

11.3 A Comparative Study between FLEXPART-WRF and HYSPLIT in an Operational Setting: Analysis of Fire Emissions across complex geography using WRF

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1. Introduction

Atmospheric transport and dispersion (T&D) models are frequently used by research and operational agencies to forecast anthropogenic, natural and accidental chemical releases of hazardous materials. T&D models often rely on gridded meteorological data from numerical models to provide accurate simulations of dispersion. T&D model applications include chemical releases, explosions of hazardous material, volcanic eruptions and fire emissions. No matter what the application, accurately forecasting the release of any hazardous material is of vital importance to life and property.

Operational offices (i.e. NOAA, NWS, etc.) typically use the Hybrid Single Particle Lagrangian Integrated Trajectory model (HYSPLIT) during hazardous pollutant episodes. Research agencies (i.e. Environmental Protection Agency, etc.) use various dispersion models to investigate air quality, emission policy and advancements to the current dispersion technology. The Flexible Particle model (FLEXPART) is a popular dispersion tool used under research settings across much of Europe with little exposure within the operational sectors, especially in the United States.

Both HYSPLIT and FLEXPART are Lagrangian dispersion models that rely on meteorological data to drive the simulations. Within operational settings, the HYSPLIT model is typically run using the North American Model (NAM) 12 km domain. The high resolution Weather, Research and Forecasting (WRF) model has been increasing in popularity within local Weather Forecast Offices. Therefore, both the 12 km and 4 km WRF are ingested into the T&D models within this study to determine if the high resolution model adds value. Such high resolution modeling is thought to improve the dispersion simulations leading to an overall better forecast of pollutant migration. The physics schemes found within the WRF model were chosen based on the terrain found within each domain. These modifications were based on sensitivity studies conducted by Challa et al. (2008) and Peffers et al. (2006).

With a push for additional dispersion models within Operational offices, a comparative study is conducted between HYSPLIT and FLEXPART-WRF to determine if FLEXPART-WRF can be used as an effective, accurate and timely dispersion model within an operational environment. In this study, an investigation of each of the T&D model applications, limitations, assumptions and approximations are revealed. An in-depth analysis of each dispersion

software package is reviewed and subsequent differences are highlighted. Such differences were found to impact the dispersion models output fields. After successful completion of the background analysis, two case studies were conducted across the complex geography of NC in an effort to challenge both the meteorological data and dispersion calculations. The case studies presented here are based on past wildfire events. The first study is conducted across the coastal plain (i.e. Evans Road Wildfire) and the second embedded within the Appalachians (i.e. South Mountain Wildfire).

2. T&D Models

2.1 HYSPLIT

HYSPLIT (version 4.9) is a system for computing trajectories and dispersion using either a puff or particle approach (Draxler and Hess, 1997). The HYSPLIT model was first introduced by the Air Resources Laboratory (ARL) of the U.S. National Oceanic and Atmospheric Administration (NOAA) and Australian Bureau of Meteorology in 1979 and has undergone many variations since this time. As research and computer capacity have increased so too have HYSPLIT's capabilities. The HYSPLIT model was once driven by rawinsonde observations ((Draxler and Taylor, 1982), but can now use various meteorological grids to help simulate the transport and dispersion of particles downwind from a source. HYSPLIT applications include, emergency response (Housiadas, 1999; Draxler, 1999; Ruminski et al., 2006), urban dispersion (Draxler, 1985; Draxler, 2006), fire weather (Ruminski et al., 2006), operations (Dreher, 2009), and pathogen transport (Main et al., 2001; Pan et al., 2006; Levetin, 1998).

Large field experiments have also been conducted to depict the accuracy of the dispersion models. HYSPLIT was evaluated based on several field campaigns (i.e. CAPTEX, ANATEX, ETEX). Draxler (1999) found that the HYSPLIT calculations were in the middle of the performance range. For a detailed description of the HYSPLIT model see Draxler and Hess (1997).

2.2 FLEXPART

Much like HYSPLIT, FLEXPART is a Lagrangian dispersion model developed by Andrea Stohl in 1995 for Austria's emergency response system and has undergone many revisions. Quick validation based on field experiments has led to its increase in popularity, especially within Europe. With over 30

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groups and 17 countries utilizing this dispersion tool, the applications range from both operational and research entities. However, the operational side of FLEXPART is not as apparent. The applications of FLEXPART include fire emissions (Kasischke et al., 2005; Wotawa and Trainer, 2000; Forster et al., 2001; Spichtinger et al., 2001), emergency response (Pechinger et al., 2001; Wenig et al., 2003; Arnold et al., 2008) urban dispersion (Fast and Easter, 2006) and most recently pathogen transport.

Stohl (1998) validated the FLEXPART (version 2.0) dispersion model by applying it to large field campaigns. Each experiment had its own unique feature that challenged the dispersion model such as terrain, weather patterns and spatial and temporal sampling and release locations. Many of the concentration results were comparable to the observed values. However, frontal passages and underestimation of the air concentration led to FLEXPART's poor performance during some of the experiments. In response to these limitations, a new convective algorithm was added and high resolution meteorological model can now be ingested into the model.

A modified version of FLEXPART (based on version 6.2) was produced to ingest the WRF model, now referred to as FLEXPART-WRF (Fast and Easter, 2006). For additional software information see Stohl et al., 2005.

2.3 Summary

Although both the dispersion models are ingesting the same meteorological data, that does not implicitly mean the models are taking in the same information. HYSPLIT and FLEXPART take in most of the same data from the WRF output, but there are a few fields that are ignored by HYSPLIT such as convective parameters and surface stress. These differences will translate into varying equations.

Based on the software description of each T&D model, there are computational similarities and differences that may lead to varying output results. Both dispersion models implement similar advection algorithms. However, the diffusion equation which adds the random turbulent component to the trajectories is handled differently. Also, the varying time steps found within the diffusion equations can have an impact on the computed concentration amount at every time step. The fall out of particles (dry deposition) is computed using the resistance method for both T&D models. FLEXPART computes an atmospheric resistance that is 4 times larger than HYSPLIT. FLEXPART also computes the quasi-laminar sublayer resistance that is 3 times larger than that of HYSPLIT. When the resistance is large, the deposition is small. Therefore, following this technique, it would seem that FLEXPART will produce a smaller concentration deposited to the surface compared to HYSPLIT.

These are just some of the large computational discrepancies found between the HYSPLIT and FLEXPART model. There are smaller features that vary between the models, but the large forcings are what drive the models and their results.

3. Configuration and Methodology

A common configuration including pre- and post-processing was created across both models to ensure a fair comparison (Fig. 1). The models are pre-processed based on initial parameters and meteorological data. Air concentration and dry deposition is calculated within each model with post-processing via Geographic Information System (GIS) for gridded analysis. The spatial and temporal concentrations are statistically analyzed and verification of the models is conducted based on remote sensing technology.

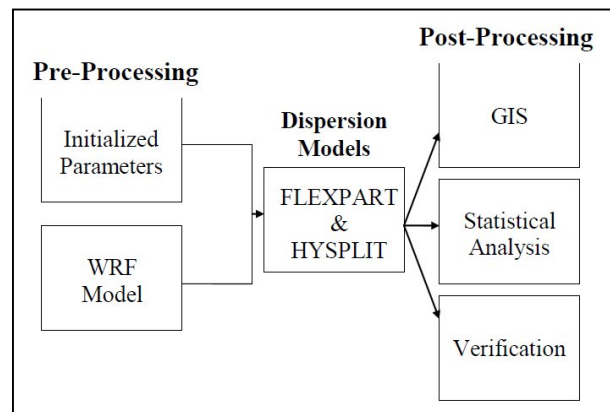


Figure 1. Flow chart of Model Configuration for the dispersion simulations.

3.1 Methodology for Analysis

Once the dispersion models complete the simulation, the output fields (i.e. air concentration and dry deposition) are post-processed via GIS. 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 resampled using a bilinear interpolation method to produce a gridded surface.

The overall computational time for both models varied. Since HYSPLIT was not automated, it took an additional 5 minutes to run each routine separately. The runtime for T&D models depend on the number of releases and the simulation duration.

Since the concentration outputs for each model is mapped on a common grid, the spatial differences can be easily evaluated. A difference field

$$D=H-F \quad [1]$$

and percent difference field

$$\%D=(H-F)/((H+F)/2)*100\% \quad [2]$$

were created every hour, where H and F are HYSPLIT and FLEXPART-WRF concentration values, respectively. Other analysis was conducted based on the concentration distribution and spatial difference (i.e. average concentration distribution, significance testing, correlation, etc.) and will be reviewed in later sections.

Given no air concentration and deposition measurements, validation was conducted based on remote sensing technologies such as NEXRAD radar and GOES satellite imagery.

4. Results

4.1 Evans Road Wildfire

A fire was reported on June 1st, 2008 in the remote location of New Lake in eastern North Carolina. With persistent drought conditions felt across the region, a lightning strike ignited the fire. By June 3rd, the fire had broke containment and raged across the Pocosin Lakes Refuge burning over 3,000 acres. Flammable organic soil made the fire impossible to control and by the afternoon, the fire had burned 8,000 acres. Fig.3 shows an aerial photograph of the smoke plume from the fire on June 12, 2008. The fire lasted approximately two months and burned over 40,000 acres. Low visibility and poor air quality conditions were the major concerns plaguing residences downwind of the wildfire. The case study presented uses a small portion of this event in an effort to evaluate two different dispersion models.



Figure 2. Evans Road Wildfire on the afternoon of June 12, 2008.

Both dispersion models released a total of 10 kg (1×10^{13} ng) into the atmosphere from the source site (latitude: 35.62, longitude: -76.452). 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 air concentration is computed using the WRF 12 km and 4 km meteorological domain. The domains are not nested within the dispersion models in an effort to separate them for comparison close to the release location.

a. Study Domain

The WRF computational area consists of a 12 km with a nested 4 km domain and is initialized by the NAM 12 km reanalysis (Fig.3). The orientation of the WRF model domain is shown in Fig.4. The outer domain contains 175 x 175 points spanning 2,100 x 2,100 km² across the eastern half of the United States. The nested domain (d02) consists of 235 x 235 points spanning 940 x 940 km² across central and eastern North Carolina and the western 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 domains. The three-day simulation was conducted from 13 UTC 09 June 09 through 12 UTC 11 June 08.

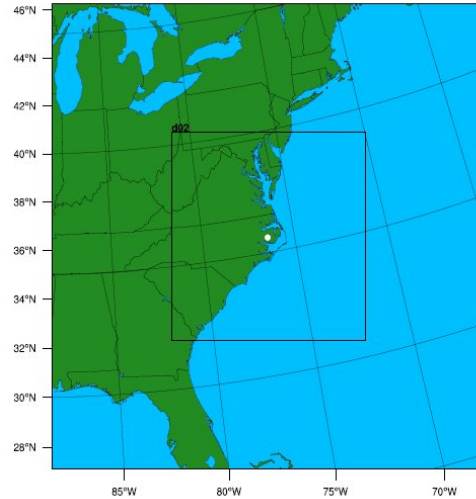


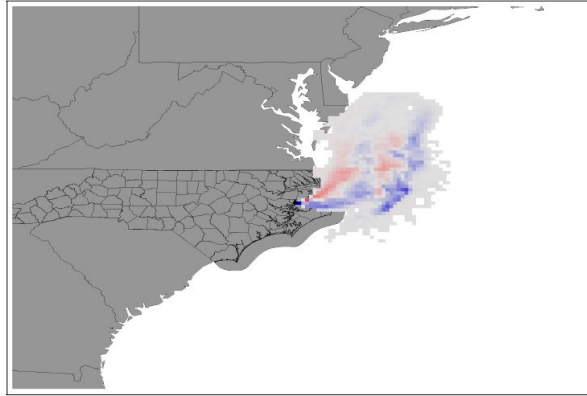
Figure 3. WRF Domain. The outer domain is 12 km with an inner domain (d02) of 4km. The white dot denotes the Evans Road wildfire location.

b. Air Concentration Plume Structure

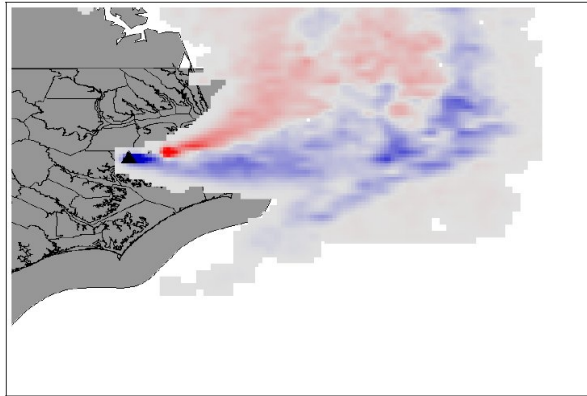
The plume patterns were in fairly good agreement till 13 hours after the start of the simulation. At this point the plumes start to diverge from the source with HYSPLIT advecting particles to the north of FLEXPART-WRF. By the morning on the 10th, Fig.4 clearly illustrates the differences in the plume pattern, emphasizing the high concentration downwind produced by FLEXPART-WRF. The trend continues through the rest of the simulation (Fig.5). At the end of the simulation, FLEXPART -WRF resolved a high concentration S-shaped signature approximately 200 miles downwind of the source that HYSPLIT did not produce.

Based on this analysis, it is clear that the two dispersion models have spatial plume structure discrepancies. To get a quantitative understanding of these differences, analysis of the distribution is reviewed. Only a small portion of the analysis is presented here.

The concentration distributions between the two T&D models across both domains were similar. However, the differences (based on the spatial plume and concentration) were found to be significant after 13 hours which corresponds well with the T&D plume divergence (Fig.6). Such differences in plume migration could impact the meteorologist and emergency manager's decision making process.



a. 12 km



b. 4 km

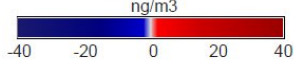
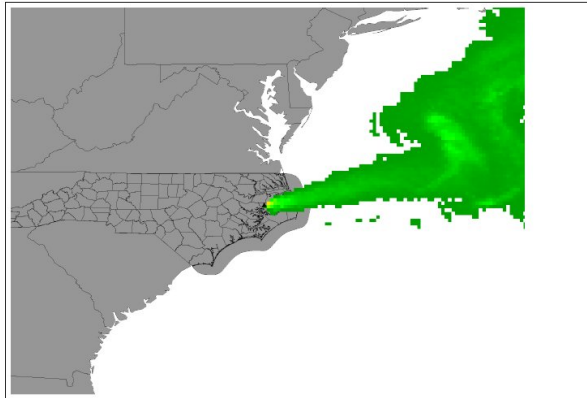
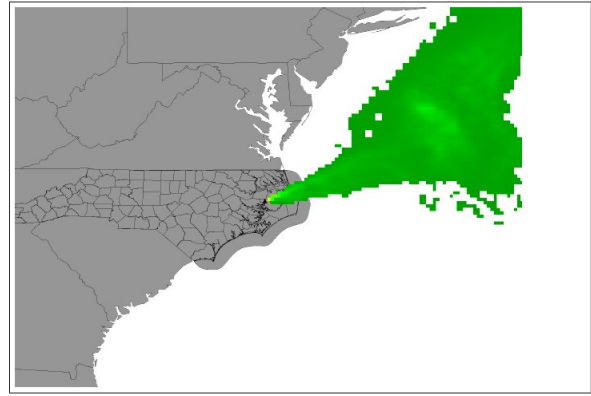


Figure 4. Difference (ng m^{-3}) in Air Concentration at 13 UTC 10 June. Positive values (red) indicate HYSPLIT has a higher concentration over that particular grid. Negative values (blue) indicate FLEXPART-WRF has a higher concentration.



a. FLEXPART-WRF



b. HYSPLIT

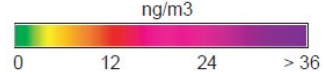


Figure 5. 12 km Air Concentration (ng m^{-3}) at 12 UTC 11 June.
P Value

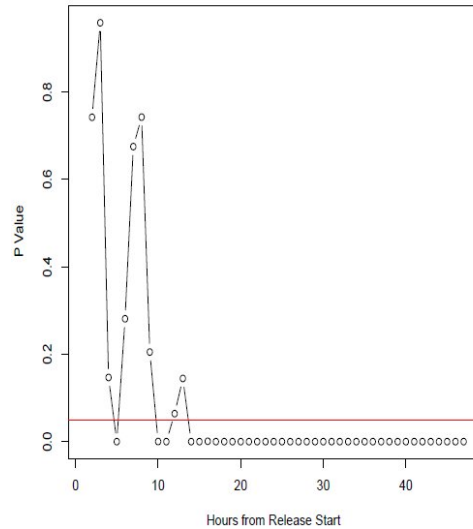


Figure 6. P-Value based on a Student-t test using a normalized distribution and 95% confidence interval.

c. Model Evaluation

There were some inconsistencies with the plume structure within the first several hours of the simulation. The observed plume illustrated a southeasterly advection of the plume while FLEXPART dispersed the particles more to the south. Also, the observed plume illustrated a downwind S-shaped signature within the first several hour of the simulation, most likely influenced by low level wind fluctuations that the T&D models did not resolve at the time (Fig. 7). FLEXPART-WRF did illustrate the S-shaped signature later on in the simulation run.

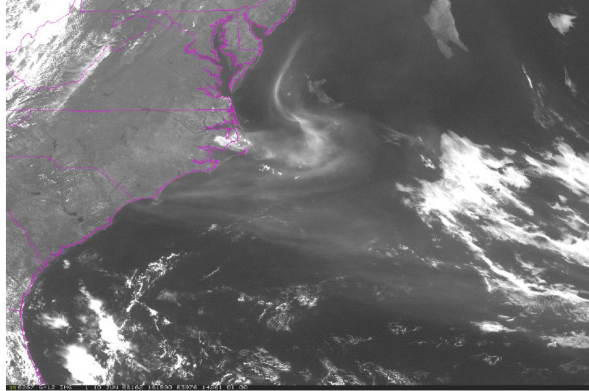


Figure 7. GOES Satellite Image at 16 UTC 10 June.

Based on NESDIS GOES satellite imagery and animation and radar signatures, FLEXPART-WRF seemed to better represent the observed plume. The two models were very comparable based on concentration and diffusion. The HYSPLIT 4 km simulation did bring the models into slightly better agreement within the first couple of hours. However, through the rest of the period the models still underwent spatial differences similar to those found within the 12 km solution. FLEXPART-WRF computed an overall higher air concentration throughout most of the simulation period, especially beyond 100 miles downwind of the wildfire.

d. Dry Deposition

The deposition concentration distribution between the models (across both domains) is very different both spatially and temporally. The discrepancies in deposition have led to statistically significant differences between the models (Fig.8). It is hard to define the actual cause of these variations, but speculation can be made on the possible contributions. Variations in equations (i.e. settling velocity, atmospheric resistance and quasi-laminar sublayer resistance, etc.) may have led to these differing results. The use of atmospheric turbulence can play a large role in the amount of particulate matter getting to the surface, especially among the atmospheric layer resistance. Also, the land-surface and vegetation cover used to modify the atmospheric layer resistance impacts the deposition rate. The deposition variations can not be contributed to the diurnal trend of the PBL. The removal method, especially within HYSPLIT, needs to be investigated further.

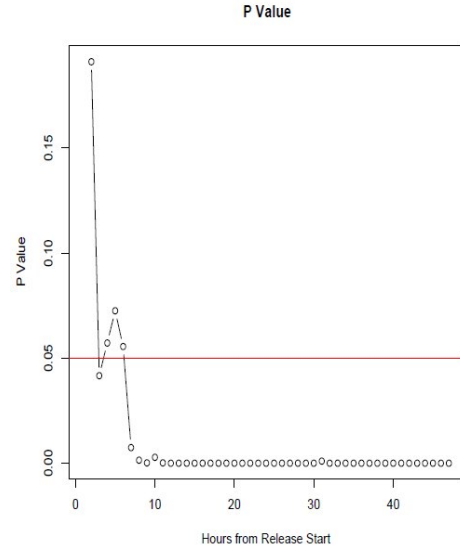


Figure 8. P-value based on Student T-test for the 12 km dry deposition concentration differences between HYSPLIT and FLEXPART. P-Values below 0.05 are statistically significant.

4.2 South Mountain Wildfire

On September 28, 2009 a wildfire was detected within the South Mountain State Park region of the southern Appalachians. With over 10,000 acres of park, there was no documentation of a fire or the extent of damage it may have caused. However, GOES satellite imagery was able to vaguely capture the smoke plume which only lasted approximately 24 hours. The South Mountain Fire was one of the only recent fires vaguely captured by satellite during fair weather conditions over the Appalachians. The case study presented here will capture most of the fires duration in an effort to evaluate the dispersion models across complex terrain.

The air concentration released a total of 10 kg (1×10^{13} ng) into the atmosphere from the source site (latitude: 35.598, longitude: -81.659). Both dispersion models continuously released a total of 2×10^6 particles tracers (.4348 kg per hour) over a 23 hour period from 150 m AGL. Dry deposition was computed based on the gravitational settling and resistances found within the lowest 75 m.

a. Study Domain

The WRF computational area consists of a 12 km and nested 4 km domain (Fig. 9) and is initialized based on the NAM 12 km reanalysis. The mother 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 22 UTC 28 Sept 07 through 21 UTC 29 Sept 07.

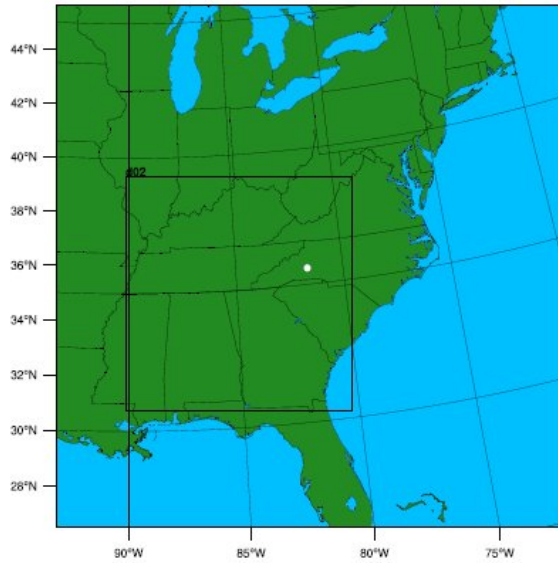
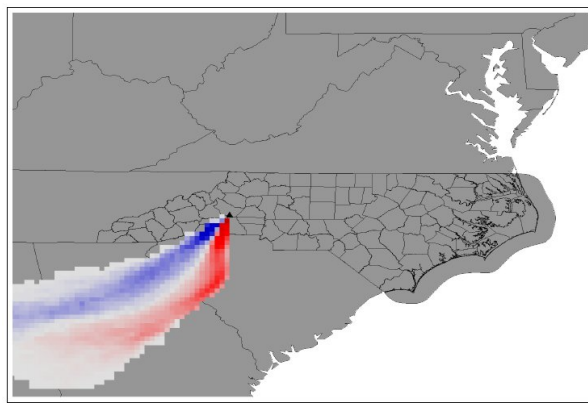


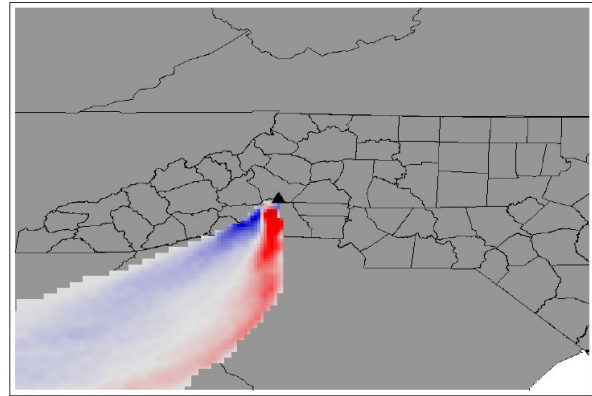
Figure 9. WRF Domain. The outer domain is 12 km with an inner domain (d02) of 4 km. The white dot denotes the South Mountain wildfire location.

b. Air Concentration Plume Structure and Evaluation

The plume migration between the two models were different within the first 12 hours of the simulation with FLEXPART-WRF dispersion to the southwest and HYSPLIT advecting the particles to the south of the release site (Fig.10). Such differences could have a dramatic impact on meteorologists and emergency management. The plumes started to come into better agreement by the end of the simulation (Fig.11).



a. 12 km



b. 4 km

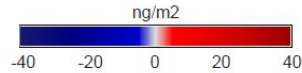
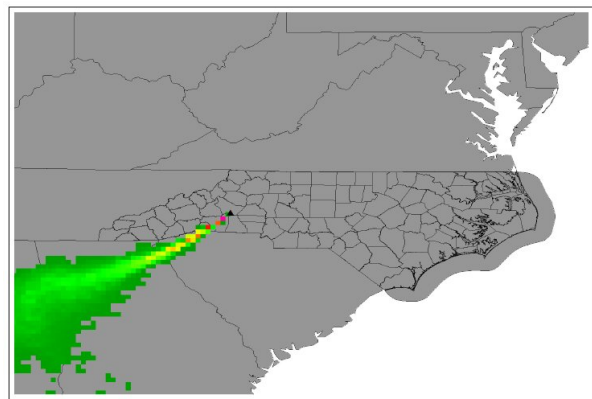
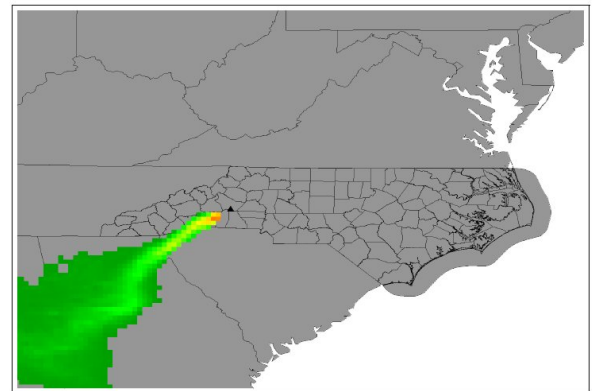


Figure 10. Difference (ng m^{-3}) in Air Concentration at 14 UTC 29 September 07. Positive values (red) indicate HYSPLIT has a higher concentration over that particular grid. Negative values (blue) indicate FLEXPART-WRF has a higher concentration.



a. FLEXPART-WRF



b. HYSPLIT

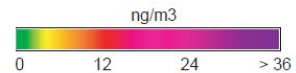


Figure 11. Air concentration (ng m^{-3}) at 21 UTC 29 September.

c. Dry Deposition

Following the air concentration, the spatial deposition pattern was quite different between the two

dispersion models. However, this was not the most significant variation found. While HYSPLIT produced high deposition through most of the simulation, especially close to the source and within localized areas, the biggest signal came several hours after the start of the release. From 13-14 UTC on the 29th, HYSPLIT deposited ($>200 \text{ ng m}^{-2}$) 10 times more particles to the surface than FLEXPART-WRF through most of the spatial plume. It is unclear at this time why HYSPLIT produced such a high deposition signature. This large deposition led to a significant difference between the models. Again, the removal methods found within the HYSPLIT model needs to be investigated. Luckily, during this simulation study, the high amount of mass being removed did not have a dramatic impact on the overall concentration within the air column. However, if this simulation is of a shorter duration with fewer particles being released over a smaller domain, it could have had a huge impact on air concentration results.

5. Summary and Discussion

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 feed into the dispersion model. The initialized parameters were identical between the dispersion model while high resolution meteorological data (WRF) guided the transport and dispersion of particles from the source. However, within each of the dispersion model configuration, there were different meteorological fields that were ingested every hour. 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, statistically analyzed and validated with remote sensing techniques.

Across both case studies there are some similar and strikingly different features noted. First, the air concentration distributions were very similar between HYSPLIT and FLEXPART-WRF across both domains. Second, the spatial plume compositions were different among both case studies with HYSPLIT dispersing to the right of FLEXPART. Thirdly, the deposition variability produced by HYSPLIT led to statistically significant differences.

It was shown that air concentration plumes between FLEXPART-WRF and HYSPLIT are similar in values but different in placement. This finding is significant given the models are run with the same initialized parameters and meteorological data. It was noted that the 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 is 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 have shown to have a large 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 (typical for operational use). 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 may cause issues.

The range of sensitivity studies for both dispersion models is endless. Studies involving different meteorological conditions, initialized parameters and computation techniques are just a few. In order to improve and advance dispersion models, research needs to continue. This study simply highlights the similarities and differences among the two dispersion models.

Operationally, FLEXPART-WRF is found to be a good candidate as an additional resource tool. In many ways, FLEXPART-WRF performed better compared to HYSPLIT based on remote sensing validation. FLEXPART-WRF was comparable in computational efficiency and performance across both wildfire cases. 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. This team relies heavily on deposition calculations which is another reason why this area needs to be investigated. Currently, FLEXPART does not have a GUI interface for forward dispersion modeling which limits the flexibility of the tool. However, a web-based version compatible with a specific application can be easily produced.

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. Much like atmospheric models, it would be wise to have multiple dispersion models during a plume episode.

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