_w}} \right)^{1/2} dW \]

(3.3)

where \( w' \) is the turbulent vertical wind component and \( \sigma_w \) is its standard deviation, \( \tau_{L_w} \) is the Lagrangian timescale for the vertical velocity autocorrelation, \( \Delta t \) is the incremental time step, \( z \) is the height, \( \rho \) is the density and \( dW \) is the Wiener process (Stohl et al., 2005). The second and third term on the right hand side correspond to the drift and density correction. This equation is similar to Legg and Raupach (1982) but with the addition of a third term to correct for atmospheric density. The Langevin equation can also be written in terms described by well mixed conditions (Thomson, 1987). Therefore, during unstable short term simulations, this equation is used. The incremental time step \( \Delta t \) follows
\[ \Delta t = \frac{1}{c_{tl}} \min(\tau_{Lw}, \tau_{min}) \left( \frac{h}{2w} \cdot \left( \frac{0.5}{\partial \sigma_w / \partial z} \right) \right) \]  

(3.4)

where \( c_{tl} \) is a time constant, \( \tau_{Lw} \) is the lagrangian timescale, \( z \) is the height, \( h \) is the PBL height, \( w \) is the turbulent wind component and \( \sigma_w \) is its standard deviation. If a particle reaches the top of the PBL then it is reflected downward changing the sign of the turbulent wind component. Parameterization of wind fluctuations under different stability conditions is taken into account using boundary layer parameters. The mesoscale vertical parameterization is turned off with high resolution input from WRF. Other boundary layer parameters are either parameterized or calculated.

By default FLEXPART computes frictional velocity, surface flux and PBL height. However, these variables are also provided by WRF. If FLEXPART-WRF does not receive these variables it will assume they are missing and will be calculated by the default methodology (Stohl et al., 2005). In the latter case, friction velocity \( (u_*) \) is first calculated as

\[ u_* = \sqrt{\tau_o / \rho} \]  

(3.5)

where \( \tau_o \) is the surface stress and \( \rho \) is the density. Friction velocity will aid in computing the Monin-Obukhov Length (L) and the PBL height. FLEXPART relies on the Richardson number \( (Ri) \) criteria to determine the PBL height defined by

\[ Ri = \frac{((g/\theta_{vn})(\theta_{vn} - \theta_{v1})(z_n - z_1))}{(u_n - u_1)^2 + (v_n - v_1)^2 + 100u_*^2} \]  

(3.6)

where \( g \) is gravity, \( \Theta_{vn} \) and \( \Theta_{v1} \) are the virtual potential temperatures, \( z_n \) and \( z_1 \) are the height, and \( (u_n, v_n) \), \( (u_1, v_1) \) are the wind components at the bottom \( (1) \) and top \( (n) \) model level. The PBL height is set to the height of the first model level for which the Richardson number exceeds the critical value of 0.25. \( Ri \) describes the ratio of buoyancy to shear forces. As the ratio nears 0.25, turbulence becomes insignificant and the top of the PBL is designated where turbulence decreases exponentially (Stohl et al., 2005).

Convective parameterization is one of the most important mechanisms for transport within the atmosphere. The scheme by Emanuel uses both the temperature and humidity fields to calculate
the necessary mass flux for particle distribution. Convection involves an updraft, downdraft and compensating subsidence on the outskirts that are all addressed within the software.

FLEXPART-WRF also accounts for minor processes that aid in replicating a typical dispersion. One of these characteristics is particle splitting. Initially when particles enter the atmosphere they take the form of a cloud that becomes distorted and large. A technique, called particle splitting, is initiated every time step as specified by the user. Particles are split into two, each with half the mass in order to correctly simulate the initial phase of dispersion.

Particles in the simulation are removed from the atmosphere through particle decay, wet deposition and dry deposition. Radioactive decay exists both within the atmosphere and once deposited. Decay can happen soon after the release which will alter the mass of the particle by loss of both energy and radiation. Both radioactive decay and wet deposition are not used within this study.

Dry deposition is another removal process within FLEXPART-WRF that deposits aerosols to the surface. There are two different parameterizations for dry deposition that depend on the form of the mass (gas or particle). If this is not specified, dry deposition will be defined as

$$
u_d(z) = \frac{F_c}{C(z)}$$  \hspace{1cm} (3.7)

where \(\nu_d\) is the deposition velocity (cm/s), \(F_c\) is the flux and \(C\) is the concentration of the species at height \(z\) within the constant flux layer. The deposition velocity of a gas is estimated using the resistance method that incorporates aerodynamic, quasi-linear sublayer and bulk surface stresses. In contrast, the deposition velocity of particles (Eq. 2.8) used within this study is influenced by gravitational velocity settling and the atmospheric and quasi-laminar sublayer resistances. The gravitational settling \((V_g)\) follows

$$V_g = g\rho_p d_p^2 C_{cun}(18\mu)^{-1}$$  \hspace{1cm} (3.8)

where \(d_p\) is the particle diameter, \(g\) is the gravitational acceleration, \(\mu\) is viscosity \((0.000018 \text{ kgm}^{-1}\text{s}^{-2})\), and \(\rho_p\) is the particle density. The Cunningham slip-flow correction \((C_{cun})\) factor follows
\[ C_{\text{cum}} = 1 + Kn[A1 + A2(-\frac{A3}{Kn})] \]  

(3.9)

where \( Kn \) (Knudsen Number) is the ratio of gas molecules to particle size, and \( A1, A2 \) and \( A3 \) are constants (Crowder et al., 2002). The atmospheric layer resistance \( (R_a) \) also contributes to dry deposition following

\[ R_a = \frac{1}{ku_{*}} \left[ \ln(z/z_o) - \Psi_h(z/L) - \Psi_h(z_o/L) \right], \]  

(3.10)

where \( u_{*} \) is the friction velocity, \( k \) is Von Karman’s constant (0.40), \( z \) is height, \( z_o \) is the roughness height, \( L \) is the Monin-Obukhov length and \( \Psi_h \) is the surface layer stability correction term for heat.

The quasi-laminar sublayer resistance \( (R_b) \) follows Erisman et al. (1994)

\[ R_b = \frac{2}{ku_{*}} \left( \frac{Sc}{Pr} \right)^{2/3} \]  

(3.11)

where \( Sc \) and \( Pr \) are the Schmidt and Prandtl numbers. Each of these resistances are parameterized according to the specie, land use type (Velde et al., 1994) and meteorological conditions.

The loss of particle mass from deposition follows

\[ \Delta m(t) = m(t)[1 - \exp\left(\frac{-v_d(h_{ref})\Delta t}{2h_{ref}}\right)] \]  

(3.12)

where \( m \) is the particle mass, \( t \) is time, \( \Delta t \) is the time step, \( h_{ref} \) is the reference height for deposition (75 m) and \( v_d \) is the deposition velocity.

The open-source nature and flexibility of the software source code allows a user to modify the program to fit a desired application. As an example, users have the option to calculate the air concentrations, mixing ratio or both. Another example of the application flexibility is the ability for users to switch on the age spectra option with age classes determined for each specie. Once the specie is older than its age class the particle is terminated within the subsequent grids.

While these options are valuable, there is no GUI for easy modification. For operational settings, this can be a disadvantage. A solution to this issue would be to automate FLEXPART within an
operational office allowing alteration to the initial conditions through an online tool. This implementa-
tion allows the end user to adapt the program to their application needs. A similar configuration
has been implemented within the State Climate Office of North Carolina for use within a Vegetable
Dispersion Forecasting Portal. A more detailed description of FLEXPART version 6.2 is provided
by Stohl et al. (2005) and the WRF modifications documented in Fast and Easter (2006a).

3.5 Applications

3.5.1 Forest Fires

Forest fires emit high concentrations of ozone, volatile organic compounds (VOC) and are a major
source of carbon monoxide (CO) and nitrogen oxide (NO) pollutants (Forster et al., 2001; Spächtger
et al., 2001; Wotawa and Trainer, 2000). It is necessary to understand the long range transport of
smoke and trace gases from wildfires in order to quantify the chemical and radioactive impacts of
forest fire emissions (Forster et al., 2001). The boreal forests in the upper latitudes are thought to
release higher concentrations of CO during fires due to their vegetation and climate (Kasischke et al.,
2005). In 1995, a field experiment in Tennessee noted very high concentrations of CO that could
not be attributed solely to anthropogenic activity (Wotawa and Trainer, 2000). Therefore, forward
and backward trajectories were run using FLEXTRA and FLEXPART. The results indicated that
the increase in CO was indeed due to the fire plumes from Canada.

Another study was conducted using data from one of the most active wildfire episodes in Cana-
dian history in August 1998. Satellites were used to detect boreal fires in Canada’s northwestern
territories where more than 1000 different fires burned causing large plumes to be advected over the
higher latitudes. During this wildfire outbreak, haze was reported as far west as Europe and an
aerosol plume was detected across Greenland (Forster et al., 2001). Smoke plumes, such as the ones
generated from the boreal forests, can linger for a long duration and can inadvertently affect the
global climate by influencing shortwave reflectivity and modifying cloud condensation nuclei within
the atmosphere (Forster et al., 2001). FLEXPART was implemented to simulate the long range
transport of the smoke plumes from the boreal forest. FLEXPART was run using the ECMWF
model with CO sources from Europe and North American via anthropogenic and smoke activity. The dispersion simulation clearly illustrated a haze lamina observed over Germany which originated from Canada. At the time of the outbreak Mace Head, Ireland had surface measurements of the emissions which compared well with the dispersion model estimates (Forster et al., 2001). Nitrogen oxide (NO), another trace gas emitted by the boreal fires, was traced over the Atlantic toward Europe (Spichtinger et al., 2001). FLEXPART was run using the ECMWF and both horizontal and vertical results were in good agreement with satellite detection. However, like most other studies, Spichtinger et al. (2001) expressed the difficulty with quantifying emissions which rely heavily on the uncertainty of the satellite data, nitrogen oxide, age spectra and removal process.

3.5.2 Emergency Response

Austria uses FLEXPART to aid in emergency response modeling for radioactive material in case of an accidental nuclear power plant release. The emergency response modeling system consists of a transport and dispersion model using diagnostic wind fields from the ECMWF (Pechinger et al., 2001). To verify the capabilities of FLEXPART an intercomparison study was conducted based on other emergency response models in Europe (Pechinger et al., 2001). Two hypothetical releases in Chernobyl and London were simulated in 1998 and the subsequent surface concentration was analyzed. Depending on the weather conditions, there is a “remarkable” difference in concentration when the meteorological input is every 3 hours compared to the 6 hourly data provided by the ECMWF (Pechinger et al., 2001). The calculated concentrations produced by the emergency response system in Austria compared well with the other 15 models. Pechinger et al. (2001), however, did not detail the individual model names, physics and assumptions, nor did it include the meteorological data on which each relied. Also, the study did not document any measurement or satellite data to validate any particular model. Pechinger’s results were based on statistical comparison of individual model concentrations.

Similar to fires, power plants are known to release chemicals such a NO into the atmosphere (Wenig et al., 2003). Wenig et al. (2003) investigated the advection of NO gas from the South American Plateau power plant to Australia in May of 1998. This study accounted for lightning
fixation, which can contribute up to 25% of the NO concentration. A simulation of this NO episode was implemented by FLEXPART using ECMWF. Observational measurements from satellite were available due to favorable weather conditions throughout this time period. A comparison between the measurements and simulation showed the emission plumes pattern matched as it traversed across the Indian Ocean to Australia (Wenig et al., 2003).

Dispersion models, RIMPUFF and FLEXPART, were compared in Spain to determine which is more suitable to detect plumes from the Almaraz nuclear power plant (Arnold et al., 2008). The Almaraz power plant is located in complex terrain, making it an ideal challenge to evaluate dispersion model capabilities. Like FLEXPART, RIMPUFF is also a Lagrangian dispersion model but uses differing model physics. For instance, RIMPUFF advects the center of the puff based on local wind rather than accounting for turbulent components. FLEXPART was run using the MM5 which better handled the effects of orography. The Hungarian Meteorological Service, which utilizes RIMPUFF, now includes FLEXPART within its emergency response system (Ferenczi, 2005).

### 3.5.3 Urban Dispersion

An adapted version of FLEXPART was introduced by Fast and Easter (2006c) to ingest the WRF mesoscale high resolution model. To evaluate this version of FLEXPART-WRF Fast and Easter (2006c) performed a series of simulations for a period in early 1997 over Mexico City where there is both complex terrain and documented air quality problems. More than 10,000 particles were released within the Mexico City valley both during the day and night. The results captured the basic assumptions of the atmospheric flow such as decoupling and diurnal variations of the PBL. The authors did recommend more evaluation be conducted based on this new configuration.
Chapter 4

Experimental Configuration and Methodology

In order to conduct a comparison between FLEXPART-WRF and HYSPLIT, a common configuration, including pre- and post-processing, was created across both models. The model analysis process flow is shown in Figure 4.2. The models are pre-processed based on initial parameters and meteorological data. Air concentration and dry deposition is calculated within each model with a Geographic Information System (GIS) post-processing for gridded analysis. The spatial and temporal concentrations are statistically analyzed and verification of the models is conducted based on GOES satellite and WSR-88D data. In the following sections, the individual components of the module configuration are discussed and major differences within these configurations are emphasized.

4.1 WRF

Both the synoptic and mesoscale flow patterns heavily manipulate the dispersion and structure of plumes from a source. It is of vital importance to correctly simulate the atmospheric conditions in an effort to guide the dispersion models toward the observed state. However, the main focus of this study is on the dispersion model comparison rather than the sensitivity of the dispersion
models to meteorological fields. In an effort to identify which dispersion model performs best as compared to satellite observations, WRF needs to adequately simulate the meteorological processes that ultimately affect dispersion. Therefore, the WRF model is evaluated to ensure that the synoptic and mesoscale patterns are correctly represented. WRF output was compared to observations from NCEP, WSR-88D radar data and sounding information from Greensboro (GSO), Morehead (MHX) and Peach Tree (FFC) upper air sites (Figure 4.1). FLEXPART-WRF and HYSPLIT use identical meteorological input from WRF to simulate the transport and dispersion of tracer particles from the source. WRF guides the dispersion model with the dynamic parameters important for dispersion calculations. It is important to note that WRF does not depict fire hot spots, which is a limitation since the atmospheric environment around the fire can be modified.

4.2 Dispersion Input Parameters

Although FLEXPART-WRF and HYSPLIT are very different models, every attempt was made to ensure the input parameters were identical for an accurate comparison. Both dispersion models released a total of 2,000,000 particles and have the same study domain with ten vertical levels at 200, 400, 600, 800, 1000, 1200, 1400, 1600, 1800, and 2000 meters above ground level (AGL). The number of particles does not define the overall concentration but the confidence of the concentration amount. The emissions from the source are assigned a pollutant mass to each virtual particle represented by the dispersion model. A total of 10 kg of mass was released during the entire simulation duration. The magnitude of the source strength will have an impact on the amount of air concentration produced. The dispersion calculations are made for air particle tracers with a diameter of 0.6 µm and density of 2.5 g/cc. Table 4.1 lists the input variables set for each dispersion model.
4.3 Model Configuration

4.3.1 HYSPLIT Configuration

The pollutant plume was diffused based on the standard 3D particle dispersion mode. Movement of each particle is computed based on the average of the three-dimensional velocity vectors and is linearly interpolated both in space and time. Turbulent velocity components are then added to incorporate diffusion in all directions (Fay et al., 1995). Turbulent velocity components are computed based on computer generated random numbers and an incremental time step. Turbulent mixing is computed using a diffusivity approach based on vertical stability estimates and the horizontal wind field deformation. The boundary layer stability (Obukhov length) is computed from heat and momentum flux with the PBL depth taken directly from the WRF. Turbulent velocity variances are computed from the TKE field.

Air concentration is computed based on incremental concentration ($\Delta c$) by a single particle of mass $m$ following the 3D particle mode

$$\Delta c = m(\Delta x \Delta y \Delta z)^{-1}$$ (4.1)

where $\Delta x, \Delta y, \Delta z$ are the grid-cell dimensions. The incremental concentrations are added to each grid cell during each advection time step for all particles and divided by the total number of times steps in the concentration averaging period. Ground level concentrations based on dry deposited matter are calculated within the lowest 75 meters of each horizontal grid cell. Dry deposition uses the resistance process and gravitational settling methods (Wesely and Hicks, 1977, 2000). Land surface information is available from an external source that modifies the atmospheric resistance parameters. Additional information regarding the dry deposition process is provided in section 4.3.3.

HYSPLIT has the ability to set a diurnal factor that modifies the horizontal and vertical turbulence based on the stability of the atmosphere. The default was set to 0.18 for both the day unstable layer and night time stable atmosphere based on experimental studies (Draxler, 2010). This factor ensures that the ratio between the horizontal ($u^2, v^2$) and vertical ($w^2$) turbulence follows
\[
\frac{w^2}{u^2 + v^2} = 0.18. 
\]  
(4.2)

Additional information regarding the HYSPLIT model is provided in Section 2.4.

### 4.3.2 FLEXPART-WRF Configuration

Similar to HYSPLIT, advection of particles in FLEXPART-WRF is computed using the “zero acceleration” scheme and the PBL height is taken directly from the WRF model. However, there are some computational differences. When computing the turbulent wind components, FLEXPART-WRF uses the Langevin equation for diffusion computation (Thomson, 1987). The Langevin equation calculates the net force on a particle tracer to the sum of a deterministic force and random force. Integration of the Langevin equation over time provides a means of calculating successive Lagrangian velocity and displacement increments of the particle (Ermak and Nasstrom, 1995). The time step prescribed for HYSPLIT and FLEXPART-WRF depend on different parameters that may lead to concentration output variations. A density correction is also implemented within FLEXPART to account for the decrease in air density with height (Stohl, 1998). FLEXPART-WRF uses TKE to compute wind fluctuations and stability. For example, the standard deviations of velocity (\(\sigma_u\), \(\sigma_v\) and \(\sigma_w\)) follows

\[
\sigma_u^2 = f_u \times TKE 
\]  
(4.3)

\[
\sigma_v^2 = f_v \times TKE 
\]  
(4.4)

\[
\sigma_w^2 = f_w \times TKE 
\]  
(4.5)

where \(f_u\), \(f_u\) and \(f_w\) are fractions of TKE estimated from the ratios of turbulence velocity components based on surface scaling and local stability (Fast and Wang, 2007). The time-averaged air concentration is computed following
\[ C_{T_c} = \frac{1}{N} \sum C_{T_s} \]  \hspace{1cm} (4.6)

where \( C_{T_c} \) is the output concentration quantity every hour based on the number \((N)\) of samples and sampled concentration \((C_{T_s})\) every minute. The removal process (dry deposition) uses the resistance method and a gravitation settling mechanism. Aerodynamic and quasi-laminar resistances are computed using theories from Stohl (1998) and Erisman et al. (1994), respectively. Additional model information is provided in Section 3.4.

### 4.3.3 Dry Deposition

In regards to dry deposition, similar methods are used within the models as previously reviewed in Chapter 2 and 3. However, there are differences within the computations that need to be emphasized. The common resistance method used in both models follows Eq. 2.8. Based on typical values \((u^*_c = .30 \text{ m/s}, k = 0.40, z = 10 \text{ m}, z_o = .10 \text{ m Pr} = 0.75, \Psi_h = 1.0, L = 100 \text{ m})\), the atmospheric layer scale analysis produces

\[ R_{ah} \approx \frac{R_{af}}{4} \]  \hspace{1cm} (4.7)

while the quasi-laminar sublayer resistance scale analysis produces

\[ R_{bh} \approx \frac{R_{bf}}{3} \]  \hspace{1cm} (4.8)

where \( R_{af}, R_{bf}, R_{ah}, R_{bh} \) are the atmospheric and quasi-laminar resistance methods based on FLEXPART-WRF and HYSPLIT, respectively. According to Eq. 4.7 and Eq. 4.8, the resistance is 4 and 3 times larger for FLEXPART-WRF than HYSPLIT. When the resistance is large, the deposition is small. Therefore, following this technique, it would seem that FLEXPART-WRF will deposit less to the surface compared to HYSPLIT. The gravitational settling term \((V_g)\) is also computed slightly different between HYSPLIT (Eq. 2.11) and FLEXPART-WRF (Eq. 3.8). According to Crowder et al. (2002), if the particle diameter \((dp)\) is less than 0.1, the slip correction factor can have a large impact on the settling velocity of the particle (Figure 4.3). For example, if a particle has a diameter
of 0.01 micron (typical of a fine smoke particulate) then the settling velocity with the Cunningham slip-correction results in $3.02 \times 10^{-7}$ cm/s while without the correction factor the settling velocity would be $6.77 \times 10^{-6}$ cm/s. Thus, it is very important to account for slip-correction, especially with small particles (Crowder et al., 2002).

By using the scale analysis and Cunningham slip-correction information above, a scale analysis can be conducted based on the deposition velocity of each of the dispersion models. When replacing the resistance variables ($R_{af}=4$, $R_{ah}=1$, $R_{bf}=3$, $R_{bh}=1$) and gravitational settling terms ($V_{gf}=6.77 \times 10^{-6}$ cm/s, $V_{gh}=3.02 \times 10^{-7}$ cm/s), the deposition velocity for HYSPLIT is 0.4967 cm/s and FLEXPART-WRF is 0.1428 cm/s. Based on these assumptions, HYSPLIT has over 3 times more deposition velocity than FLEXPART-WRF. Again, this would equate to FLEXPART-WRF yielding less deposition than HYSPLIT.

### 4.3.4 Summary

In an effort to provide a fair comparison between FLEXPART-WRF and HYSPLIT, the input parameters are set to be as close to identical as possible. Table 4.1 describes the input parameters that are set for each dispersion model. In addition, both dispersion models use common WRF inputs with exceptions as noted in Table 4.2. For example, FLEXPART ingests surface stress components from the meteorological data while HYSPLIT computes this parameter.

The computational methods within each dispersion model are similar. However, difference were found, such as the diffusivity computation in HYSPLIT which uses a 3D particle dispersion method. This mode of dispersion advects particles and adds a random component to the particle motion. Conversely, FLEXPART-WRF uses the Langvein equation for diffusion as described in Chapter 3. Dry deposition, as noted Section 4.3.3, is also computed differently between the models which may have led to some output discrepancies. A complete list of the configuration for each dispersion model is provided in Table 4.3. Additional details on the dispersion model physics is provided in Chapter 2 and Chapter 3 and is well documented by Stohl et al. (2005)and Draxler and Hess (1998).
4.4 Methodology for Analysis

Both dispersion models are run with inputs from WRF ARW version 3.1. WRF forecast is ingested hourly by both FLEXPART-WRF and HYSPLIT for transport and dispersion calculations. FLEXPART-WRF uses an executable code that outputs dispersion (i.e. air concentration, dry deposition and wet deposition) every hour into netCDF files, that are then converted to text files. HYSPLIT output is provided in ascii text format. Output text files contain a list of locations with corresponding concentration amounts. The output text files are then placed into GIS for post-processing. The GIS software (GRASS version 6.3) takes the computed air concentration and deposition values and maps each value onto identical grids for analysis. Point values are then resampled using a bilinear interpolation method to produce a gridded surface.

Computational time for the two models were different. Data formatting and analysis for HYSPLIT required pre- and post-processing routines to be run separately. Processing for FLEXPART-WRF was more easily integrated and automated due to the availability of the source code. Hence, the simulation runtime was affected. The average time of computation for HYSPLIT was 15 minutes and for FLEXPART-WRF it was approximately 10 minutes for a 48 hour simulation.

Since both dispersion models are post-processed on the same grid, spatial differences can be easily evaluated. A difference field ($D$)

$$D = H - F$$

(4.9)

and percent difference field ($\%D$)

$$\%D = \frac{H - F}{H + F} \times 100\%.$$  (4.10)

are created every hour where $H$ and $F$ are HYSPLIT and FLEXPART-WRF output fields, respectively. Based on Eq. 4.9, positive values indicate HYSPLIT has a higher concentration value at that specific grid point. Negative values correspond to higher FLEXPART-WRF concentrations. In regards to Equation 4.10, a 0% difference is optimal suggesting the two simulations are the same, while larger magnitudes suggest they are less similar compared to one another. This method is
appropriate when comparing two experimental datasets where the values are calculated using two different methods (Winkler, 1985). Percent error ($\%_{\text{error}}$) is another technique used to determine how accurate an experimental value is to an accepted value following

$$\%_{\text{error}} = \frac{H - F}{F} \times 100\%$$  \hspace{1cm} (4.11)

where FLEXPART-WRF (F) is the true (accepted) value based on positive verification from the case study analysis and HYSPLIT is the experimental value. Other analysis methods used to investigate FLEXPART-WRF and HYSPLIT concentration and deposition (i.e. average difference, concentration distribution, diffusion from source, etc.) will be examined in later sections.

Observed air concentration and deposition measurements were not available during these events leading to a lack in quantitative verification. However, validation of the spatial and temporal plume structure were conducted using GOES satellite information at 15 minute intervals during both case studies.
Pre-Processing

- Input Parameters
- WRF Model

Dispersion Models

- FLEXPART
- HYSPLIT

Post-Processing

- GIS
- Statistical Analysis
- Verification

Figure 4.1: Upper Air Sites

Figure 4.2: Flow Chart of the Model Configuration for the dispersion simulations.
Table 4.1: Initialized Parameters for June 9, 2008 Case Study

<table>
<thead>
<tr>
<th>Initial Parameters</th>
<th>FLEXPART-WRF</th>
<th>HYSPLIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Forward Simulation Start</td>
<td>June 09 13 UTC 08</td>
<td>June 09 13 UTC 08</td>
</tr>
<tr>
<td>Simulation End</td>
<td>June 11 12 UTC 08</td>
<td>June 11 12 UTC 08</td>
</tr>
<tr>
<td>Time Averaged Output (s)</td>
<td>3600</td>
<td>3600</td>
</tr>
<tr>
<td>Sampling Rate of Output (s)</td>
<td>60</td>
<td>60</td>
</tr>
<tr>
<td>Lower Left Output Grid (lat,lon)</td>
<td>33.00,-81.00</td>
<td>-</td>
</tr>
<tr>
<td>Upper Right Output Grid (lat,lon)</td>
<td>37.50,-72.00</td>
<td>-</td>
</tr>
<tr>
<td>Grid points in X</td>
<td>301</td>
<td>-</td>
</tr>
<tr>
<td>Grid points in Y</td>
<td>301</td>
<td>-</td>
</tr>
<tr>
<td>Span (lat,lon)</td>
<td>-</td>
<td>2.25,4.5</td>
</tr>
<tr>
<td>Spacing (lat,lon)</td>
<td>-</td>
<td>0.15,0.03</td>
</tr>
<tr>
<td>Number of Vertical levels (200m)</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>Vertical Height of each level (m)</td>
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<td>200</td>
</tr>
<tr>
<td>Number of Releases</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Start time of release</td>
<td>June 09 13 UTC</td>
<td>June 09 13 UTC</td>
</tr>
<tr>
<td>End time of release</td>
<td>June 11 12 UTC</td>
<td>June 11 12 UTC</td>
</tr>
<tr>
<td>Latitude of release (degrees)</td>
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</tr>
<tr>
<td>Longitude of release (degrees)</td>
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<td>-76.452</td>
</tr>
<tr>
<td>Total Number of Particles Released</td>
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<td>2,000,000</td>
</tr>
<tr>
<td>Release height (m)</td>
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<td>150</td>
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<tr>
<td>Amount Released (kg)</td>
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<td>10</td>
</tr>
<tr>
<td>Age Spectra</td>
<td>Off</td>
<td>Off</td>
</tr>
<tr>
<td>Radioactive Decay</td>
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<td>Off</td>
</tr>
<tr>
<td>Wet Deposition</td>
<td>Off</td>
<td>Off</td>
</tr>
<tr>
<td>Dry Deposition</td>
<td>On</td>
<td>On</td>
</tr>
<tr>
<td>Particle Density</td>
<td>2500 (kg/m3)</td>
<td>2500 (kg/m3)</td>
</tr>
<tr>
<td>Particle Diameter</td>
<td>0.6 (µm)</td>
<td>0.6 (µm)</td>
</tr>
</tbody>
</table>
Table 4.2: WRF Output Variables used within Dispersion Model

<table>
<thead>
<tr>
<th>Variables from WRF</th>
<th>FLEXPART-WRF</th>
<th>HYSPPLIT</th>
</tr>
</thead>
<tbody>
<tr>
<td>U wind component</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>V wind component</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Temperature (T)</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Height (Z)</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Pressure (P)</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Surface Pressure (Po)</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Vertical Wind (W)</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Relative Humidity</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Cloud Cover</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Dew Point Temperature (Td)</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Sensible Heat Flux</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Convective Parameters</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>Solar Radiation</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Surface Stress</td>
<td>Yes</td>
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* Available but not used within this Study
Chapter 5

Case Study: Evans Road Wildfire

5.1 Evans Road Wildfire

On June 1st, 2008 a fire was reported on private property in the New Lake vicinity of eastern North Carolina, south of the Pocosin Lakes National Wildlife Refuge (Figure 5.1). A combination of drought conditions and a lightning strike resulted in the ignition of the fire. By June 3rd, the fire had broken containment and raged across the Pocosin Lakes Refuge burning over 3,000 acres. By that afternoon, the fire had burned 8,000 acres and with persistent drought, windy conditions and flammable organic soil, it could not be contained. Figure 5.2 shows an aerial photograph of the smoke plume from the fire on June 12, 2008. The fire lasted for approximately two months and burned over 40,000 acres. Low visibility and poor air quality conditions were the major concerns plaguing locations downwind of the wildfire. The case study presented uses a small portion of this event, from 13 UTC 09 June 08 through 12 UTC 11 June 08, in an effort to evaluate two dispersion models.
5.2 Study Domain

The baseline WRF computational area consists of an outer domain of 12 km resolution with a nested 4 km resolution gridded domain and is initialized by the North American Model (NAM) re-analysis. The goal of nesting down to the 4 km inner domain is to explore any additional information that may be gained with higher resolution data. The 4 km resolution inner domain provides data to test the hypothesis that the plumes may better agree with each other, especially near the source where operational forecasters are most concerned. The location and orientation of the WRF model domain is shown in Figure 5.3. The outer domain contains 175 x 175 points spanning 2,100 x 2,100 km$^2$ across the eastern half of the United States. The inner domain consists of 235 x 235 points spanning 940 x 940 km$^2$ across central and eastern North Carolina and the northwestern North Atlantic. The domain locations were chosen based on typical operational needs. Both FLEXPART-WRF and HYSPLIT were designed to calculate dispersion using the WRF computational 12 km and 4 km domains, now referred to as EVANS12 and EVANS4, respectively.

A discussion on the WRF configuration used is provided in Section 1.3. For this case study, the PBL scheme was set to the MYJ. As previously mentioned, a sensitivity study conducted by Challa et al. (2008) indicated that this scheme is the most appropriate for coastal regions.

5.3 Meteorological Conditions

5.3.1 Surface Conditions

In an effort to simulate the observed plume, the meteorological conditions produced by WRF must be representative of the actual atmosphere. Surface analysis produced by NCEP is used as confirmation for the WRF surface output fields. Figure 5.4 illustrates the synoptic and mesoscale patterns observed throughout the simulation. The map analysis is compared closely with the WRF surface analysis as seen in Figure 5.5 and Figure 5.6.

At the start of the simulation period, the Bermuda High sitting off the southeast US coastline produced southwesterly winds across portions of the southern coastal plain region of NC. In addition, the WRF simulation, as shown in Figure 5.5a and Figure 5.6a, generated a weak surface trough over
this same region producing northerly winds in the mid-Atlantic that eventually migrated to the south as the trough moved slowly eastward which compared well to observations (Figure 5.4a). On June 9th, a weak high pressure system formed over the Appalachians instigating northerly flow. However, southerly flow began to dominate by 21 UTC which is shown in observations (Figure 5.4b) and captured in the WRF simulations (Figure 5.5b and Figure 5.6b). Through the early morning hours on the 10th, the high pressure system off the southeast coast helped to veer the wind southwesterly by 12 UTC according to observations (Figure 5.4c). The model derived simulation, show in Figure 5.5c and Figure 5.6c, also captures this signature. The observed winds, as shown in Figure 5.4d, started to back at the surface ahead of the cold front through the afternoon hours on the 10th which compared well with the WRF simulation (Figure 5.5d and Figure 5.6d). The model derived migration of the cold front (Figure 5.5e and Figure 5.6e) was also representative of the observed frontal propagation in Figure 5.4e. The front eventually stalled across the coastal plain, west of the source allowing the flow to be westerly by the end of the simulation period.

Very hot and dry conditions were observed across the region with pyroconvection (an area of convection that forms over a wildfire due to excessive heat) occurring late in the simulation. Although instability was high (CAPE >3000 J/kg) during day time hours, there was no lifting mechanism apart from the wildfire to induce thunderstorms. Pyroconvection was produced over the wildfire (18 UTC 10 June) and WRF was unable to simulate this mesoscale process. Since WRF is not able to simulate pyroconvection, a solution would be to modify the release height. However, doing this would not represent the atmosphere during most of the simulation period. A more sophisticated solution would be for the models to adjust the height of release based on the thermal buoyancy (i.e. afternoon heating). The pyroconvection in this case was remote, of short duration and did not significantly affect the overall results.

Along the coastal plain, the diurnal temperature swing was about 15 degrees Fahrenheit with temperatures in the upper 80’s to lower 90’s during the two day period as shown in Figure 5.5b and Figure 5.5d and mid 70’s at night as shown in Figure 5.5c and Figure 5.5e. This pattern was consistent with observations and continued throughout the simulation period with the high pressure ridge largely dominating the atmospheric pattern across the coastal plain. The winds were
approximately 5-10 kts near the surface with occasional gusts during the daytime mixing and below 5 kts at night.

### 5.3.2 Boundary Layer Conditions

Apart from surface conditions, other important factors that influence atmospheric dispersion are in the PBL. Vertical profiles of temperature, dew point, wind speed and direction as well as convective parameters from WRF is compared to observations from the Morehead City (MHX) radiosonde site. The location of the MHX site is provided in Figure 4.1. The WRF simulated moisture, temperature and wind profiles, as shown in Figure 5.7, compared well to the MHX sounding at this time and throughout the simulation period. Based on the EVANS12 mixing height estimates shown in Figure 5.8, the atmosphere was very dry with a typical diurnal fluctuation. Near the beginning of the simulation (12 UTC 09 June), the nocturnal inversion (300 m) produced light winds at the surface with little vertical mixing as shown in Figure 5.9a. By 21 UTC, the mixing height was well above 2 km with winds averaging from the south at 5 kts and veering winds through the column (Figure 5.9b). At this time, the plume structure was most likely analogous to a fumigating or looping plume. Relatively weak low level winds shifted overnight to westerly by the morning of June 10th (Figure 5.9c). As seen in Figure 5.9d, winds had shifted southwesterly ahead of the front by 21 UTC. The winds veered westerly and increased in magnitude as the pressure gradient tightened by the end of the simulation (Figure 5.9e). As seen in Figure 5.10, the WRF upper air analysis for 12 km were very similar to those produced by the 4 km domain.

### 5.4 Air Concentration Results

Air concentrations are analyzed to compare the relative performance of each dispersion simulation. Each simulation is driven by meteorological conditions provided from WRF output using the configuration strategies described earlier. Meteorological model evaluation (as described above) is conducted before the dispersion simulations are initiated to ensure the weather conditions are being handled properly. Both FLEXPART-WRF and HYSPLIT are run using the same WRF data and
dispersion parameters. Total air concentration (surface to 2 km AGL) and the subsequent distribution are analyzed for differences and compared with available satellite imagery. Possible mechanisms associated with observed differences between the models is discussed in Chapter 4.

5.4.1 Model Configuration

Both dispersion models released a total of 10 kg ($1 \times 10^{13}$ng) into the atmosphere from the source site (latitude: 35.62, longitude: -76.452). Due to the nature of the simulation (wildfire), a total of $2 \times 10^6$ particles tracers are continuously released from 150 m above ground level (AGL) is simulated. An hourly release rate of .2127 kg into the atmosphere is simulated over a 47 hour period. The air concentration is defined within a 2000 m column AGL. The concentration is estimated as an integrated mass of individual particles as they pass over the concentration grid which is a matrix of cells, each with a volume defined by its dimensions. The air concentration was computed based on EVANS12 and EVANS4. The domains were not nested within the dispersion models in an effort to separate them for comparison close to the release location. A more detailed description of the equations is provided in Chapter 2 and Chapter 3 and the technical manuals for HYSPLIT (Draxler and Hess, 1998) and FLEXPART (Stohl et al., 2005).

5.4.2 Plume Spatial Structure

Figures 5.10-5.27 show the air concentrations for FLEXPART-WRF and HYSPLIT at select times during the simulation period. Within the first few hours of the simulation, particles were slow to migrate away from the source due to light winds at the surface and aloft as shown in Figure 5.11 and Figure 5.12. By 22 UTC 09 June, the FLEXPART-WRF plume extends to the south and pollutants close to the source start to advect northward as the trough dissipates and mixing within the boundary layer is well underway (Figure 5.13a). In Figure 5.13b, HYSPLIT does not illustrate the southerly extent of the plume within the EVANS12 simulation and keeps the concentration closer to the source. However, EVANS4 shows signs of dispersion to the southeast among both models (Figure 5.14) based on higher resolution wind fields. As a frontal system approaches from the west and the high pressure offshore strengthens by 04 UTC on the 10th, winds shift southwesterly advecting the
particles to the northeast as shown in Figure 5.15 and Figure 5.16. While both dispersion models illustrate the same horizontal plume composition, it is evident that FLEXPART-WRF simulates a higher concentration ($\sim 5$ ng m$^{-3}$), especially downwind, as compared to HYSPLIT ($\sim 3$ ng m$^{-3}$).

At 07 UTC 10 June, FLEXPART-WRF shows a line structure of higher downwind concentration ($>5$ ng m$^{-3}$) as compared to HYSPLIT ($<5$ ng m$^{-3}$) shown in Figure 5.17. EVANS4 resolved the signature but further inland as shown in Figure 5.18. By 11 UTC 10 June, as shown in Figure 5.19 and 5.20, the models start to diverge spatially with HYSPLIT dispersing air concentration to the northeast and FLEXPART-WRF to the east-northeast across both resolutions. The models diverge by an approximate angle of 10 degrees throughout the rest of the simulation with the HYSPLIT plume illustrating a more northerly component as compared to FLEXPART-WRF. Approximately 160 km downwind, concentrations are higher within FLEXPART-WRF ($>7$ ng m$^{-3}$). In Figure 5.21 and Figure 5.22, particles are advecting to the east with plume veering through 18 UTC. As illustrated in Figure 5.23 and Figure 5.24, a strong wind shift disperses the plume to the north advecting a local maximum of air concentration approximately 48 km downwind of the source by 23 UTC 10 June. Thereafter, the primary flow is from the southwest, dispersing particles in a northeasterly direction. At 8 UTC on the 11th, slow veering begins and continues throughout the rest of the simulation (Figure 5.25, Figure 5.26) with the particles dispersing in an eastward direction by 12 UTC 11 June (Figure 5.27, Figure 5.28).

### 5.4.3 Model Evaluation

Results from the two dispersion models show some consistency and variation in plume composition and concentration. Figures 5.28-5.36 shows the model differences at selected times during the simulation period. At 19 UTC on the 9th, the plumes spatial distribution suggests divergence between the models as shown in Figure 5.29 with EVANS4 depicting the dividing line between the model solutions. During this time, FLEXPART-WRF is dispersing to the south, while the EVANS12 HYSPLIT simulation kept its concentration more confined to the release site. Notably, both dispersion models have similar concentration magnitudes. Figure 5.30 illustrates comparable plume advection at 05 UTC on the 10th with differing concentration distribution among the plumes. As
shown in Figure 5.31, the air concentration produced by the EVANS12 HYSPLIT solution is 31% lower approximately 80 km downwind than that of FLEXPART-WRF and 82% higher between the source release and 96 km downstream. The overall strength of these features is also captured in EVANS4 with exception to the higher concentration downstream produced by the EVANS12 HYSPLIT simulation. The modeled plume movement and air concentration amounts start to deviate by 13 UTC 10 June as shown in Figure 5.32. At this time, HYSPLIT is advecting the plume to the northeast while FLEXPART-WRF has a more easterly component. The percent difference field as shown in Figure 5.33 clearly illustrates this pattern with better model agreement in the middle of the plume (≈0%) with extreme values (≈±200%) further out. The HYSPLIT plume starts to back around at 17 UTC while FLEXPART-WRF is still dispersing the plume southward and with a higher downwind concentration (>10 ng m$^{-3}$) approximately 321 km away from the source (Figure 5.34). At 22 UTC 10 June, as shown in Figure 5.35, HYSPLIT advects the pollutants to the north and FLEXPART-WRF to the northeast. FLEXPART-WRF simulates a well defined “S-shape” high concentration signature more than 240 km downwind that is not resolved by HYSPLIT. In Figure 5.36 HYSPLIT is near 300% higher in air concentration where the plume is advecting to the north of FLEXPART-WRF and 30% smaller on average over the rest of the plume. Model divergence (HYSPLIT dispersing to the north of FLEXPART-WRF) is evident by 06 UTC on the 11th as shown in Figure 5.37. The difference in the spatial structure and air concentration (FLEXPART-WRF higher in concentration, especially downwind) continues throughout the rest of the simulation (Figure 5.38, Figure 5.39). Parts of the northern edge of HYSPLIT produced concentrations that are locally 250% higher than FLEXPART-WRF while over the remaining region of the dispersion plume HYSPLIT simulates air concentrations that are 40% lower than FLEXPART-WRF as shown in Figure 5.40. For this case study, HYSPLIT and FLEXPART-WRF demonstrate differences in both the spatial plume patterns and relative downwind concentrations. Below, an analysis is conducted based on the quantitative distribution of the air concentration data for each model and domain.

Although some features well offshore were not captured by EVANS4, the plume distribution within the domain seems unchanged compared to EVANS12. From the plume analysis, EVANS4 appears to add little value to the dispersion forecast. There is one exception which occurred within
the first few hours of the simulation where the HYSPLIT spatial plume structure differed compared to the EVANS12 simulation. This result did bring the dispersion models into better agreement and helped in verification based on the observed plume. The only added benefit beyond this is the high resolution output which will clarify the direction and location of the plume.

5.4.4 EVANS12 Air Concentration Evaluation

Figure 5.41 shows the variation in average air concentration in the EVANS12 simulation during the simulation period. The average air concentration difference between FLEXPART-WRF and HYSPLIT ranged from 2.24 ng m\(^{-3}\) at the beginning of the simulation to -0.09 ng m\(^{-3}\) by the end. HYSPLIT produces an overall higher average air concentration (\(\sim 1.0\) ng m\(^{-3}\)) within the first eight hours of the simulation with FLEXPART-WRF producing a higher air concentration (\(\sim 0.2\) ng m\(^{-3}\)) throughout the rest of the simulation. According to the percent error as shown in Figure 5.42, HYSPLIT produces on average 46% higher air concentration within the first 8 hours and 27% lower air concentration as compared to FLEXPART-WRF during the remaining simulation period. Therefore, FLEXPART-WRF yields a 15% higher air concentration on average through the entire simulation. Since the average concentration is influenced by the increasing number of particles released in the atmosphere, the distribution of particles in each simulation is analyzed in more detail. Figure 5.43 shows the air concentration distribution between FLEXPART-WRF and HYSPLIT with a box plot series. The dispersion models show similar patterns with three peaks in air concentration occurring during the day time hours. The first peak produced by FLEXPART-WRF reaches a maximum of 41.9 ng m\(^{-3}\), seven hours after the release start. HYSPLIT peaks 4 hours after the release start with a concentration of 38.9 ng m\(^{-3}\). The second peak in air concentration occurs at the 27th and 28th hour with 17.6 ng m\(^{-3}\) and 26.2 ng m\(^{-3}\) for FLEXPART-WRF and HYSPLIT, respectively. Both models indicated a peak in concentration at the end of the simulation with 9.4 ng m\(^{-3}\) (FLEXPART-WRF) and 15.1 ng m\(^{-3}\) (HYSPLIT). The maximums in concentration described above are outliers outside the one standard deviation of the mean. Although HYSPLIT illustrated outliers (extremes) that were higher in air concentration, especially among the last two concentration peaks (hour 28 and 47), FLEXPART-WRF was found to have a higher median average concentration.
concentration through most of the simulation period. Figure 5.44 shows the first, second (median) and third quartile of data based on the box plot series air concentration distribution. FLEXPART-WRF shows a higher third quartile than HYSPLIT indicating that FLEXPART-WRF has a 28\% higher concentration within the lowest 75\% of the data. In addition, the median is also 33\% higher (~0.15 ng m$^{-3}$) for FLEXPART-WRF. The spatial differences in Figure 5.45 shows a box plot series with the quartiles skewed negative (~0.20 ng m$^{-3}$) highlighting FLEXPART-WRF’s slightly higher air concentration signal compared to HYSPLIT. It should be noted that the spatial difference is centered around zero and is both influenced by the concentration distribution and spatial plume pattern.

While the differences between the models do appear small compared to the total source release (1x10$^{13}$ ng), a student t-test was conducted to identify the significance of the resultant difference. The student-t test was constructed to test if the mean spatial difference distribution is equal to zero (null hypothesis: H$_{0}$(D) = 0). P-values calculated from this test highlight if the null hypothesis of the student-t test is accepted (>0.05) or rejected (<0.05). Figure 5.47 shows, using a 95\% confidence interval over a normalized distribution (Figure 5.46), the p-values produced each hour, with values that fall below the 0.05 threshold (indicated as a red line) rejecting the null hypothesis. The log form of the p-value emphasize the magnitude of the p-values produced. Within the first several hours, there are periods (hour 5, 10 and 11) where the differences between the model air concentrations was significant (p-values < 0.05). However, after the 13th hour, the difference is significant (p-values < 0.05) throughout the rest of the simulation. This pattern follows closely with the spatial plume model divergence which occurred around the 13th hour of the simulation. In addition, the correlation between FLEXPART-WRF and HYSPLIT was found to decrease with time as shown in Figure 5.48 and Figure 5.49.

Based on the analysis above, one of the major discrepancies is the plume placement of the two dispersion models which is influenced by the diffusion methods embedded within the software. To investigate the downwind horizontal diffusion, polygons are strategically placed 40, 120, 240 and 400 km downwind from the release site in an effort to capture the maximum air concentration every hour for both dispersion models (Figure 5.50). Figure 5.51 and 5.52 show the maximum concentrations
in each polygons during the simulations period. Both FLEXPART-WRF and HYSPLIT illustrates diffusion especially within the first three polygons. Comparatively, the models show very similar diffusion patterns, especially within 240 km from the source. Beyond 240 km, the diffusion signal is clearly visible within FLEXPART-WRF while HYSPLIT shows little signature. Air concentration is slightly higher (>0.5 ng m$^{-3}$) for FLEXPART-WRF, especially beyond 240 km downstream. This result coincides with the dispersion simulations which illustrated that FLEXPART-WRF produced a higher air concentration downwind. This difference may be associated with differing diffusion equations used by each model and their subsequent incremental time steps. During times when HYSPLIT had slightly lower concentration amounts, diffusion above 2000 m or deposition to the ground may have been occurring.

5.4.5 EVANS4 Air Concentration Evaluation

Figure 5.53 shows EVANS4 average air concentration distribution, which encompasses an area closer to the source. HYSPLIT has a $\sim 0.4$ ng m$^{-3}$ higher air concentration throughout the first 11 hours with FLEXPART-WRF beginning to show signs of higher concentration ($\sim 0.1$ ng m$^{-3}$) after 15 hours. Based on the percent error as shown in Figure 5.54, HYSPLIT computes on average 34% higher air concentration within the first 15 hours of the simulation and 32% lower air concentration during the remaining period. Therefore, FLEXPART-WRF yields a 9% higher air concentration on average through the entire simulation. A box plot series shown in Figure 5.55 highlights the higher concentration values computed by each model. Three peaks in air concentration are identified, much like those simulated by EVANS12 and the timing of these concentration spikes is very similar between the two dispersion models. The air concentration is higher within EVANS4, especially the extreme values, due to the increased resolution leading to less diffusion within a grid box. In an effort to emphasize the majority of the data, quartiles are analyzed during the model period. Figure 5.56 illustrates the 25th, 50th (median) and 75th percentiles of the air concentration data between both dispersion models based on the box plot distribution. Consistent with the average concentration distribution, HYSPLIT’s 75th percentile is approximately 30% higher than FLEXPART-WRF within the first 15 hours of the release. Thereafter, FLEXPART-WRF’s 75th percentile is $\sim 25\%$
higher in air concentration. The FLEXPART-WRF median air concentration is 26% higher in air concentration throughout the simulation than HYSPLIT. Another box plot series, representing the spatial difference between the dispersion models, is given in Figure 5.57, and illustrates a symmetric distribution. The outliers highlighted in this figure, identify the 3 peaks in concentration at hours 4, 28, and 47 which occurred from spatial plume divergence and concentration variability. The distribution of these differences becomes centered very close to zero by the end of the simulation. The majority of the distribution represented by the quartiles are skewed negative (-2.0 ng m$^{-3}$) indicating that FLEXPART-WRF has a higher air concentration aside from the outlier values based on the plume placement and concentration values.

The differences between the models are small compared to the total amount released, but may be significant. To evaluate this possibility, a student-t test is conducted using a 95% confidence interval over a normalized distribution. This analysis follows the one described in Section 5.4.4. Figure 5.58 shows that during the first several hours of the simulation (hour 1, 3-5 and 10), the p-values were above 0.05 allowing the null hypothesis ($H_0(D = 0)$) to be accepted. After this point the differences were found to be significant with an exception of a couple of hours (24 and 41-43). The correlation between FLEXPART-WRF and HYSPLIT did decrease with time with the values falling from 0.8 to 0.08 from hour 13 through 27 as shown in Figure 5.59. However, the correlation did improve from hour 28 through 37 as the correlation increased to near 0.6.

Although significant differences were observed between the two models, the diffusion properties were very analogous. Similar to the EVANS12 simulation, 3 polygons are placed 40, 120 and 240 km downwind of the source release (Figure 5.60). As shown in Figure 5.61, the maximum concentration was captured within these polygons at every hour to demonstrate diffusion of pollutants. The signal of air concentration migrating across the polygons is noted throughout the simulation for both models. The magnitude and timing of the maximum air concentration is comparable between the two models as shown in Figure 5.62. Across polygons 2 and 3, FLEXPART-WRF had on average a 10% higher maximum concentration than HYSPLIT.

Within EVANS4, there are differences in plume composition and concentration distribution. HYSPLIT produced on average an 34% higher air concentration during the first 15 hours while
FLEXPART-WRF produced a 32% higher air concentration through the remaining 22 hours of the simulation. The spatial plume distribution between the models is similar within the first 12 hours. Through the rest of the simulation, HYSPLIT disperses the plume to the right (north) of FLEXPART-WRF with lower concentration downwind. Both models diffused the air concentration in similar ways. The EVANS4 concentrations were comparable to those produced by EVANS12 with exception to the extreme values which were at times 35% higher.

5.4.6 Summary

Although the differences in air concentration values across both resolutions (EVANS12 and EVANS4) were not substantial compared to the amount of concentration being released, the spatial plume distribution lead to significant differences among the dispersion models. The variability between the models is based on the spatial distribution of the pollutants and concentration amounts. The spatial distribution is most likely affected by the diffusion equations. The resultant concentration distribution is influenced by many factors such as transport and diffusion out of the layer, deposition and time steps. Overall, based on the quantitative analysis in combination with the spatial plume analysis, especially in regards to the percent error computations, FLEXPART-WRF was found to produce a higher air concentration through most of the simulation period. Dry deposition differences between the two models is discussed in Section 5.5 in an effort to identify the fall out of particles that may have led to air concentration differences between the models.

5.4.7 Verification

The hourly air concentration plume composition from each dispersion model is compared to GOES Satellite data from the National Environment Satellite Data and Information Service (NESDIS). Analysis of satellite imagery at the beginning of the study simulation will show pollutants downwind that originated from the source long before the start of the experimental simulation. Therefore, model verification is conducted several hours after the release start to allow for particle dispersion.

At 22 UTC on the 9th, the GOES satellite image shown in Figure 5.63 depicts a plume dispersing
to the southeast of the wildfire. Figure 5.11 shows the FLEXPART-WRF EVANS12 simulation, which does illustrate southerly advection of particles, while HYSPLIT kept the particles closer to the source. However, the EVANS4 simulation did clearly illustrate dispersion to the south and east for both dispersion models (Figure 5.14). Across both EVANS12 and EVANS4 at 22 UTC, FLEXPART-WRF dispersed more to the south compared to the actual plume. By 11 UTC 10 June, the satellite image shows an eastward advection with an S-shaped plume structure offshore as shown in Figure 5.64. Close to the source, the observed plume was advecting eastward, which corresponds closely with the FLEXPART-WRF dispersion, especially using the EVANS4 solution (Figure 5.20). Prior to 11 UTC 10 June, the plume was transported to the north and veered to the east which is captured by both dispersion models. However, both FLEXPART-WRF and HYSPLIT do not clearly identify this S-shape plume at this time (Figure 5.19). FLEXPART does note higher air concentrations downwind from the source, which HYSPLIT does not resolve. A couple of hours later, the observed plume migrated east southeast with lingering concentration offshore as shown in Figure 5.65. FLEXPART-WRF is more representative of the observed plume across both EVANS12 and EVANS4 (Figure 5.21 and Figure 5.22).

Two hours later (18 UTC 10 June), pyroconvection forms over the wildfire due to excessive heat. Figure 5.66 and Figure 5.67 show the GOES and Aqua satellite imagery at 18 UTC on June 10. Some of the pollutants were ejected out of the PBL and dispersed north due to the southerly winds aloft. However, since the fire was widespread at this time, some of the downwind pollutants stayed within the PBL. The amount of air concentration may be affected by the pyroconvection, ejecting particles outside of the computational layer. As shown in Figure 5.68 and Figure 5.69, both models and domains show dispersion to the southeast with no pollutant ejection since pyroconvection is not modeled by WRF. Within both EVANS12 and EVANS4, FLEXPART-WRF shows a southeasterly dispersion of the plume while HYSPLIT transports the pollutants to the east. The offshore S-shaped plume is still identified by satellite at 18 UTC and is simulated by FLEXPART-WRF as shown in the EVANS12 simulation (Figure 5.68). HYSPLIT does not resolve higher concentration downwind or an observed “S-shape” plume. The plume migrated to the north shortly after the pyroconvection formed and dissipated as shown in the NEXRAD radar imagery (Figure 5.70).
Near the end of the simulation (08 UTC 11 June), both FLEXPART-WRF and HYSPLIT disperse the plume in an eastward direction (Figure 5.25). The observed plume, as shown in Figure 5.71, is advecting the particles to the east, which corresponds well with the FLEXPART-WRF simulation. Meanwhile, HYSPLIT disperses the plume to the northeast. Throughout the simulation, based on the 15 minute satellite imagery and animation, FLEXPART-WRF appears to have a better handle on the wildfire plume compared to HYSPLIT.

5.5 Dry Deposition

As pollutants are released into the atmosphere, gravitational settling and resistances lead to the fall out of particles from the atmosphere. As the particles deposit to the ground, the mass of pollutants within the atmosphere decreases. In the previous sections it was concluded that FLEXPART-WRF over both domains and through most of the simulations had a slightly higher air concentration. One hypothesis is that HYSPLIT deposits slightly more matter to the ground. Although the resistance method is used for both dispersion models, computational variability within the model documentations may play a role in deposition concentrations. In the next section, each dispersion model will be analyzed and compared based on dry deposition concentration found within the lowest 75 meters of the atmosphere.

5.5.1 Spatial Deposition Structure

At 22 UTC 09 June, FLEXPART-WRF illustrates dry deposition south of the source following the air concentration plume while HYSPLIT produces high deposition values over the release location as shown in Figure 5.72 and Figure 5.73. HYSPLIT deposits on average 30 ng m$^{-2}$ more matter than FLEXPART-WRF as indicated in Figure 5.74. At 02 UTC on the 9th, Figure 5.75 and Figure 5.76 shows the plume migration northward with HYSPLIT’s dry deposition decreasing (<5 ng m$^{-2}$) and little change among the FLEXPART-WRF simulation. In the early morning hours of the 10th (5 UTC), the EVANS12 FLEXPART-WRF plume starts to deposit higher amounts near the source while HYSPLIT deposits very little (<3 ng m$^{-2}$) to the surface as shown in Figure 5.77
and Figure 5.79a. According to Figure 5.78 and Figure 5.79b HYSPLIT resolved localized higher deposition downwind (>20 ng m$^{-2}$). By 08 UTC 10 June, Figure 5.80 and Figure 5.82a shows the EVANS12 HYSPLIT solution depositing over 30 ng m$^{-2}$ 40 km downwind of the source while FLEXPART-WRF deposits less than 10 ng m$^{-2}$ through the entire plume. Figure 5.81 and Figure 5.82b depicts localized deposition downwind of over 100 ng m$^{-2}$ within the EVANS4 solution. On the morning of the 10th (10 UTC), both dispersion models are illustrating deposition to the northeast with HYSPLIT producing 20 ng m$^{-2}$ higher concentration close to the source as shown in Figure 5.83 and Figure 5.84. Following the air concentration plume, HYSPLIT starts to deposit to the north of FLEXPART-WRF at 14 UTC (Figure 5.85, Figure 5.86). During this time, HYSPLIT deposits higher pockets of matter (∼60 ng m$^{-2}$) to the northeast while FLEXPART-WRF deposits approximately 5 ng m$^{-2}$ to the east. Analysis shows that the EVANS4 deposition solution at 14 UTC is more eastward compared to the EVANS12 solution. At 18 UTC on the 10th, HYSPLIT is depositing on average over 40 ng m$^{-2}$ more particles to the ground both 32 km and approximately 321 km downwind of the source as shown in Figure 5.87. By 20 UTC, a wind shift advects particles back to the north. FLEXPART-WRF and HYSPLIT deposit matter to the north of the source with HYSPLIT producing on average 10 ng m$^{-2}$ higher deposited concentration. This trend continues through 23 UTC 10 June as shown in Figure 5.88 and Figure 5.89. However, one hour later, HYSPLIT substantially decreases the amount of particles being deposited to the surface by 30 ng m$^{-2}$ (Figure 5.90). In Figure 5.91 and Figure 5.92, HYSPLIT deposition increases by 04 UTC 11 June with pockets of higher deposition (>30 ng m$^{-2}$) downwind extending back to the source through the next several hours. Figure 5.93 illustrates the HYSPLIT deposition occurring to the north FLEXPART-WRF. By the end of the simulation, HYSPLIT is still producing high deposition amounts >40 ng m$^{-2}$ in the EVANS12 solution and >100 ng m$^{-2}$ in the EVANS4 while FLEXPART-WRF is depositing to the east northeast at a constant rate of 5 ng m$^{-2}$ as shown in Figure 5.94, Figure 5.95 and Figure 5.96. The divergence between the two dispersion plumes is evident even among the deposition solution as FLEXPART-WRF removes matter to the south of HYSPLIT.
5.5.2 EVANS12 Dry Deposition Evaluation

Dry deposition produced by HYSPLIT and FLEXPART is very different both in regards to composition and concentration values. Figure 5.97 illustrates both the average and variances of the deposition concentration between the dispersion models. FLEXPART-WRF averages less than 3 ng m\(^{-2}\) throughout the simulation while HYSPLIT shows a spike in deposition (38.6 ng m\(^{-2}\)) within the first 10 hours of the simulation. HYSPLIT variance is large with a deposition standard deviation of 77.6 ng m\(^{-2}\), six hours after the release start. The total difference based on the average in deposition concentration is 255 ng m\(^{-2}\). As shown in Figure 5.98, HYSPLIT deposits \(~4000\%\) more matter on average during the 5th hour of the simulation than FLEXPART-WRF. The variability decreases rapidly between 10 and 20 hours. However, after the 20th hour, the variance begins to rise periodically throughout the rest of the simulation. This coincides with Figure 5.99 which highlights the extreme deposition values based on a box plot series. Based on these outliers, HYSPLIT computed a higher amount of deposited matter to the surface than FLEXPART-WRF. The maximum deposition concentration values during the first several hours were 88.8 ng m\(^{-2}\) and 21.2 ng m\(^{-2}\) for HYSPLIT and FLEXPART-WRF, respectively. Periodically after this time, HYSPLIT computed outliers of deposition concentration above 40 ng m\(^{-2}\). FLEXPART-WRF’s outliers average 2 ng m\(^{-2}\) throughout the rest of the simulation period. Following the air concentration plume, both dispersion models emphasize 4 peaks in concentration but they occur at difference times and magnitudes.

The outliers investigated do not fully reflect the whole data distribution. Figure 5.100 conveys 50\% of the data distribution around the median using percentiles. HYSPLIT computes on average an 86\% higher concentration within the first 15 hours than FLEXPART-WRF based on the upper quartile of data. Although there are large peaks in HYSPLIT concentration throughout the forecasting period, the average deposited concentration and percentiles deceased with time. These peaks are influenced by the increasing number of particles depositing to the ground. However, the spatial difference in deposition clearly identifies the peaks in concentration as shown in Figure 5.101. There are periods where FLEXPART-WRF does produce slightly higher deposition amounts (> 8 ng m\(^{-2}\)) than its counterpart (11-17 hours after the release start). The spatial difference is influenced by both
the spatial plume pattern and deposition concentrations. Given a normalized dataset, a student-t test was conducted to determine if the deposition differences between the dispersion models were significant. The student-t test verifies that the differences are significant over the majority of the forecast period (hour 2 and 7-47) as shown in Figure 5.102. The correlation between the models decrease with time in Figure 5.103.

5.5.3 EVANS4 Dry Deposition Evaluation

Similar to the EVANS12 solution, the average dry deposition, as shown in Figure 5.104, illustrates a peak in HYSPLIT deposition (~50 ng m\(^{-2}\)) six hours into the simulation. The standard deviation of deposition produced by HYSPLIT six hours after the start of the simulation are well above 150 ng m\(^{-2}\). The total difference based on the average of the deposition concentration yielded 160 ng m\(^{-2}\). In Figure 5.105, HYSPLIT deposits over 3000\% more matter to the ground than FLEXPART-WRF from hour 5 through 7 of the simulation period. The deposition distribution of each model over the forecast period is emphasized in Figure 5.106. At times the outlier deposition amounts within the EVANS4 simulation are 3 and 4 times larger in magnitude than those found within the EVANS12 solution. As illustrated, HYSPLIT is much larger in concentration amount (>300 ng m\(^{-2}\)) than FLEXPART-WRF with several deposition peaks identified. These peaks coincide with the spatial plume deposition structures. In an effort to highlight the majority of the data distribution based on the box plot series, Figure 5.107 emphasizes 50\% of the concentration distribution around the median. HYSPLIT has a 93\% higher concentration distribution based on the 75th quartile than FLEXPART-WRF within the first 15 hours similar to the EVANS12 simulation. This is an indication that the data distribution between the two domains is similar with exception to the extreme deposition values. After the 15th hour, the variability in HYSPLIT’s deposition decreases with an 80\% higher upper quartile compared to FLEXPART-WRF. Although, HYSPLIT has larger outlier concentrations, the increasing number of particles being deposited will have an impact on the average. An emphasis is placed on the actual spatial differences which is influenced by the spatial plume composition and deposition distribution as shown in Figure 5.108. With a positive difference, it is evident that HYSPLIT does indeed have a higher deposition during most of the simulation.
The deposition difference is centered near zero after 27 hours. Common to the EVANS12 data distribution, FLEXPART-WRF had a period of time (hour 11-17) where it had a slightly higher deposition than that of HYSPLIT. The significance of these differences are evaluated through a student-t test. In Figure 5.109, p-values are less than 0.05 through the whole simulation period making the differences in deposition concentration significant every hour.

### 5.5.4 Dry Deposition Summary

Based on the air concentration differences analyzed in Section 5.4, higher deposition rates were predicted for HYSPLIT, but not to this extent. It is hard to define the actual cause of these variations, but speculation can be made on the possible contributions. The equations used to calculate deposition for each model affects the overall result. Therefore, based on the deposition computations described in Chapter 4, the atmospheric and quasi-laminar resistances used to compute the deposition velocity have most likely led to these statistically significant differences. In addition, the atmospheric turbulence can play a large role in the amount of particulate matter getting to the surface, especially among the atmospheric layer resistance. This may explain the localized pockets of higher deposition concentration produced by HYSPLIT. Also, the land-surface and vegetation cover used to modify the atmospheric layer resistance impacts the deposition rate. After analysis of the deposition trend compared to the diurnal fluctuation of the temperature and subsequent boundary layer height, the variability in deposition can not be contributed to a diurnal feedback. Verification of dry deposition is very difficult and requires concentration measurements at or near the surface level. For this case study, there are no measurements available. Such differences in the spatial and temporal deposition concentration between the models and domains needs to be investigated in the future. In an effort to identify how much mass was lost within the air column due to dry deposition, Figure 5.111 illustrates the percent of the air column concentration (2000 m) that was deposited throughout the simulation. Although HYSPLIT is depositing at times over 3000% more matter to the surface than FLEXPART-WRF, it is only removing at most 1.3% of the total mass within the column. This spike in mass removal was not coupled with air concentration. Total, HYSPLIT removed 8.52% of mass from the air column compared to FLEXPART-WRF’s 2.2%.
This removal of mass only accounts for part of the air concentration differences between the models. Another attempt was made to help explain the slight differences in air concentrations between the models. Similar to the air concentration simulations described above, the EVANS12 simulation air concentration column was increased to 10000 m AGL in an effort to capture diffusion above the 2 km column top. Figure 5.112 illustrates the concentration between the two dispersion models under this constraint. Based on this analysis, FLEXPART-WRF produces ~15% higher air concentrations through a majority of the simulation period verified by the upper quartiles and median distribution. This finding still does not explain the slight air concentration difference produced by EVANS12 and EVANS4.

5.6 Summary

A comparative study was conducted using two dispersion models for the Evans Road wildfire in an effort to highlight any differences produced by the models. According to both EVANS12 and EVANS4, FLEXPART-WRF produced a ~12% higher air concentration values through a majority of the simulation. The overall air concentration distribution between the two models were very similar in magnitude, with the biggest differences found among the spatial plume composition. After 12 hours, the FLEXPART-WRF and HYSPLIT model solutions diverge. Analysis indicates that both dispersion models have similar horizontal diffusion patterns with the maximum air concentration signal produced by HYSPLIT decreasing approximately 400 km downwind. A sensitivity study based on the diffusion equations within the dispersion models may need to be investigated in order to fully comprehend these findings. Also, the high resolution model added some value at the beginning of the simulation, especially among the HYSPLIT solution, but did not bring the two models into better agreement later in the period.

Based on NESDIS satellite data, FLEXPART-WRF performed well through a majority of the simulation and is able to better replicate the observed plume as compared to HYSPLIT. Quantitatively, the differences between the models are found to be significant through a portion of the simulation. Dry deposition is investigated in an effort isolate the differing concentration values pro-
duced by the models. HYSPLIT is found to deposit a higher amount of particles to the ground compared to its counterpart, with no diurnal trend found. The peaks in deposition typically occur near the source, but do appear periodically downstream of the source. The areas of deposition tend to reduce downwind concentrations which can affect the overall diffusion of particles. It is unclear why HYSPLIT spikes in deposition at different times, but the differing equation (as reviewed in Chapter 4) may have had an impact. For example, the settling velocity and atmospheric and quasi-laminar resistance methods were different between the models. FLEXPART-WRF produces 3 to 4 times larger resistance than HYSPLIT, leading to smaller deposition. Although deposition is removing mass from the air column (especially within the first several hours), the deposition and air concentration seem to be decoupled with little reduction in air concentration noticed among the HYSPLIT simulations. The HYSPLIT deposition only accounts for part of the air concentration differences. In an attempt to explain other factors influencing the slight differences in air concentrations between the models, modification of the air concentration column was made. The EVANS12 air concentration column was increased to 10000 m AGL in an effort to capture vertical diffusion above the 2000 m. FLEXPART-WRF still produces ~15% higher air concentrations through a majority of the simulation period which does not help explain the air concentration differences. A vertical analysis of the dispersion process within each model, similar to that conducted by (Peffers, 2008), would highlight the particles entering and exiting the air column which may help explain some of the findings within this document. A sensitivity study based on the deposition equations would also be useful.
Figure 5.1: Evans Road Wildfire on June 9th, 2008 in the Pocosin Lakes National Wildlife Refuge within eastern NC.

Figure 5.2: Evans Road Wildfire on the afternoon of June 12th, 2008.
Figure 5.3: WRF Domain. The outer (12 km) domain is comprised of the eastern Continental U.S. with an inner (4 km) domain encompassing the eastern mid-Atlantic and northwestern Atlantic Ocean. The white dot denotes the location of the Evans Road Wildfire.
Figure 5.4: NCEP Surface Analysis
Figure 5.4: (cont.) NCEP Surface Analysis with wind, pressure, temperature and dew point temperature
Figure 5.5: WRF 12 km simulation of surface winds (kts), temperature (F) and pressure (hPa).

(a) 12 UTC 09 June

(b) 21 UTC 09 June
Figure 5.5: (cont.) WRF 12 km simulation of surface winds (kts), temperature (F) and pressure (hPa).
Figure 5.6: WRF 4 km simulation of surface winds (kts), temperature (F) and pressure (hPa).
Figure 5.6: (cont.) WRF 4 km simulation of surface winds (kts), temperature (F) and pressure (hPa).
Figure 5.7: Observed and WRF simulated sounding for the MHX observation site at 12 UTC 10 June.
Figure 5.8: WRF 12 km simulation of PBL Height (m) with diurnal trends noted by the large fluctuation in PBL height.
Figure 5.8: (cont.) WRF 12 km simulation of PBL Height (m) with diurnal trends noted by the large fluctuation in PBL height.
Figure 5.9: 12 km Sounding at the source site (Evans Road Wildfire).
Figure 5.10: 4 km Sounding at the source site (Evans Road Wildfire).
Figure 5.11: EVANS12 Air Concentration (ng m\(^{-3}\)) 19 UTC 09 June.
Figure 5.12: EVANS4 Air Concentration (ng m\(^{-3}\)) 19 UTC 09 June.
Figure 5.13: EVANS12 Air Concentration (ng m$^{-3}$) 22 UTC 09 June.
Figure 5.14: EVANS4 Air Concentration 22 UTC 09 June.
Figure 5.15: EVANS12 Air Concentration (ng m$^{-3}$) 04 UTC 10 June.
Figure 5.16: EVANS4 Air Concentration 04 UTC 10 June.
Figure 5.17: EVANS12 Air Concentration (ng m$^{-3}$) 07 UTC 10 June.
Figure 5.18: 4km Air Concentration 07 UTC 10 June.
Figure 5.19: EVANS12 Air Concentration (ng m$^{-3}$) 11 UTC 10 June.
Figure 5.20: 4km Air Concentration 11 UTC 10 June.
Figure 5.21: EVANS12 Air Concentration (ng m$^{-3}$) 16 UTC 10 June.
Figure 5.22: EVANS4 Air Concentration 16 UTC 10 June.
Figure 5.23: EVANS12 Air Concentration 23 UTC 10 June.
Figure 5.24: EVANS4 Air Concentration (ng m$^{-3}$) 23 UTC 10 June.
Figure 5.25: EVANS12 Air Concentration (ng m$^{-3}$) 08 UTC 11 June.
Figure 5.26: EVANS4 Air Concentration (ng m\(^{-3}\)) 08 UTC 11 June.
Figure 5.27: EVANS12 Air Concentration (ng m$^{-3}$) 12 UTC 11 June.
Figure 5.28: 4km Air Concentration (ng m$^{-3}$) 12 UTC 11 June.
Figure 5.29: Difference (ng m$^{-3}$) in Air Concentration at 19 UTC 09 June. Positive values (red) indicate HYSPLIT has a higher concentration over that particular grid. Negative values (blue) indicate FLEXPART-WRF has a higher concentration.
Figure 5.30: Difference (ng m$^{-3}$) in Air Concentration at 05 UTC 10 June.
Figure 5.31: Percent error between HYSPLIT and FLEXPART-WRF at 05 UTC 10 June. The percentage indicates how much higher or lower HYSPLIT air concentration is compared to the accepted FLEXPART-WRF concentration. Positive values (red) indicate HYSPLIT has a higher concentration over that particular grid. Negative values (blue) indicate FLEXPART-WRF has a higher concentration.
Figure 5.32: Difference (ng m\(^{-3}\)) in Air Concentration at 13 UTC 10 June.
Figure 5.33: Percent Difference (%) between FLEXPART-WRF and HYSPLIT at 13 UTC 10 June. Positive values (red) indicate HYSPLIT has a higher concentration over that particular grid. Negative values (blue) indicate FLEXPART-WRF has a higher concentration. The lighter shades indicated better precision between the two models, while darker shades indicate less precision.
Figure 5.34: Difference (ng m$^{-3}$) in Air Concentration at 17 UTC 10 June.
Figure 5.35: Difference (ng m$^{-3}$) in Air Concentration at 22 UTC 10 June.
Figure 5.36: Percent error between HYSPLIT and FLEXPART-WRF at 22 UTC 10 June.
Figure 5.37: Difference (ng m$^{-3}$) between FLEXPART-WRF and HYSPLIT at 06 UTC 11 June.
Figure 5.38: Difference (ng m\(^{-3}\)) in Air Concentration at 12 UTC 11 June.
Figure 5.39: Percent Difference (%) between FLEXPART-WRF and HYSPLIT at 12 UTC 11 June.
Figure 5.40: Percent error between HYSPLIT and FLEXPART-WRF at 12 UTC 11 June.
Figure 5.41: EVANS12 Average Air Concentration every hour throughout the simulation.
Figure 5.42: EVANS12 Percent Error of Air Concentration every hour throughout the simulation. Values >0% indicate that HYSPLIT is higher in air concentration on average and values <0% indicate that HYSPLIT is lower in air concentration on average.
Figure 5.43: Box Plot of the EVANS12 Air Concentration distribution. The bottom and top of the box plots are the 25th and 75th percentiles and the whiskers are one standard deviation away from the mean. The median is the dark line within the box. The small circles represents outliers of higher air concentrations.
Figure 5.44: EVANS12 Air Concentration distribution shown in Quartiles for FLEXPART-WRF and HYSPLIT (Q1 is the 25th percentile and Q3 is the 75th percentile).
Figure 5.45: Spatial Difference distribution of Air Concentration between FLEXPART-WRF and HYSPLIT throughout the simulation.
Figure 5.46: A sample of the Normalized Distribution of the Difference field at 07, 08, 09 and 10 UTC 10 June 08.
Figure 5.47: P-Values from Student-T test based on the Difference between FLEXPART-WRF and HYSPLIT.
Figure 5.48: 6 hr Log Correlation between FLEXPART-WRF and HYSPLIT within the first 24 hours of the start of release.
Figure 5.49: EVANS12 Correlation between FLEXPART-WRF and HYSPLIT.
Figure 5.50: Polygons assigned to EVANS12. The center of each polygon is placed 25 (1), 75 (2), 150 (3) and 250 (4) miles downwind of the source release.
Figure 5.51: EVANS12 Maximum Air Concentration Diffusion within Polygon 1, 2, 3 and 4.
Figure 5.52: EVANS12 Maximum Air Concentration shown for each Polygon.
Figure 5.53: EVANS4 Average Air Concentration every hour throughout the simulation.
Figure 5.54: EVANS4 Percent Error of Air Concentration every hour throughout the simulation. Values >0% indicate that HYSPLIT is higher in air concentration on average and values <0% indicate that HYSPLIT is lower in air concentration on average.
Figure 5.55: Box Plot of the EVANS4 Air Concentration distribution. The bottom and top of the box plots are the 25th and 75th percentiles and the whiskers are one standard deviation away from the mean. The median is the dark line within the box. The small circles represent outliers of higher air concentrations.
Figure 5.56: EVANS4 Air Concentration distribution shown in Quartiles for FLEXPART-WRF and HYSPLIT (Q1 is the 25th percentile and Q3 is the 75th percentile).
Figure 5.57: EVANS4 Spatial Difference distribution of Air Concentration between FLEXPART-WRF and HYSPLIT.
Figure 5.58: P-Values from Student-T test based on the Difference between FLEXPART-WRF and HYSPLIT
Correlation between FLEXPART and HYSPLIT 2008-06-09

Hours from Start of Release

Correlation

Figure 5.59: EVANS4 correlation between FLEXPART-WRF and HYSPLIT.

Figure 5.60: Polygons assigned to EVANS4. The center of each polygon is placed 25 (1), 75 (2) and 150 (3) miles downwind of the source release.
Figure 5.61: EVANS4 Maximum Air Concentration Dispersion within Polygon 1, 2 and 3
Figure 5.62: EVANS4 Maximum Air Concentration shown for each Polygon.
Figure 5.63: GOES Satellite Image at 22 UTC 09 June.
Figure 5.64: GOES Satellite Image at 11 UTC 10 June.
Figure 5.65: GOES Satellite Image at 16 UTC 10 June.
Figure 5.66: GOES Satellite Image at 18 UTC June 10.
Figure 5.67: AQUA high resolution satellite image at 18 UTC June 10.
Figure 5.68: Air Concentration (ng m$^{-3}$) at 18 UTC 10 June under the EVANS12 simulation.
Figure 5.69: Air Concentration (ng m$^{-3}$) at 18 UTC 10 June under the EVANS4 simulation.
Figure 5.70: NEXRAD Radar Image at 22 UTC June 10 with the pyroconvection to the left of the plume signature.
Figure 5.71: GOES Satellite Image at 08 UTC 11 June.
Figure 5.72: EVANS12 Dry Deposition (ng m²) 22 UTC 09 June.
Figure 5.73: EVANS4 Dry Deposition (ng m$^{-2}$) 22 UTC 09 June.
Figure 5.74: Difference (ng m$^{-2}$) in Dry Deposition at 22 UTC 09 June.
Figure 5.75: EVANS12 Dry Deposition (ng m$^{-2}$) 02 UTC 10 June.
Figure 5.76: EVANS4 Dry Deposition (ng m$^{-2}$) 02 UTC 10 June.
Figure 5.77: EVANS12 Dry Deposition (ng m$^{-2}$) 05 UTC 10 June.
Figure 5.78: EVANS4 Dry Deposition (ng m$^{-2}$) 05 UTC 10 June.
Figure 5.79: Difference (ng m$^{-2}$) in Dry Deposition at 05 UTC 10 June.
Figure 5.80: EVANS12 Dry Deposition (ng m$^{-2}$) 08 UTC 10 June.
Figure 5.81: EVANS4 Dry Deposition (ng m$^{-2}$) 08 UTC 10 June.
Figure 5.82: Difference (ng m$^{-2}$) in Dry Deposition at 08 UTC 10 June.
Figure 5.83: EVANS12 Dry Deposition (ng m^{-2}) 10 UTC 10 June.
Figure 5.84: EVANS4 Dry Deposition (ng m\(^{-2}\)) 10 UTC 10 June.
Figure 5.85: EVANS12 Dry Deposition (ng m\(^{-2}\)) 14 UTC 10 June.
Figure 5.86: EVANS4 Dry Deposition (ng m\(^{-2}\)) 14 UTC 10 June.
Figure 5.87: Difference (ng m$^{-2}$) in Dry Deposition at 18 UTC 10 June.
Figure 5.88: EVANS12 Dry Deposition (ng m$^{-2}$) 23 UTC 10 June.
Figure 5.89: EVANS4 Dry Deposition (ng m$^{-2}$) 23 UTC 10 June.
Figure 5.90: HYSPLIT Dry Deposition (ng m\(^{-2}\)) 00 UTC 10 June.
Figure 5.91: EVANS12 Dry Deposition (ng m$^{-2}$) 04 UTC 11 June.
Figure 5.92: EVANS4 Dry Deposition (ng m$^{-2}$) 04 UTC 11 June.
Figure 5.93: Difference (ng m$^{-2}$) in Dry Deposition at 06 UTC 11 June.
Figure 5.94: EVANS12 Dry Deposition (ng m\(^{-2}\)) 12 UTC 11 June.
Figure 5.95: EVANS4 Dry Deposition (ng m$^{-2}$) 12 UTC 11 June.
Figure 5.96: Difference (ng m$^{-2}$) in Dry Deposition at 12 UTC 11 June.
Figure 5.97: EVANS12 Average Dry Deposition every hour throughout the simulation.
Figure 5.98: EVANS12 Percent Error of Dry Deposition every hour throughout the simulation. Values >0% indicate that HYSPLIT is higher in air concentration on average and values <0% indicate that HYSPLIT is lower in air concentration on average.
Figure 5.99: Box Plot of the EVANS12 Dry Deposition distribution. The bottom and top of the box plots are the 25th and 75th percentiles and the whiskers are one standard deviation away from the mean. The median is the dark line within the box. The small circles represent the outliers of higher deposition concentrations.
Figure 5.100: EVANS12 Dry Deposition distribution shown in quartiles for FLEXPART-WRF and HYSPLIT (Q1 is the 25th percentile and Q3 is the 75th percentile).
Figure 5.101: EVANS12 Spatial Difference Distribution of Dry Deposition between FLEXPART-WRF and HYSPLIT.
Figure 5.102: P-Values from Student-T test based on the Difference between FLEXPART-WRF and HYSPLIT
Figure 5.103: Dry Deposition Correlation between FLEXPART-WRF and HYSPLIT within the EVANS12 Simulation.
Figure 5.104: EVANS4 Average Dry Deposition every hour throughout the simulation. The variance is denoted by the average standard deviation (SD).
Figure 5.105: EVANS4 Percent Error of Dry Deposition every hour throughout the simulation. Values >0% indicate that HYSPLIT is higher in air concentration on average and values <0% indicate that HYSPLIT is lower in air concentration on average.
Figure 5.106: Box Plot of the EVANS4 Dry Deposition distribution. The bottom and top of the box plots are the 25th and 75th percentiles and the whiskers are one standard deviation away from the mean. The median is the dark line within the box. The small circles represent the outliers of higher deposition concentrations.
Figure 5.107: EVANS4 Dry Deposition distribution shown in quartiles for FLEXPART-WRF and HYSPLIT (Q1 is the 25th percentile and Q3 is the 75th percentile).
Figure 5.108: EVANS4 Spatial Difference Distribution of Dry Deposition between FLEXPART-WRF and HYSPLIT.
Figure 5.109: P-Values from Student-T test based on the Difference between FLEXPART-WRF and HYSPLIT from the EVANS4 simulation.
Figure 5.110: Dry Deposition Correlation between FLEXPART-WRF and HYSPLIT within the EVANS4 Simulation.
Figure 5.111: Fraction of Column Mass that was deposited to the surface within the EVANS12 simulation
Figure 5.112: Box Plot of the EVANS12 Air Concentration distribution with the air column modified to 10000 m AGL. The bottom and top of the box plots are the 25th and 75th percentiles and the whiskers are one standard deviation away from the mean. The median is the dark line within the box. The small circles represents outliers of higher air concentrations.
Chapter 6

Case Study: South Mountain Wildfire

6.1 South Mountain State Park Wildfire

On the afternoon of September 28th, 2007, GOES satellite imagery captured a smoke plume from the South Mountain State Park region in North Carolina (Figure 6.1). With over 10,000 acres of park, there was no documentation of a fire or the extent of damage it may have caused. However, based on the images, the fire burned a little over 24 hours. The South Mountain Fire was one of the only recent fires captured by satellite during fair weather conditions over the Appalachians. The case study presented here will capture most of the fire’s duration in an effort to evaluate the dispersion models over more complex terrain.

6.2 Study Domain

The baseline WRF computational area consists of a 12 km and nested 4 km domain and is initialized by the NAM 12 km analysis. The model domain is shown in Figure 6.2. The outer domain contains 175 x 175 points spanning 2,100 x 2,100 km² across the eastern half of the United States.
The inner domain (d02) consists of 235 x 235 points spanning 940 x 940 km² encompassing part of the southeast. The two-day period of study was conducted from 28-29th September 2007. Both FLEXPART-WRF and HYSPLIT were designed to calculate air concentration and dry deposition using the WRF 12 km and 4 km domain, now referred to as SOUTH12 and SOUTH4, respectively.

6.3 WRF Configurations

The specific configuration regarding the WRF model can be found within Chapter 1. For this case study, the PBL scheme was set to the MYNN. As previously mentioned, a sensitivity study conducted by Olson and Brown (2009) and research findings by Peffers and Fuelburg (2009), indicated that this scheme may be most appropriate across regions of complex terrain.

6.4 Meteorological Conditions

6.4.1 Surface Conditions

Figure 6.3 shows high pressure across most of the central and eastern U.S leading to northerly winds during the simulation period. With a relaxed pressure gradient and minimal upper level forcing, the winds were light at 5 knots with occasional gusts due to turbulent mixing. As the high pressure system slowly migrated east, the winds at the surface veered with time helping to lower temperatures and mixing heights. Maximum temperatures were in the lower 80’s on the 28th and upper 70’s on the 29th with low relative humidity. Figure 6.4 and Figure 6.5 detail the WRF 12 km and 4 km simulation of temperature, pressure and wind direction and speed. The WRF simulated a high pressure system across the central U.S. which moved slowly eastward throughout the simulation period. The temperatures moderated from the lower 80’s on the afternoon of the 28th to the upper 70’s on the 29th as the winds veered from north to northeast. The WRF simulation compared well to observations.
6.4.2 Boundary Layer

The WRF simulated upper air analysis within both domains illustrated similar features to those observed at the Greensboro (GSO) and Peach Tree City (FFC) upper air sites as shown in Figure 6.6 and Figure 6.7. However, the layer above the PBL is substantially more dry in the WRF soundings. While this is a notable difference, it does not impact the dispersion process which typically involves transport winds and PBL depth.

In Figure 6.8, the dry air aloft and the aforementioned surface high induced stable conditions (CAPE<500 Jkg$^{-1}$) across the region throughout the simulation period. A diurnal trend of the planetary boundary layer was also observed. As shown in Figure 6.9, the PBL height rose to 1700 m during the afternoon hours (on the 29th) with a nocturnal inversion at 250 m across the South Mountain region.

6.5 Air Concentration Results

The air concentration was computed based on SOUTH12 and SOUTH4. Each simulation is driven by WRF output using the configurations emphasized in Chapter 1 and 4. Both models use the same WRF configurations and initialized parameters. The air concentration released a total of 10 kg (1x10$^{13}$ng) into the atmosphere from the source (latitude: 35.598, longitude: -81.659). Both dispersion models continuously released a total of 2 x 10$^6$ particles tracers (.4348 kg per hour) over a 23 hour period from 150 m AGL. The total air concentration is based on a 2 km air column from the surface. Following similar methods found in Chapter 5, air concentration is analyzed.

6.5.1 Plume Spatial Structure

Within the first couple hours of the simulation, the particles are displaced to the south of the source. Five hours after the start of the simulation, Figure 6.10 and Figure 6.11 suggest that the downwind particles produced by FLEXPART-WRF move to the south southwest while HYSPLIT advects the pollutants to the south as the high pressure system anchored across the central U.S. shifts to the east. The SOUTH12 simulation shows FLEXPART-WRF producing higher air concentration
(~6 ng m\(^{-3}\)) throughout the plume compared to HYSPLIT which produces higher concentration (~4 ng m\(^{-3}\)) closer to the source release. However, the SOUTH4 solution illustrates higher concentration values through both the FLEXPART-WRF (~8 ng m\(^{-3}\)) and HYSPLIT (~12 ng m\(^{-3}\)) plume. At 05 UTC the FLEXPART-WRF simulated plume starts to veer southwesterly while the HYSPLIT solution is still advecting particles to the south as shown in Figure 6.12 and Figure 6.13. The winds continue to veer throughout the rest of the simulation dispersing the particles to the southwest by the end of the simulation period (Figure 6.14 and Figure 6.15).

### 6.5.2 Model Evaluation

Within the first several hours the dispersion models diverge spatially. In Figure 6.16 HYSPLIT disperses particles south-southeast while FLEXPART-WRF advects particles south-southwest. By 14 UTC, HYSPLIT is dispersing particles to the south and FLEXPART-WRF to the southwest as illustrated in Figure 6.17. As noted in the previous section, HYSPLIT does eventually disperse particles to the southwest and it isn’t until after 14 UTC that the models come into better model agreement throughout the remaining simulation period. By the end of the simulation, both models are dispersing to the southwest with downwind divergence of air particles occurring over 320 km from the source as shown in Figure 6.18. In Figure 6.19, HYSPLIT produces on average 40% lower air concentration than FLEXPART-WRF within 80 km from the source. Although the spatial plume divergence between the two models is evident, it is hard to conclude based on this analysis which dispersion model produces an overall higher air concentration. In an effort to answer this question, a quantitative assessment of the air concentration distribution is discussed below.

### 6.5.3 SOUTH12 Air Concentration Evaluation

According to the average air concentration, as shown in Figure 6.20, HYSPLIT computes higher concentration (~4.1 ng m\(^{-3}\)) compared to FLEXPART-WRF (~2.8 ng m\(^{-3}\)) within the first few hours of the simulation. HYSPLIT computes on average 80% higher concentration than FLEXPART-WRF two hours after the start of the simulation as illustrated in Figure 6.21. Models concentration values come into better agreement 5 hours after the start of the simulation with the average dif-
ference in model magnitude quite minimal and the percent error approaching 0%. After the 15th hour of the simulation, FLEXPART-WRF computes a 20% higher air concentration. As a result, FLEXPART-WRF yields a 15% higher air concentration on average throughout the simulation. As previously mentioned, the average is influenced by the increasing number of particles in the atmosphere. Therefore, the concentration distribution between the two models needs to be emphasized. Figure 6.22 shows the air concentration distribution which is very similar in magnitude between the two dispersion models, with extreme values of concentration increasing over time. Based on this analysis, HYSPLIT produced a $\sim 5\%$ larger upper quartile and $\sim 3\%$ higher median values within the first five of hours. Thereafter, FLEXPART-WRF produced a $\sim 17\%$ larger upper quartile and $\sim 85\%$ higher median values than HYSPLIT through the rest of the simulation. While the dispersion models may show commonalities in the magnitude of concentration, there are spatial differences that are illustrated in Figure 6.23. The box plot series is skewed toward negative values indicating that FLEXPART-WRF produced higher air concentration values based on the plume placement and concentration. The outliers produced by HYSPLIT were higher than those produced by FLEXPART-WRF which increased HYSPLIT’s average air concentration values. Based on a normalized dataset, as shown in Figure 6.24, a student-t test is conducted using a 95% confidence interval to determine if the model spatial differences are significant (Figure 6.25). Through a majority of the simulation (hour 2, 4-8, 10 and 16-21) the differences were found to be significant ($p<0.05$).

Within the SOUTH12, the magnitude of air concentration was similar with the plume’s spatial structure being the biggest difference among the models. Again, it is hypothesized that the spatial extent of the plumes are being influenced by the diffusive nature of the models. Polygons set 80, 160 and 320 km downwind of the release location are used to compare the diffusion patterns of the particles within each model. Figure 6.26 shows the locations of each of the polygons relative to the release location. The maximum air concentration is captured by each polygon to evaluate the strength and pattern of the diffusion within both dispersion models. Based on this analysis, the diffusion strength is substantially different between the models with an average $2 \text{ ng m}^{-3}$ maximum air concentration difference as shown in Figure 6.27. In Figure 6.28, the diffusion signal through the polygons are evident among both models, but the temporal patterns of each model differ. The
FLEXPART-WRF solution keeps a strong concentration signal throughout all the polygons, especially within the first 10 hours of the simulation. HYSPLIT illustrates diffusion within the first two polygons with the concentration signal becoming weak beyond 320 km.

### 6.5.4 SOUTH4 Air Concentration Evaluation

The SOUTH4 quantitative concentration distribution shown in Figure 6.29 suggests that on average the HYSPLIT concentration is higher than FLEXPART-WRF until hour 16 as opposed to hour 7 within the SOUTH12 solution. In Figure 6.30, the percent error also indicates that HYSPLIT is producing on average a \(~20\%\) higher concentration within the first 16 hours of the simulation compared to FLEXPART-WRF. From hour 16 through the 21, HYSPLIT has 7% smaller air concentration compared to FLEXPART-WRF. As a result, HYSPLIT is 25% higher in air concentration on average throughout the simulation. Unlike the SOUTH12 solution, HYSPLIT computes a \(~5\%\) higher air concentration during the last 2 hours of the simulation period. One interesting feature captured by Figure 6.30 is the spike once produced (at 23 UTC 28 September) by the SOUTH12 average air concentration solution is reduced within the SOUTH4 simulation. This reduction was also observed in the Evans Road case study discussed in Chapter 5. With higher resolution modeling, there is more data which can influence the overall average by filtering out more of the higher concentration values. The air concentration values after the 5th hour come into better agreement. Again, this could be influenced heavily by the increasing number of particles in the atmosphere. In an effort to combat this issue, concentration distribution is investigated within each dispersion model. In Figure 6.31, HYSPLIT has larger extreme concentration values (\(~40\) ng m\(^{-3}\)) compared to FLEXPART-WRF (\(~25\) ng m\(^{-3}\)). However, the majority of the data (50%) centered around the mean would suggest that FLEXPART-WRF has a higher concentration overall with 0.1 ng m\(^{-3}\) difference in the upper quartile and median values. FLEXPART-WRF has a 53% higher upper quartile and a 25% higher median. Therefore, FLEXPART-WRF seems to produce a higher air concentration through the majority of the plume although the average air concentration (which is being heavily influenced by extreme values) suggests HYSPLIT produces a higher concentration. In Figure 6.32, the spatial difference in air concentration highlights the HYSPLIT outliers which
reached over 50 ng m$^{-3}$. Based on a 95% confidence interval over a normalized distribution, the differences are significant at hour 3-7, 11, and 16-17 as shown in Figure 6.33. This result is an overall improvement compared to the significance testing found in the SOUTH12 simulation.

While the concentration distribution patterns appear very comparable between FLEXPART-WRF and HYSPLIT, the differences in spatial distribution are significant. Such deviations can be produced by differing diffusion equations among the models. To investigate the horizontal diffusion pattern, polygons are placed 40, 120 and 240 km downwind of the source to capture the maximum air concentration values (Figure 6.34). The diffusion pattern within the SOUTH4 dispersion models is shown in Figure 6.35 with the maximum FLEXPART-WRF concentration peaking at the 2nd hour (4th for HYSPLIT) and diffusing throughout the polygons. FLEXPART-WRF produced a peak in concentration (6.3 ng m$^{-3}$) 7 hours into the simulation that did not get diffused through the downwind polygons. Also, HYSPLIT illustrated a maximum air concentration at the 12th hour that did diffuse downstream but was not simulated by FLEXPART-WRF. The HYSPLIT diffusion signal did improve compared to the SOUTH12 diffusion solution.

Based on the SOUTH12 evaluation, the air concentration magnitudes are very similar between the two dispersion models. Although HYSPLIT produces high concentration values, especially close to the source, FLEXPART-WRF simulates a higher air concentration through the plume over a majority of the simulated period. Again, the biggest difference is not the concentration values but the plume’s spatial and diffusive patterns produced by each of the models.

### 6.5.5 Verification

GOES Satellite images were able to approximately capture a plume from the South Mountain State Park region on September 28th, 2007. It is typically very difficult to observe a smoke plume, especially overland, such in this case (Li et al., 2000). However, the images during the early morning and evening time frames clearly depict the plume migration away from the source. Verification of these simulations also involves analysis of the animated satellite imagery which can lead to a better illustration of the plume migration. In the early morning hours on September 29th, a plume is observed (as a streak of white) just west of the North Carolina-Tennessee line as shown in Figure
6.37. At this time, FLEXPART-WRF’s southwesterly dispersion accurately captured the observed plume migration compared to the more southern stream solution produced by HYSPLIT (Figure 6.38). A couple of hours later, the plume is continuously migrating to the southwest (Figure 6.39) with FLEXPART-WRF better replicating the plume direction compared to HYSPLIT as shown in Figure 6.40. Near the end of the simulation, the observed plume is dispersing to the south-southwest as shown in Figure 6.41. Figure 6.42 shows the models coming in better agreement dispersing the particles to the southwest.

It is evident, especially when observing the animated plume, that FLEXPART-WRF has an overall better handle of the plume dispersion pattern. HYSPLIT forecasts the plume to go more south during the first several hours when in actuality the smoke plume was confined to the southwest as light northeasterly winds circulate around the high pressure system.

6.6 Dry Deposition

As particles are being released into the atmosphere, gravitational settling combined with atmospheric and quasi-laminar resistances will inevitably lead to the natural fall out of pollutants from the atmosphere. The particles will exit the column reducing the air concentration mass within the air column. Deposition is calculated within the lowest 75 m of the atmosphere. Following the methods found in Chapter 5, dry deposition is analyzed.

6.6.1 Spatial Plume Structure and Model Evaluation

In Figure 6.43, the SOUTH12 FLEXPART-WRF solution at 09 UTC on the 29th deposits a constant amount of matter to the ground throughout the simulation (<5 ng m$^{-2}$) with HYSPLIT producing a slightly higher deposition concentration (∼5 ng m$^{-2}$). In addition, the SOUTH4 HYSPLIT solution illustrates localized higher deposition (∼10 ng m$^{-2}$) approximately 240 km downwind of the source as shown in Figure 6.44. The spatial deposition pattern is illustrated in Figure 6.45 where HYSPLIT is depositing matter to the right of FLEXPART-WRF with higher concentration amounts highlighted in red. At 13 UTC on the 29th, the SOUTH12 HYSPLIT solution increases
deposition by almost 700% throughout the plume with deposition values ranging from 5 to over 200 ng m$^{-2}$ as shown in Figure 6.46 and Figure 6.48a. The SOUTH4 simulation, shown in Figure 6.47, illustrates a similar pattern with deposition ranging from 5 to over 500 ng m$^{-2}$ (Figure 6.48b). During the last couple hours of the simulation, HYSPLIT produces locally higher amounts of deposition ($\sim$40 ng m$^{-2}$) downwind that are resolved by the SOUTH12 solution (Figure 6.49 and Figure 6.51a) but are not simulated in the SOUTH4 as shown in Figure 6.50 and Figure 6.51b.

6.6.2 SOUTH12 Dry Deposition Evaluation

The average concentration distribution in Figure 6.52 suggests that both models are similar in deposition magnitude until the 15th hour of the simulation. HYSPLIT increased deposition by $\sim$7500% between hour 14 and 15 according to Figure 6.53. Based on this analysis, HYSPLIT yields a 150% higher deposition throughout the entire simulation. At this time, based on a box plot series of the deposition concentration shown in Figure 6.54, HYSPLIT deposition concentration is $\sim$8 times higher than that produced by FLEXPART-WRF. During the last couple of hours of the simulation, HYSPLIT returns to its original deposition rate ($\sim$10 ng m$^{-2}$) but produces deposition to localized areas which are illustrated by the outliers between hour 19 and 23.

The spatial difference distribution, as shown in Figure 6.55, is centered near zero, except from 13 UTC through 14 UTC. Using the student-t test under the assumption of a 95% confidence interval across a normalized distribution, Figure 6.56 shows the difference is found to be significant (p<0.05) during part of the simulation (hours 3, 4, 6-8, 15-19 and 22-23), most notably corresponding with the spike in deposition produced by HYSPLIT.

Analysis of mass continuity was investigated in an effort to quantitatively assess how much matter was being removed from the air concentration column based on dry deposition. Figure 6.62 illustrates that little mass ($<$1%) was removed during most hours of the simulation with over 2% being removed during the high deposition episode at the 15th and 16th hour.
6.6.3 SOUTH4 Dry Deposition Evaluation

The average concentration distribution among the SOUTH4 simulation, as shown in Figure 6.57, follows a similar trend found in the SOUTH12 solution. However, as noted throughout this document, the SOUTH4 produces higher extreme concentration amounts across both dispersion models, especially close to the source. Based on the percent error (Figure 6.58) of the dry deposition distribution between the two dispersion model, HYSPLIT deposits on average 8000% more matter to the surface than that produced by FLEXPART-WRF between the 15th and 16th hour of the simulation period. Based on this analysis, HYSPLIT yields a 287% higher deposition than FLEXPART-WRF. In Figure 6.59, a box plot series of the deposition distribution shows the extremely large outliers (>800 ng m\(^{-2}\)) produced by HYSPLIT as compared to FLEXPART-WRF (< 30 ng m\(^{-2}\)) from hour 15 to 16. Also, within the first 5 hours, 50% of the data centered around the mean (based on the upper quartiles) suggests that HYSPLIT is producing \(\sim\)80% higher deposition compared to FLEXPART-WRF. The spatial difference in deposition concentration between two models, as shown in Figure 6.60, also highlights the high deposited values produced by HYSPLIT during the 15th and 16th hour of the simulation. Based on the student-t test, these deposition differences are significant with p-values well below the 0.05 threshold (except hour 21 which had a p-value of 0.07) as shown in Figure 6.61.

6.7 Summary

A comparative study was conducted based on the South Mountain State Park wildfire in an effort to highlight the performance of the dispersion models across complex terrain. Similar to the previous study, the overall air concentration distribution between the two models were very comparable. The largest differences between the models are the spatial plume composition and dry deposition. During most of the simulation, HYSPLIT dispersed well to the right of FLEXPART-WRF leading to statistically significant differences between the models. Due to this discrepancy, we hypothesized that diffusion may play a role in the differing plume composition produced by each of the dispersion models. Based on the horizontal diffusion analysis, FLEXPART-WRF illustrated the
transport of high concentration particles through space and time more clearly than HYSPLIT among
the SOUTH12 simulation. However, HYSPLIT diffusion patterns improved within the SOUTH4
simulation. While diffusion is noted among each model, the temporal patterns are different. This
result may be a sign of diffusion issues within the models that have lead to spatial variability. The
high resolution model did add some benefit as the solution produced a less significant differences
between the model.

Based on NESDIS satellite data, FLEXPART-WRF performed well compared to the observed
plume transporting the particles to the southwest. HYSPLIT produced dispersion to the south
during the first several hours. The dispersion plumes did come into better agreement near the end
of the simulation.

Dry deposition is an important feature within dispersion models that represents the fall out
of particles from pollutant plumes. Similar to the previous case, HYSPLIT was found to deposit
much higher amounts of matter to the ground, with no diurnal trend found. The percent of mass
removed from the total air column due to deposition was less than 1% during most of the simulation.
However, high deposition led to a larger percent of mass (>2%) being removed at hour 15 and 16.
The removal of air concentration by dry deposition impacted the diffusive nature of the particles.

While the high deposition rates produced in this case study have little impact on the air con-
centration, other simulation circumstances (e.g. episode duration, weather conditions, etc.) may be
more heavily influenced by deposition. Again, it is unclear why HYSPLIT spikes in deposition at
different times, but the differing deposition equations within the models may have had an impact.
Unfortunately, deposition can not be verified due to lack of observation. It should be noted though,
that these differences are significant and should be studied in more detail. A vertical analysis and
sensitivity study may be required in order to achieve a concrete understanding of these results.
Figure 6.1: South Mountain Wildfire location embedded within the Appalachians of North Carolina. Warmer colors indicating higher elevation.

Figure 6.2: WRF Domain. The outer 12 km domain spans across most of the eastern United States. The inner 4 km domain (d02) encompasses part of the southeast. The white dot denotes the South Mountain Wildfire location.
Figure 6.3: NCEP Surface Analysis.
Figure 6.4: WRF SOUTH12 simulation of surface winds (kts), temperature (F) and pressure (hPa).
Figure 6.5: WRF SOUTH4 simulation of surface winds (kts), temperature (F) and pressure (hPa).
Figure 6.6: Sounding for the GSO observation site at 12 UTC 29 September.
Figure 6.7: Sounding for the FFC observation site at 12 UTC 29 September.
Figure 6.8: Sounding at the source site (South Mountain State Park).

(a) 12 km Sounding at 00 UTC 29 September 07
(b) 12 km Sounding at 12 UTC 29 September 07
(c) 4 km Sounding at 00 UTC 29 September 07
(d) 4 km Sounding at 12 UTC 29 September 07
Figure 6.9: WRF SOUTH12 simulated PBL Height (m)
Figure 6.10: SOUTH12 Air Concentration (ng m$^3$) 03 UTC 29 September.
Figure 6.11: SOUTH4 Air Concentration (ng m$^3$) 03 UTC 29 September.
Figure 6.12: SOUTH12 Air Concentration (ng m$^3$) 05 UTC 29 September.
Figure 6.13: SOUTH4 Air Concentration (ng m$^3$) 05 UTC 29 September.
Figure 6.14: SOUTH12 Air Concentration (ng m\(^3\)) 21 UTC 29 September.
Figure 6.15: SOUTH4 Air Concentration (ng m$^3$) 21 UTC 29 September.
Figure 6.16: Difference (ng m\(^3\)) in Air Concentration at 03 UTC 29 September. Positive values (red) indicate HYSPLIT has a higher concentration over that particular grid. Negative values (blue) indicate FLEXPART-WRF has a higher concentration.
Figure 6.17: Difference (ng m$^3$) in Air Concentration at 14 UTC 29 September.
Figure 6.18: Difference (ng m$^3$) in Air Concentration at 21 UTC 29 September.
Figure 6.19: Percent error between FLEXPART-WRF and HYSPLIT at 21 UTC 29 September.
Figure 6.20: SOUTH12 Average Air Concentration every hour throughout the simulation.
Figure 6.21: SOUTH12 Percent Error of Air Concentration every hour throughout the simulation. Values >0% indicate that HYSPLIT is higher in air concentration on average and values <0% indicate that HYSPLIT is lower in air concentration on average.
Figure 6.22: Box plot of the SOUTH12 Air Concentration distribution. The bottom and top of the box plots are the 25th and 75th percentiles and the whiskers are one standard deviation away from the mean. The median is the dark line within the box. The small circles represents outliers of higher air concentration.
Figure 6.23: Spatial Difference distribution of Air Concentration between FLEXPART-WRF and HYSPLIT throughout the simulation.
Figure 6.24: A sample of the Normalized Distribution of the Difference field between 12 and 15 UTC 29 September 07.
Figure 6.25: P-Values from Student-T test based on the Difference between FLEXPART-WRF and HYSPLIT
Figure 6.26: Polygon Map for the SOUTH12 simulation. Polygons are set 80, 160 and 320 km downwind of the release source.
Figure 6.27: SOUTH12 Maximum Air Concentration Diffusion within Polygon 1, 2 and 3.
Figure 6.28: SOUTH12 Maximum Air Concentration shown for each Polygon.
Figure 6.29: SOUTH4 Average Air Concentration every hour throughout the simulation.
Figure 6.30: SOUTH4 Percent Error of Air Concentration every hour throughout the simulation. Values >0% indicate that HYSPLIT is higher in air concentration on average and values <0% indicate that HYSPLIT is lower in air concentration on average.
Figure 6.31: Box plot of the SOUTH4 Air Concentration distribution. The bottom and top of the box plots are the 25th and 75th percentiles and the whiskers are one standard deviation away from the mean. The median is the dark line within the box. The small circles represents outliers of higher air concentration.
Figure 6.32: Spatial Difference distribution of Air Concentration between FLEXPART-WRF and HYSPLIT throughout the simulation. Positive values correspond with larger HYSPLIT values while negative values with FLEXPART-WRF values.
Figure 6.33: P-Values from Student-T test based on the Difference between FLEXPART-WRF and HYSPLIT
Figure 6.34: Polygon Map for the SOUTH4 simulation. Polygons set 40, 120 and 240 km downwind of the source release site.
Figure 6.35: SOUTH4 Maximum Air Concentration Diffusion within Polygon 1, 2 and 3.
Figure 6.36: SOUTH4 Maximum Air Concentration shown for each Polygon.
Figure 6.37: GOES Satellite Image 1215 UTC 29 September 07.
Figure 6.38: Air Concentration (ng m$^3$) 12 UTC 29 September 07.
Figure 6.39: GOES Satellite Image 15 UTC 29 September 07.
Figure 6.40: Air Concentration (ng m$^3$) 12 UTC 29 September 07.
Figure 6.41: GOES Satellite Image 2132 UTC 29 September 07.
Figure 6.42: Air Concentration (ng m$^3$) 21 UTC 29 September 07.
Figure 6.43: SOUTH12 Dry Deposition (ng m$^2$) 09 UTC 29 September.
Figure 6.44: SOUTH4 Dry Deposition (ng m$^2$) 09 UTC 29 September.
Figure 6.45: Difference (ng m$^2$) in Dry Deposition 09 UTC 29 September.
Figure 6.46: SOUTH12 Dry Deposition (ng m\(^2\)) 13 UTC 29 September 07.
Figure 6.47: SOUTH4 Dry Deposition (ng m$^2$) 13 UTC 29 September.
Figure 6.48: Difference (ng m$^2$) in Dry Deposition 13 UTC 29 September 07.
Figure 6.49: SOUTH12 Dry Deposition (ng m$^2$) 21 UTC 29 September 07.
Figure 6.50: SOUTH4 Dry Deposition (ng m$^2$) 21 UTC 29 September 07.
Figure 6.51: Difference (ng m$^2$) in Dry Deposition 21 UTC 29 September 07.
Figure 6.52: SOUTH12 Average Dry Deposition every hour throughout the simulation.
Figure 6.53: SOUTH12 Percent Error of Dry Deposition every hour throughout the simulation. Values >0% indicate that HYSPLIT is higher in air concentration on average and values <0% indicate that HYSPLIT is lower in air concentration on average.
Figure 6.54: Box plot of the SOUTH12 Dry Deposition distribution. The bottom and top of the box plots represent the 25th and 75th percentiles and the whiskers are one standard deviation away from the mean. The median is the dark line within the box. The small circles represent the outliers of the higher deposition concentrations.
Figure 6.55: SOUTH12 Spatial Difference Distribution of Dry Deposition between FLEXPART-WRF and HYSPLIT.

(a) Spatial Difference

(b) Range between -2 and 2 ng m$^{-2}$
Figure 6.56: P-Value from Student-T test based on the Difference between FLEXPART-WRF and HYSPLIT
Figure 6.57: SOUTH4 Average Dry Deposition every hour throughout the simulation.
Figure 6.58: SOUTH4 Percent Error of Dry Deposition every hour throughout the simulation. Values >0% indicate that HYSPLIT is higher in air concentration on average and values <0% indicate that HYSPLIT is lower in air concentration on average.
Figure 6.59: Box plot of the SOUTH4 Dry Deposition distribution. The bottom and top of the box plots represent the 25th and 75th percentiles and the whiskers are one standard deviation away from the mean. The median is the dark line within the box. The small circles represent the outliers of the higher deposition concentrations.
Figure 6.60: SOUTH4 Spatial Difference Distribution of Dry Deposition between FLEXPART-WRF and HYSPLIT.
Figure 6.61: P-Value from Student-T test based on the Difference between FLEXPART-WRF and HYSPLIT.
Figure 6.62: Percent (%) of mass removed from the air column due to deposition within the SOUTH12 domain.
Chapter 7

Summary and Conclusions

Atmospheric transport and dispersion models are widely used across operational and research settings. Operational forecasters work closely with emergency managers and the public to provide site specific information and dispersion forecasts. Operational agencies within the U.S. often use the HYSPLIT model for chemical, accidental and natural pollutant releases. Research agencies utilize many dispersion models for air quality and chemical studies. No matter what the application, hazardous material entering the atmosphere can impact life and property. Therefore, accurately forecasting the transport and dispersion of pollutants is extremely valuable.

A comparative study between two Lagrangian dispersion models (i.e. HYSPLIT and FLEXPART-WRF) was conducted to determine which model performed best across the complex terrain and geography of NC. In an effort to identify the physics, limitations and assumptions embedded within each dispersion model, an in depth analysis of the underlying software was reviewed. The largest computational discrepancies found within the dispersion models were the diffusion methods, time steps and removal techniques. These differences can have a profound impact on both the plume structure and concentration values as seen in this study. The dispersion models are sensitive to the input meteorological models and the initialized parameters that are ingested. The mesoscale meteorological model WRF was used by both the dispersion models. A typical 12 km and high resolution 4 km domain are used within both case studies in an effort to determine if the high resolution would
bring the dispersion models into better agreement. One limitation of the WRF is its inability to
depict a fire high spot which can have an impact on the accuracy of the stability and atmospheric
environment around the wildfire. Both dispersion models have been used for similar types of studies
(i.e. smoke emissions, urban dispersion, air quality, etc.). However, HYSPLIT is most widely used
under operational settings, especially within the United States. FLEXPART-WRF is used very little
within the U.S. and most of its applications are research-based. This study evaluates the versatility,
accuracy and efficiency of FLEXPART-WRF within an operational setting.

The focus of this study was to compare FLEXPART-WRF and HYSPLIT across complex terrain
and geography using two wildfire case studies. The research configuration required pre-processing
of initialized parameters and meteorological data that were fed into the dispersion model. The
initialized parameters were identical between the dispersion model while high resolution meteo-
rological data (WRF) guided the transport and dispersion of particles from the source. However,
each dispersion model was configured to ingest different meteorological data which led to differing
computations embedded within the software. Once the dispersion models simulate the transport
and dispersion of particles and calculate the resultant air and deposited concentration, the output
is post-processed using GIS, analyzed and validated with remote sensing information.

7.1 Evans Road Wildfire

A prolonged wildfire within the coastal plain of NC was simulated from 13 UTC 09 June 08
through 12 UTC 11 June 08. High pressure was in control over much of the southeast. A cold front
approached from the west by the end of the simulation period. The WRF model was validated based
on NCEP surface observations and upper air soundings. Although identical meteorological condi-
tions and initialized parameters were used, FLEXPART-WRF and HYSPLIT produced significantly
different dispersion plumes. While air concentration magnitudes were similar, the spatial plume
compositions were found to be substantially different. Twelve hours after the simulation start, the
HYSPLIT plume started to migrate to the north (right) of FLEXPART-WRF. This trend continued
for the rest of the simulations leading to statistically significant differences between the model
solutions. The spatial differences in plume placement is thought to be due to differences in model diffusion dynamics. Spatial differences were found to be significant at hours 5, 10-11 and 13-47 within the EVANS12 simulation and hours 1, 3-5, 10, 13-23, 24-40 and 44-47 within the EVANS4 simulation. The horizontal diffusion pattern were similar between the models. However, HYSPLIT did not produce strong concentrations 400 km downwind which led to weak diffusion signals. The plume spatial structure between the two models illustrated divergence after 12 hours with HYSPLIT dispersion to the right of FLEXPART-WRF by approximately 10 degrees. A sensitivity study based on the diffusion mode within each model is warranted. Based on statistical analysis, FLEXPART-WRF was found to have a on average a 25% higher air concentration (based on EVANS12 and EVANS4) through most of the simulation with larger concentrations downwind of the source compared to HYSPLIT. One hypothesis being that HYSPLIT either deposits slightly more matter to the ground or diffuses more mass above the 2 km air column. Dry deposition was extensively investigated for this reason and will be reviewed below. A simulation was constructed to increase the air concentration column (surface-10000 m) in an effort to capture diffusion above the original column top (2000 m). Based on this modified simulation, HYSPLIT is on average 25% smaller in air concentration compared to FLEXPART-WRF through a majority of the simulation. This result indicates that HYSPLIT does not diffuse more mass above above 2 km than FLEXPART-WRF.

Forecasting offices typically use a 12 km domain when forecasting pollutant releases. Not all operational offices have high resolution nested domains across their local area, but this trend is growing in popularity. Therefore, the case studies presented here were run using both a 12 km and 4 km resolution (referred to as EVANS12 and EVANS4, respectively). The hypothesis being that EVANS4, given a more accurate and extensive data set, would result in a better dispersion forecast. Many of the variables that were once parameterized in EVANS12 can be explicitly resolved by EVANS4 leading to a better representation of the atmosphere. Within the first several hours, the EVANS4 dispersion solution did extend the HYSPLIT plume to the south which compared better with observations. Also, the EVANS4 solution eliminated a erroneous spike in air concentration once produced by the EVANS12 FLEXPART-WRF solution. However, the EVANS4 simulation still resulted in HYSPLIT dispersing to the north of FLEXPART-WRF after 12 hours. The higher
resolution did bring the dispersion models into better agreement and verification was improved within the first few hours. During the remaining simulation period, the EVANS4 solutions still diverged. The high resolution provides a clearer depiction of the concentration pockets and plume location. If given the opportunity to run the dispersion model with a high resolution it would be wise to do so. Based on both domain simulations, FLEXPART-WRF was found to better represent the observed plume according to GOES satellite imagery.

Dry deposition is the fall out of particles from the atmosphere. Since FLEXPART-WRF had a slightly higher concentration, especially downwind from the source, deposition was hypothesized to be slightly higher for HYSPLIT. HYSPLIT did indeed produce higher deposited concentration to the ground and to an extent that was not forecasted. Throughout the simulation across both domains, HYSPLIT calculated at times over 3000% higher deposition than FLEXPART-WRF. The EVANS4 solution produced localized higher deposition amounts that are not resolved by the EVANS12 simulation. Following the air concentration plume, HYSPLIT was depositing matter to the north of FLEXPART-WRF during most of the simulation. The concentration values and spatial plume differences led to statistically significant differences in deposition at the 95th confidence interval between the two dispersion models. It is unclear from this analysis why HYSPLIT is producing localized high deposition. Based on dry deposition computation, the FLEXPART-WRF equations result in higher resistances (i.e. atmospheric and quasi-laminar) leading to less deposition. However, this still does not explain the pockets of higher deposition and variability that occurred throughout HYSPLIT’s experimental study. Although deposition is quite large across HYSPLIT, it has little impact on the overall air concentration amounts produced. Many other studies have shown issues with deposition values (Wain et al., 2006; Draxler, 1999). An in depth analysis needs to be conducted based on the HYSPLIT removal methods and output to better investigate the possible causes of the high deposition and slightly lower concentrations in HYSPLIT.
7.2 South Mountain Wildfire

A short lived wildfire embedded within the Appalachian mountains of NC was observed by satellite on September 28, 2007. The fire was visible with GOES satellites and lasted approximately 24 hours. This fire event both challenged the meteorological and dispersion models while also producing a reasonable forecast duration. Using the same analysis methodology used for the Evans Road event, the South Mountain wildfire was simulated by both FLEXPART-WRF and HYSPLIT in an effort to compare the dispersion models across complex terrain. With dominant high pressure over the central U.S., the WRF model had a good handle on the atmosphere through most of the simulation.

The fire was simulated from 21 UTC 28 September 07 through 22 UTC 29 September 07 across a 12 km (SOUTH12) and 4 km (SOUTH4) domain. Much like the Evans Road wildfire study, concentration magnitudes were similar between the models and the SOUTH4 solution produced higher concentration values. While HYSPLIT illustrated larger extreme (outlier) concentrations, FLEXPART-WRF produced an overall higher air concentration throughout much of the simulation period. Within the first several hours, the spatial plume composition diverged quite a bit between the two models with HYSPLIT dispersing particles to the right of FLEXPART-WRF. After 10 hours, the model plumes came into better agreement within 80 km of the source. However, the downwind plumes were still diverging with FLEXPART-WRF advecting particles to the left of HYSPLIT. Differences in plume placement and concentration led to statically significant differences in air concentration between the models (hour 2, 4-8, 10 and 16-21 for SOUTH12 and 3-7, 11 and 16-17 for the SOUTH4). Based on plume composition alone, the higher resolution meteorological data did not seem to bring the models into better agreement. However, the significance testing illustrates that the differences within the SOUTH4 solution decreased between the two models through a portion of the simulation period. Again, this finding reemphasizes that if a high resolution meteorological model is available it should be used for dispersion modeling at local scales. Since there were significant differences in the model air concentration based on spatial plume composition, the horizontal diffusion patterns are investigated. The pattern between HYSPLIT and FLEXPART-WRF were dissimilar with diffusion illustrated best in the SOUTH4 simulations. The differences in
horizontal diffusion are thought to be based on the large spatial spread between the modeled plumes. As noted in the previous case study, vertical diffusion needs to be investigated across both dispersion models in an effort to understand the spatial discrepancies. Overall, FLEXPART-WRF performed best compared to the satellite images. Although, the images alone are very hard to analyze, the animated plumes further suggest that FLEXPART-WRF performed better than HYSPLIT.

Dry deposition was investigated for this case study. The deposition pattern between FLEXPART-WRF and HYSPLIT were found to be significantly different. Fifteen hours into the simulation, HYSPLIT produced 8000% higher deposition compared to FLEXPART-WRF across a large portion of the air concentration plume. This period of high deposition lasted only a couple of hours before returning to its original deposition rate. Throughout most of the simulation the dispersion models compared well in deposition concentration with localized higher values produced by HYSPLIT. Such differences led to statistically significant differences in dry deposition concentration between the models. Although the mass removed from deposition is small compared to the overall column of air concentration, spikes in deposition produced by HYSPLIT could have a large impact on air concentration amounts under special circumstances. This area needs to be investigated to determine the causes of the differences in model dry deposition amounts.

7.3 Conclusions

Among both case studies and across both resolutions, HYSPLIT dispersed particles to the right of FLEXPART-WRF. Within the Evans Road case study, HYSPLIT dispersed particles 10 degrees to the north (right) of FLEXPART-WRF at the source after the 12th hour of the simulation. Conversely, HYSPLIT advected particles 20 degrees to the right of FLEXPART-WRF within the first 12 hours of the South Mountain case study simulation. The plume composition differences are most likely linked to the differing diffusion equations found within the model software. The dispersion of particles is also influenced by HYSPLIT’s large concentration removal via deposition. Analysis found that FLEXPART-WRF produced a higher concentration throughout both of the case study simulations. While the differences in air concentration between the two dispersion models are small.
compared to the source strength, the spatial difference in concentration values led to statistically significant differences between the two dispersion models across both cases based on plume placement and concentration. In an effort to isolate the reason for these differences, deposition was investigated.

HYSPLIT produced higher deposition in both the Evans Road and South Mountain case studies, at times removing 2% of mass from the air column. Large fluctuations in HYSPLIT deposition were observed close to the source with localized areas of high deposition occurring downwind. For approximately 2 hours of the simulation of the South Mountain case study, HYSPLIT deposited 10 times more matter to the ground compared to FLEXPART-WRF. This combined with deposition placement led to statistically significant spatial deposition differences between the two models. Again, these areas of deposition can impact the diffusion of particles within the atmosphere. The reason for such large deposition differences is not clear, but the differing deposition resistance equations have an impact. Although HYSPLIT does remove more mass out of the air column compared with FLEXPART-WRF, this did not fully account for the air concentration differences. Therefore, a modified simulation was conducted to account for a larger air column of concentration. The air column was increased to 10000 m (top of the model) to investigate any diffusion occurring above the original column top (2000 m). Based on the continuity of mass, the air concentration should be nearly identical between the two models. However, FLEXPART-WRF was still found to be higher in air concentration by approximately 15%. It should be emphasized that such differences in air concentration and dry deposition as well as plume composition from dispersion models can have a considerable influence on decisions made by forecasters and emergency managers. Therefore, additional work must be conducted on this topic which will be reviewed in Section 7.5.

Based on remote sensing technologies, FLEXPART-WRF appeared to better replicate the observed plume across both wildfire case studies. Therefore, based on the results of this study, FLEXPART-WRF appears to be a more accurate operational tool. Following the case studies presented here, both dispersion models are very operationally efficient taking approximately 10 minutes to run.
7.4 Impacts of Research

Air concentration values produced by both dispersion models across each wildfire case study were comparable. The spatial distribution of the air concentration was one of the biggest differences found between the models. Within both case studies, HYSPLIT illustrates a rightward diffusion of particles compared to FLEXPART-WRF. Such difference in the spatial plume structure could largely impact operational forecasters and emergency managers. Forecasters rely on the modeled simulations of the plume placement and concentration distribution when issuing air quality and dense smoke advisories. Also, emergency managers collaborate with forecasters to determine evacuation areas and routes. An inaccurate forecast of the plume dispersion could be costly to both life and property.

Operational forecasters, such as those forecasting the transport of disease spores from vegetation, rely heavily on particle deposition produced by the dispersion models. There were statistically significant differences in deposition among both case studies based on concentration and location. At times throughout each simulation, HYSPLIT deposited a larger amount of mass to the surface compared to FLEXPART-WRF. In addition, HYSPLIT deposited particles to the right of FLEXPART-WRF following the air concentration plume. Such differences in deposition concentration and placement could impact the forecast. These forecasts will help determine if farmers need to spray for disease spores across their crop. Over spraying can be very costly to the farmers and the end users (consumers).

The comparative study highlights the differences between HYSPLIT and FLEXPART-WRF so they can be run simultaneously in the future with the basic understanding of their limitations, assumptions and approximations. Their deficiencies have been noted within this document and the operational assessment of FLEXPART-WRF is reviewed in Section 7.5.

7.5 Future Work

The study presented highlights the differences produced by two very similar Lagrangian dispersion models, one of which is used frequently as an operational tool within many governmental
agencies. The differences in model output could have substantial ramifications during the decision making process leading to impacts on life and property. Therefore, it is imperative that future work be done in this area to ensure accurate dispersion modeling is being simulated.

It was shown that air concentration plumes between FLEXPART-WRF and HYSPLIT are similar in magnitude but different in placement. It was noted that the diffusion equations embedded within each model were different and thus could impact the overall result. Although horizontal diffusion was tested, vertical diffusion of particles in and out of the air column needs to be investigated in an effort to understand the results found within this document. A sensitivity study based on the diffusion mode should also be researched in the future. Since the time steps between both models are very complex it may be difficult to test this parameter.

One of the biggest differences between the models are the dry removal concentrations. The deposition resistance methods between the two models are different by factors of 3 and 4 based on the quasi laminar sublayer and atmospheric resistance techniques, respectively. Such differences could impact the overall result. Based on personal communication with Draxler (2010), HYSPLIT dry deposition could produce high values of deposition if there are not enough particles released both spatially and temporally. However, within this study over 2 million particles were released ranging from 23 to 47 hours. An in depth investigation needs to be conducted on the removal methods, especially those found within HYSPLIT. Although deposition was found to hold little impact on the air concentration values within the study, under certain conditions it can cause issues (i.e. short releases, little matter being released, short vertical extent of the air concentration column, etc.).

Within this study, the spatial divergence and concentration distribution were being influenced by the continuous release of mass into the atmosphere. Therefore, a similar study investigating an instantaneous source release would help to clearly identify spatial divergence and air concentration and deposition fluctuations found within each of the dispersion models.
7.6 Operations

FLEXPART-WRF will be implemented as an operational tool for the Cucurbit Downey Mildew forecasting team at North Carolina State University in the Summer of 2010. The forecasting team will use a 72 hour FLEXPART-WRF simulation to aid in vegetable disease dispersion. Using a web-based tool, forecasters can indicate the location of disease spore(s), the release amount and duration which is then feed into the dispersion model. FLEXPART-WRF, which is run at the NC State Climate Office, will ingest the 06 UTC WRF model and compute the transport and dispersion of disease spores. The simulation time varies based on the number of releases. The dry deposition concentrations will be post-processed in GIS where the forecasters can visualize the data via Google Maps. Forecasters can then place polygons within the Google framework over the high risk locations to warn of the impending crop hazards. Originally the forecast team at NC State worked with the HYSPLIT online version to create trajectory and concentration maps, but found this process to be quite tedious.

From this application, it is evident that dry deposition is an important output. Forecasters who are attempting to forecast the fall out of pollutants need an accurate depiction of deposition both spatially and temporally. This reiterates the importance for an accurate simulation of not only air concentration but dry deposition as well.

In conclusion, both dispersion models can be utilized under an operational setting across one platform. Based on the study presented here, FLEXPART-WRF has proved to be an accurate, timely and versatile dispersion tool based on the research presented. Much like atmospheric models, it would be wise to have multiple dispersion models to analyze during a plume episode.
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