EPA United States Environmental Protection Agency

Assessment of the "VISTAS" Version of the CALPUFF Modeling System

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PREFACE

This report summarizes the process undertaken and documents the results of EPA's assessment of the "VISTAS" version of the CALPUFF modeling system, which lead to EPA's approval of CALPUFF (v5.8), CALMET (v5.8) and CALPOST (v5.6394) as the "EPA-approved" version, announced on June 29, 2007.

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1.0 INTRODUCTION

The CALPUFF Modeling System, consisting of the CALPUFF dispersion model, CALMET meteorological processor, and CALPOST postprocessor, was promulgated by EPA as the preferred model for long-range transport (LRT) regulatory modeling applications for purposes of demonstrating compliance with Class I PSD increments.[1] As with any modeling system, periodic updates are anticipated as part of the standard software life cycle to address bugs that are identified, as well as enhancements that may be needed to address new data formats or other needs that may arise. To address the need for a systematic process to assess impacts of modifications to the CALPUFF modeling system, EPA established a standard "Protocol for Updating the CALPUFF Modeling System" and developed a "CALPUFF Assessment Tool" to support that process.[2] Such a process is vital to preserving the integrity of the preferred status of models recommended by EPA in the *Guideline on Air Quality Models* (40 CFR Part 51, Appendix W).[1]

This report summarizes the process undertaken, and documents the results of EPA's assessment of the "VISTAS" version of the CALPUFF modeling system, which lead to EPA's approval of CALPUFF (v5.8), CALMET (v5.8) and CALPOST (v5.6394) as the "EPA-approved" version, announced on June 29, 2007. As part of this assessment, EPA performed several tests to compare modeled impacts based on the then-current VISTAS versions of CALMET (v5.726) and CALPUFF (v5.756) to impacts based on the previous EPA-approved versions of CALMET (v5.53a) and CALPUFF (v5.711a), for the purpose of assessing whether to update the EPA-approved version of the modeling system.

2.0 CALPUFF ASSESSMENT TOOL OVERVIEW

The CALUFF Assessment Tool consists of 11 scenarios designed to test the modeling system across a range of possible applications in terms of modeling domain, meteorological data options, and source types. The CALPUFF Assessment Tool prepares summaries of differences in predicted concentrations between two versions of the CALPUFF Modeling System, the "Base" version referring to the current EPA-approved version, and the "Beta" version referring to the updated version of the modeling system that is the subject of the assessment. The CALPUFF Assessment Tool was successfully applied to support EPA's adoption of CALPUFF (v5.711a) and CALMET (v5.53a) as the EPA-approved versions in June 2006.[3]

The following list provides a brief description of the 11 scenarios included in the CALPUFF Assessment Tool:

1.   Large-scale domain in Pacific NW – NWS met data only
2.   Same as Scenario 1 with MM5 NOOBS option
3.   Medium-scale domain in Pacific NW (subset of 1) with MM5&NWS data
4.   Medium-scale domain near Shenandoah NP – NWS met data only
5.   Small-scale complex flow with deep valley – NWS met data only
6.   Idealized hill with steady-state met, with similarity dispersion
7.   Same as Scenario 6, with PG dispersion
8.   Flat terrain with steady-state met, with similarity dispersion
9.   Same as Scenario 8, with PG dispersion
10.   Idealized hill with simulated wind shear, profile met data
11.   Same as Scenario 3, with chemistry and deposition included (optional)

The following list provides a brief description of the sources included in the different scenarios:

- Four core sources included in all scenarios:
  - Ground-level area source (20m by 200m)
  - 10m volume source
  - 30m non-buoyant point source
  - 65m buoyant point source
- Two sets of core sources included in Scenarios 1, 2, and 5 at different locations within domain
- Scenario 3 also includes 99m buoyant stack near coast
- Scenario 4 also includes buoyant area source
- Scenarios 6 and 7 also include three PRIME downwash sources (35m buoyant, 35m capped, 50m buoyant)

More details regarding the scenarios included in the CALPUFF Assessment Tool are provided in a presentation submitted at EPA's 8th Modeling Conference held in RTP, NC in September, 2005.[4]

3.0 SUMMARY OF CALPUFF ASSESSMENT RESULTS

3.1   PRELIMINARY ASSESSMENT OF VISTAS VERSION

EPA initiated an assessment of the latest "Beta" version of the CALPUFF modeling system in June 2006, based on the version being distributed at that time by TRC as the "VISTAS" version. The initial application of the CALPUFF Assessment Tool to the "VISTAS" version indicated significant differences between the VISTAS version and the then-current EPA-approved version across all scenarios, except for Scenario 10, which does not utilize CALMET. A brief summary of the initial comparison results are provided in Table 1, which shows the range of absolute maximum percent differences, computed as [100*(Beta-Base)/Base], for the high ranked values by scenario across all sources and averaging periods by scenario. Note that Scenario 11 is not included in the summary of comparison results presented here. Scenario 11 is based on Scenario 3, but also includes chemistry and deposition. The magnitude of differences found between the VISTAS and prior EPA-approved versions necessitated a thorough assessment of the factors contributing to those differences before EPA could make a determination of whether to approve the VISTAS version as an update to the previous regulatory version. The CALPUFF Assessment Tool also attributed most of the differences in Table 1 to changes in CALMET, rather than CALPUFF. The only scenario that showed differences due to CALPUFF was Scenario 5, with a maximum percent difference due to CALPUFF of about 7 percent.

Table 1: Range of Maximum Absolute Percent Differences by Scenario for Initial Application of Assessment Tool	
Scenario 1	-22.0 to +23.3
Scenario 2	-0.2 to +83.4
Scenario 3	-17.7 to +60.8
Scenario 4	-13.6 to +28.1
Scenario 5	-46.0 to +21.1
Scenario 6	-10.3 to +6.3
Scenario 7	-1.7 to +1.0
Scenario 8	-10.0 to +5.4
Scenario 9	-1.2 to +1.0
Scenario 10	No differences

Due to limited documentation available at that time, it was impossible to determine which model changes were contributing to the differences. Under the auspices of VISTAS, TRC provided additional documentation regarding the changes between the previous EPA-approved versions of CALMET (v5.53a) and CALPUFF (v5.711a) and the then-current VISTAS versions of CALMET (v5.726) and CALPUFF (v5.756). This additional documentation included:

    (1)   tables derived from in-code documentation of changes to each model component, annotated to indicate the category of each change and whether each change may

affect results;

(2)   Model Change Bulletin B (MCB-B), for CALPUFF v5.711a/ v5.711b and CALMET v5.53a/v5.53b (available from TRC CALPUFF website);

(3)   Model Change Bulletin C (MCB-C), for CALPUFF v5.711b/v5.756 and CALMET v5.53b/v5.726;

(4)   Model Change Bulletin D (MCB-D), for CALMET v5.726/v5.730; and

(5)   a summary of model tests performed by TRC.

The changes identified by the annotated tables of in-code documentation were classified as follows:

(1) bug fixes;

(2) non-optional technical enhancements;

(3) optional technical enhancements;

(4) non-technical enhancements;

(5) enhancement adjustments; or

(6) coordinate conversion fixes.

In order to facilitate isolating the potential impact of changes identified as (1) bug fixes, and (2) non-optional technical enhancements, TRC provided to EPA the following interim versions of CALMET and CALPUFF:

CALMET (5.53c)   = CALMET (5.53a) + bug fixes
CALMET (5.53c2) = CALMET (5.53c) + non-optional technical enhancements
CALPUFF (5.711c) = CALPUFF (5.711a) + bug fixes

Another potential source of differences identified by TRC in the summary of their comparison test related to new CALMET parameters associated with optional technical enhancements for which new default values had been specified in the VISTAS versions that differed from values that would be needed to maintain equivalence with the previous EPA-approved version. As implemented in the VISTAS version, these options required the user to manually override the new default values in the appropriate input file for the VISTAS version to maintain consistency with the EPA-approved version. The following list identifies the new default parameters within the VISTAS version of CALMET, along with the non-default value required to manually override the default in the CALMET.INP file for consistency with the EPA-approved version:

(1)   IMIXH = -1 for convective mixing height option based on Maul-Carson for land cells only and Original OCD mixing height overwater (default value of 1 would be selected to use Maul-Carson for land and water cells if IMIXH is omitted);

(2)   THRESHL = 0.0 for threshold buoyancy energy flux per meter of boundary layer required for Mixing Height Growth over land (default value of 0.05 $W/m^2/m$ would be selected if THRESHL is omitted);

(3)   THRESHW = 0.0 for threshold buoyancy energy flux per meter of boundary layer required for Mixing Height Growth over water (default value of 0.05 $W/m^2/m$ would be selected if THRESHW is omitted); and

(4)   ICOARE = 0 for option to use delta-T method for the Coupled Ocean Atmosphere

Response Experiment (COARE) bulk flux model for computing wave heights and boundary layer parameters overwater (default value of 10 for COARE method with COARE wave option 0 would be selected if ICOARE is omitted).

The following new defaults in the VISTAS version of CALPUFF were also identified, requiring manual override with the specified value in the CALPUFF.INP file to maintain consistency with the then-current EPA-approved version:

SVMIN(6:12) = 0.50 for minimum sigma-v value (m/s) for over water cells for stability classes 1 through 6 (default value of 0.37 m/s would be used for each stability class for over water grid cells if these parameters are omitted).

3.2   RESULTS OF ADDITIONAL TESTS

Based on the interim versions of CALMET and CALPUFF provided by TRC, and the additional clarification regarding input file modifications needed for the VISTAS version to maintain consistency with the EPA-approved version for certain parameters, EPA conducted the following initial set of test runs in order to compare and isolate affects of the Bug Fixes, the Non-optional Technical Enhancements, and the New Defaults for Optional Technical Enhancements that require manual override in the CALPUFF/CALMET input files:

Test 1. CALPUFF (5.711c) and CALMET (5.53c)   vs. VISTAS (CALPUFF v5.756 and CALMET v5.726) without modified inputs for new default parameters;

Test 2. CALPUFF (5.711c) and CALMET (5.53c2) vs. VISTAS (5.756/5.726) without modified inputs for new default parameters;

Test 3. CALPUFF (5.711c) and CALMET (5.53c)   vs. VISTAS (5.756/5.726) with modified inputs to override new default parameters; and

Test 4. CALPUFF (5.711c) and CALMET (5.53c2) vs. VISTAS (5.756/5.726) with modified inputs to override new default parameters.

TRC asserted, citing results of their comparison tests[5], that "the VISTAS code is equivalent to the EPA-approved code once the coding errors in the EPA code are corrected." Based on this assertion, the results for Test No. 1 should demonstrate equivalency. Section 3.2.2 of Appendix W establishes a maximum threshold of 2 percent differences between the maximum or highest, second-highest (H2H) results as the criterion for equivalence between an alternative model and the preferred model. This 2 percent threshold has often been used as a benchmark for assessing differences between models or model versions, and is useful in the context of this assessment.

Summaries of comparison results obtained from EPA's preliminary tests are presented below in order to provide an initial indication of whether the criterion of equivalence was met. It is important to note in assessing the results from these comparisons that the current regulatory niche for the CALPUFF modeling system in Appendix W is for modeling compliance with NSR/PSD permitting requirements for long range transport (> 50km) applications at Class I areas. In light of this, differences between various versions of the CALPUFF modeling system for design values representative of such regulatory applications are a necessary part of any

comparison study intended to support adoption of an updated version of the model. The summaries presented here are limited in scope, focusing on the percent differences in high ranked values without explicit regard to transport distances, and may significantly understate differences found across the full modeling domain.

The results for Test No. 1, showing the impact of bug fixes without modifications to input files to override new default parameters, are summarized in Table 2 as the range of absolute maximum percent differences, computed as [100*(Beta-Base)/Base], for high ranked values across all sources and averaging periods by scenario.

Table 2: Results for Test No.1: Range of Maximum Absolute Percent Differences by Scenario	
Scenario 1	-22.0 to +24.5
Scenario 2	-21.7 to +81.8
Scenario 3	-17.9 to +60.3
Scenario 4	-3.3 to +30.5
Scenario 5	-41.8 to +19.5
Scenario 6	-9.7 to +6.3
Scenario 7	-1.7 to +1.0
Scenario 8	-9.3 to +5.6
Scenario 9	-1.2 to +1.0
Scenario 10	No differences

These results clearly did not support the assertion that "the VISTAS code is equivalent to the EPA-approved code once the coding errors in the EPA code are corrected." In fact, the range of differences was quite similar to the range of differences found from the initial comparison of the then-current EPA-approved version vs. the current VISTAS version. This did not necessarily imply that the impact of bug fixes on model results was insignificant, as will be shown later.

At the other end of the spectrum of initial tests, Test No. 4 was designed to eliminate all of the documented causes of potential differences relative to the VISTAS version, including Bug Fixes, Non-optional Technical Enhancements, and New Default Parameters for Optional Technical Enhancements. Table 3 summarizes the range of maximum percent differences of high ranked values by scenario for Test No. 4, which shows better overall agreement than initial test results.

Table 3: Results for Test No.4: Range of Maximum Absolute Percent Differences by Scenario	
Scenario 1	-17.7 to +0.6
Scenario 2	-20.9 to +10.3
Scenario 3	-0.4 to +5.1
Scenario 4	No differences
Scenario 5	No differences
Scenario 6	No differences
Scenario 7	No differences
Scenario 8	No differences
Scenario 9	No differences
Scenario 10	No differences

While no differences were found for several scenarios, some significant differences remained for Scenarios 1, 2 and 3, indicating that other undocumented factors were contributing to differences in concentrations. Preliminary analysis of the spatial pattern of differences across the domain showed much larger differences in high ranked values for distance ranges typical of long range transport/Class 1 area impact assessments, as shown in Figure 1 for the Jordan Valley 65m buoyant source within Scenario 2, confirming the caution stated above that differences based solely on high ranked values may significantly understate the magnitude of differences found across the full modeling domain.

The causes of differences found for Test No. 4 were initially unresolved based on the documentation available at the time. However, given the results summarized above for Tests 1 and 4, additional tests were performed to further isolate the differences that could be attributed to each of the three known causes identified above: 1) bug fixes; 2) non-optional technical enhancements; and 3) new default parameters for optional technical enhancements. Results from the following additional tests are presented below:

> Test 5. CALPUFF (5.711a) and CALMET (5.53a) vs. CALPUFF (5.711c) and
>   CALMET (5.53c) – Differences Due to Bug Fixes;
> Test 6. CALPUFF (5.711c) and CALMET (5.53c) vs. CALPUFF (5.711c) and
>   CALMET (5.53c2) – Differences Due to Non-optional Technical Enhancements;
>   and
> Test 7. CALPUFF (5.576) and CALMET (5.526) without modified inputs for new default
>   parameters vs. CALPUFF (5. 576) and CALMET (5. 526) with modified inputs
>   for new default parameters – Differences Due to New Default Parameters

The range of maximum absolute percent differences of high ranked values by scenario for Test 5 (Bug Fixes), Test 6 (Non-optional Technical Enhancements), and Test 7 (New Default Parameters are presented in Table 4.

Figure 1: Contour Plot of Percent Differences for Scenario 2
Jordan Valley 65m Point Source; 4th-Highest 24-Hour Averages

Test 4 - CALPUFF (5.711c) and CALMET (5.53c2) vs. VISTAS (5.756/5.726)
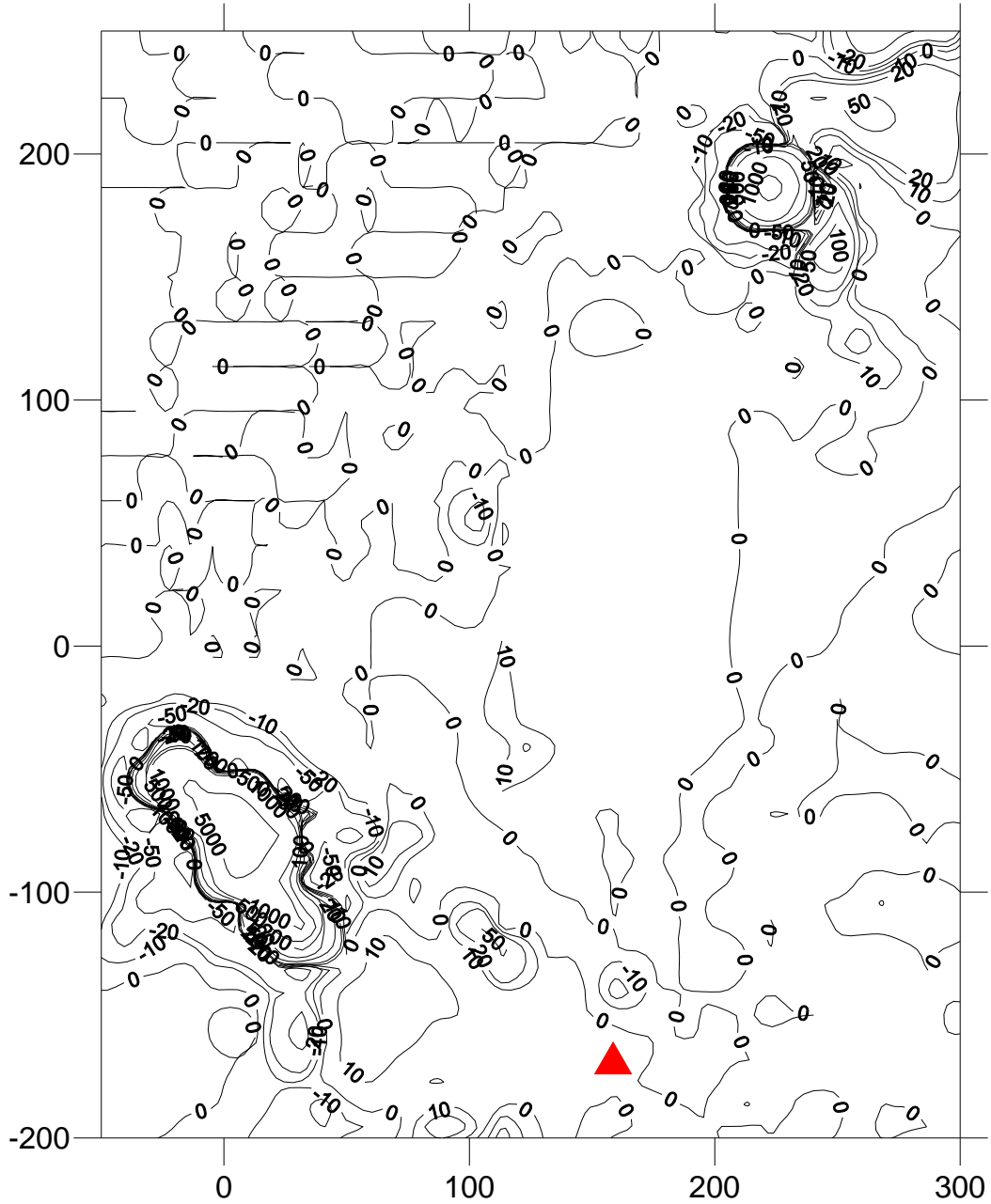(with modified inputs to override new default parameter)

Figure 1. Contour plot of percent differences in 4th-highest 24-hour averages for
Scenario 2 from Test 4.

	Table 4: Range of Maximum Absolute Percent Differences by Scenario		
	Test 5 – Bug Fixes	Test 6 – Non-Optional Technical Enhancements	Test 7 – New Default Parameters
Scenario 1	-1.0 to +22.6	-18.6 to +1.9	-22.0 to +24.4
Scenario 2	-15.4 to +27.8	-30.5 to +0.7	-21.8 to +118.3
Scenario 3	-5.1 to +6.0	-0.8 to +1.7	-19.3 to +60.8
Scenario 4	-18.4 to +8.4	-0.7 to +4.2	-3.2 to +30.5
Scenario 5	-32.4 to +9.5	-9.2 to +0.6	-41.8 to +20.9
Scenario 6	-1.4 to +0.6	-2.0 to +6.3	-12.6 to +5.5
Scenario 7	No differences > |0.01|	-1.7 to +1.0	0.0 to +0.4
Scenario 8	-1.4 to +0.6	-2.0 to +3.1	-12.1 to +5.5
Scenario 9	No differences > |0.01|	-1.2 to +1.0	No differences > |0.01|
Scenario 10	No differences	No differences	No differences

3.3 SUMMARY OF SIGNIFICANT FINDINGS

While the summaries of comparison results presented above are limited in scope, based only on the comparison of high ranked values, a few significant findings are worth noting:

1. Significant differences could be attributed to each of the three known factors that had been identified (Bug Fixes, Non-optional Technical Enhancements, and New Default Parameters for Optional Technical Enhancements);
2. Of the three known factors, the New Default Parameters for Optional Technical Enhancements appeared to cause the largest differences overall;
3. Differences varied significantly across different scenarios and source types, with no significant overall bias evident, although there appeared to be some tendency for the Non-optional Technical Enhancements to decrease concentrations, while the New Default Parameters for Optional Technical Enhancements showed an opposite trend, to some degree.

The significant contribution of New Default Parameters for Optional Technical Enhancements to differences between the then-current EPA-approved version and the current VISTAS version was somewhat unexpected, based on the limited documentation of differences between the two versions. These additional tests confirmed previous results indicating that most of the differences were due to CALMET rather than CALPUFF. The only significant differences attributable to CALPUFF were for the valley sources in Scenario 5, which is a near-field complex flow scenario along the Columbia River gorge. These additional tests indicated that <u>all</u> of the differences attributable to CALPUFF were due to the New Default Parameter for minimum sigma-v over water, which was reduced from 0.5m to 0.37m in the VISTAS version. The maximum percent differences for Scenario 5 due to this new default in parameter in CALPUFF ranged from -0.2 to +7.0.

Further evaluation of results related to the New Default Parameters in CALMET indicated that the new default threshold buoyancy energy flux for convective mixing heights over land (THRESHL) and over water (THRESHW) were the major factors contributing to these differences. This finding supported earlier indications that differences in mixing heights between the then-current EPA-approved version and the VISTAS version could be a major factor contributing to the differences in concentrations. Technical concerns regarding the implementation of these new default parameters for convective mixing heights were shared with TRC, but these concerns remain unresolved. The importance of convective mixing to both near field and long range dispersion estimates for many sources, the lack of adequate technical justification or validation for these new default parameters, and the significance of their impact on results based on these tests, presented an insurmountable obstacle to approval of the VISTAS version of the CALPUFF modeling system. These technical concerns regarding the new default parameters for convective mixing heights are described in more detail in the next section.

4.0 DESCRIPTION OF TECHNICAL ISSUES

4.1 ISSUE WITH NEW DEFAULT MIXING HEIGHT PARAMETERS

In 2006, significant modifications to the CALPUFF modeling system were introduced by Earth Tech under contract to the U.S. Department of the Interior Minerals Management Service (MMS) for overwater and coastal applications of the modeling system. These include the option to use similarity profiles and bulk flux algorithms based upon observations from the Coupled Ocean-Atmosphere Response Experiment (COARE) and use of the convective boundary layer algorithms in marine environments. These efforts were motivated in part by a recognition that CALMET formulations for overwater dispersion based on the Offshore and Coastal Dispersion (OCD) model lacked a convective mixing component, and could significantly underestimate turbulence levels and boundary layer depths over the Gulf of Mexico.

With the addition of the option to compute convective boundary layer heights over water, the model developer noted the potential for unrealistic growth of the convective boundary layer heights over areas with significant and sustained values of surface energy flux. According to the report entitled "Development of the Next Generation Air Quality Models for Outer Continental Shelf (OCS) Applications, Final Report: Volume 1",[6] it was noted that observed positive values of surface buoyancy flux over warm bodies of water such as the Gulf of Mexico were persistent for days during situations with cold air advection from continental air masses. Observed marine boundary layer heights were at equilibrium even in the presence of sustained surface buoyancy fluxes, supporting the notion that sustained convective mixing growth must be offset by some form of energy dissipation. Without some mechanism of buoyant energy dissipation in the model, convective mixing heights would grow continuously without interruption in these cases.

In order to prevent the continual growth of the convective boundary layer, the model developer introduced a threshold surface buoyancy energy flux necessary to sustain growth of the convective boundary layer. It was conjectured that as the marine convective boundary would grow, so would the energy requirements to sustain that growth. A similar threshold (THRESHL) was encoded for overland convective mixing heights for consistency. The model developers conjectured that the overland threshold would be much less important because of diurnal variations as well as the much higher values of surface heat flux overland.

The threshold buoyancy energy flux is characterized as the quantity of surface heat flux required to sustain the convective mixing height growth, expressed in W/m^2 per meter of mixing height. Separate threshold terms were added for land (THRESHL) and water (THRESHW), and were incorporated into both the Maul-Carson (current recommended) and new Gryning-Batchvarova mixing height algorithms. Default values of 0.05 $W/m^2/m$ were set for both THRESHL and THRESHW. The magnitude of the threshold kinematic heat flux at the surface is computed by the following equation:

$$\left(w'\theta'\right)_{th} = \frac{\left(THRESH\right)\left(Zic_{h-1}\right)}{\left(\rho\right)\left(c_p\right)} \tag{1}$$

where

$(w'\theta')_{th}$ = threshold kinematic heat flux (K m/s)
THRESH = threshold buoyancy energy flux parameter = 0.05 W/m^2/m
Zic_{h-1} = convective mixing height from previous hour (m)
ρ = density of air (kg/m^3)
c_p = specific heat at constant pressure (J/kg/K)

At each time step, CALMET checks to see whether sufficient buoyant energy is available to sustain the growth of the convective boundary layer by simply subtracting the threshold quantity necessary to sustain the growth based on Equation 1 from the hourly buoyant energy flux. While the documentation provided describes this threshold as a threshold to "sustain the growth" of the boundary layer, a review of its implementation in the CALMET code indicated that once the difference falls below zero, CALMET resets the convective boundary layer height for the current time step to zero. The effect of setting the convective mixing height to zero would be partially masked in most applications because the hourly mixing height output from CALMET for these cases would be higher of the default minimum mixing height (Z_{min}=50m) and the daytime mechanical mixing height (Z_{mech}), and also due to the default option for upwind averaging of mixing heights. However, the convective velocity scale (w_*), which is used by CALPUFF to scale vertical turbulence under convective conditions, is based only on the convective mixing height.

As noted previously, EPA's assessment found that significant differences between the previous EPA-approved version and the VISTAS version were attributable to the implementation of these new mixing height parameters. Visualization of the CALMET mixing heights from Scenario 4, a typical LRT Class I area scenario including the Shenandoah National Park and other nearby Class I areas, showed multiple periods when the convective boundary layer would collapse over large areas over land, contrary to the conjecture that the overland threshold would be much less important. For example, at the location identified in Figure 2, the overland convective boundary layer collapsed during the middle of the day on three out of four consecutive simulation days (Figure 3). The boundary layer heights on these three days (10/17, 10/18, and 10/20) changed from 957m, 598m, and 1088m to 0m and then back to 599m, 437m, and 267m within a span of three hours on each of the three respective days. A very small difference between the buoyant energy flux and the threshold is all that is necessary to cause the complete collapse of the convective boundary layer. Note that the convective mixing heights presented in these figures were generated using no minimum mixing height and no upwind averaging of mixing heights in CALMET.

4.2   POTENTIAL RAMIFICATIONS OF TECHNICAL ENHANCEMENT

When this anomalous behavior was confirmed in the CALMET meteorological fields, some important implementation issues were raised by EPA. First, the sudden collapse and regeneration of the convective boundary layer creates physically unrealistic mixing height patterns with extremely tight spatial gradients that would not normally be observed in the

atmosphere. When using CALMET with meteorological observations only (no prognostic meteorological datasets used for the first guess windfield), certain derived meteorological values rely upon data from the nearest surface or upper air meteorological site in the modeling domain. These create physical discontinuities in two-dimensional meteorological fields when relying upon nearest station data. In CALMET, the surface buoyant energy flux calculation found in both the Maul-Carson and the Gryning-Batchvarova convective mixing height schemes relies upon the conversion of sensible heat flux which is in turn derived from the nearest station with non-missing cloud cover data. When the buoyant energy flux is derived in such a way and the energy is insufficient to sustain the convective boundary layer growth, the convective boundary layer will collapse at every grid point which derives sensible heat flux from cloud cover observations at a particular surface station. This anomalous convective mixing height behavior is illustrated in Figure 5 as a series of contour plots of convective mixing height for a 3-hour period on Oct. 19, 1992 based on Scenario 4. The visualization shows that the collapse of convective mixing height occurs over distances of more than 100 km.   Derived micrometeorological values such as convective velocity scale (w_*), which contains the convective boundary layer height in its equation, will exhibit the same spatial patterns as the convective boundary layer.

Another important issue is the impact that unrealistic changes in micrometeorological parameters have on dispersion. When employing dispersion coefficients from internally computed micrometeorological variables (MDISP=2), these unrealistic changes to the micrometeorological variables will have a significant impact upon puff growth rates. The collapse of the convective boundary layer and associated changes in dispersion will have varying impacts on surface concentrations depending upon source type. For low-level sources, this sudden collapse of the daytime boundary layer is likely to significantly increase ground level concentrations by essentially trapping the puffs within an artificially compressed daytime boundary layer. For elevated point sources, the opposite effect may manifest itself, as these sources will be emitting puffs well above the mixing height. Comparison results from Test 7 show evidence of these patterns of impact where the largest positive percent difference of +188 percent (VISTAS version > EPA-approved version) was for a low-level area source in Scenario 2, and the largest negative difference of -41.8 percent was for a 65m buoyant source in Scenario 5.
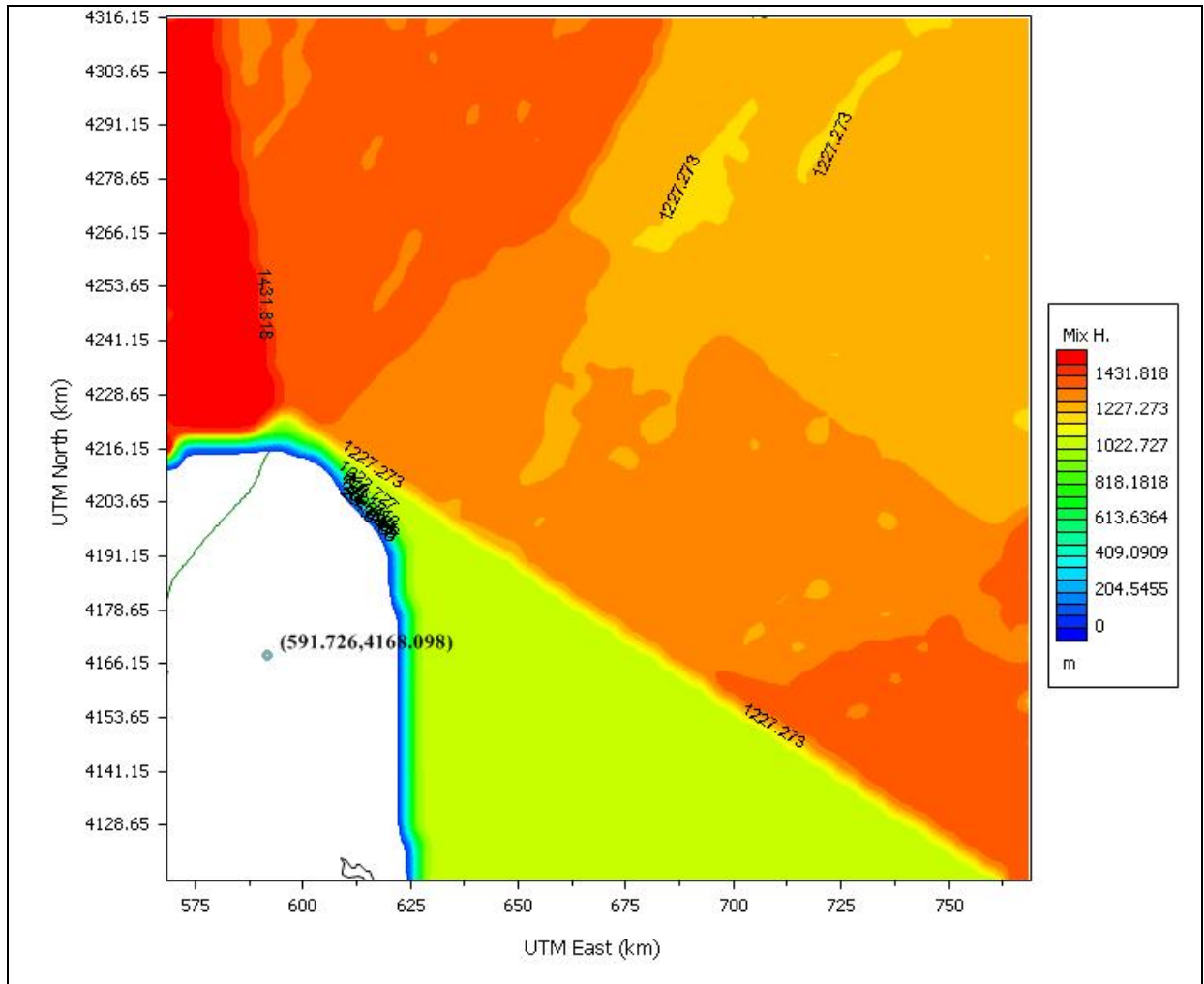
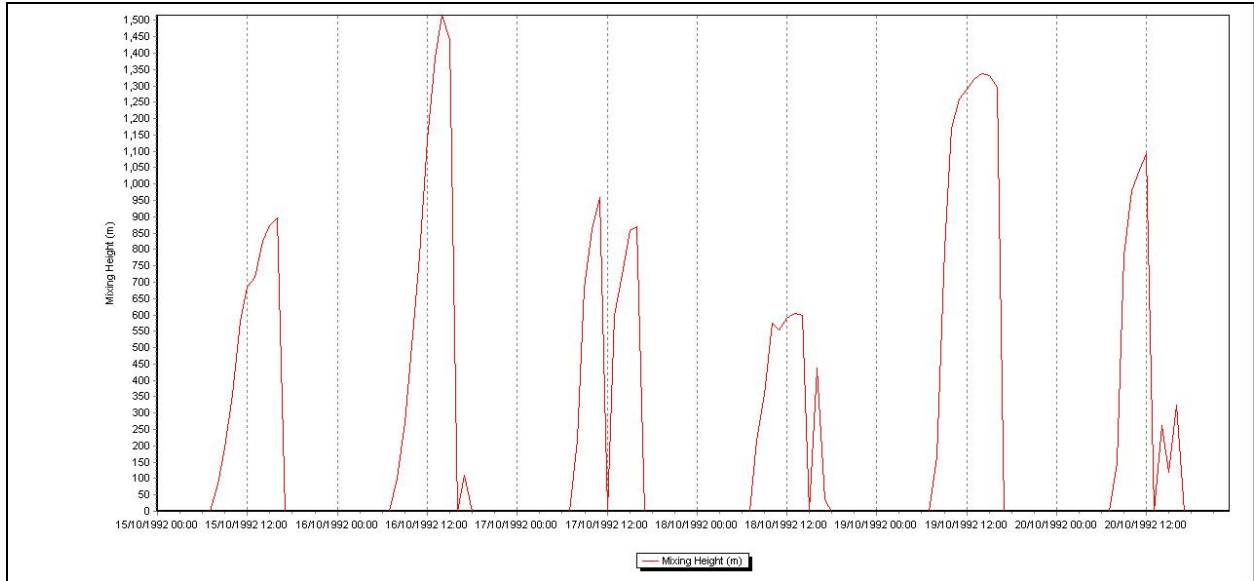Figure 2. CALMET convective mixing heights for one time step, Test 4.

Figure 3. Time series of convective mixing height from point identified in Figure 1.
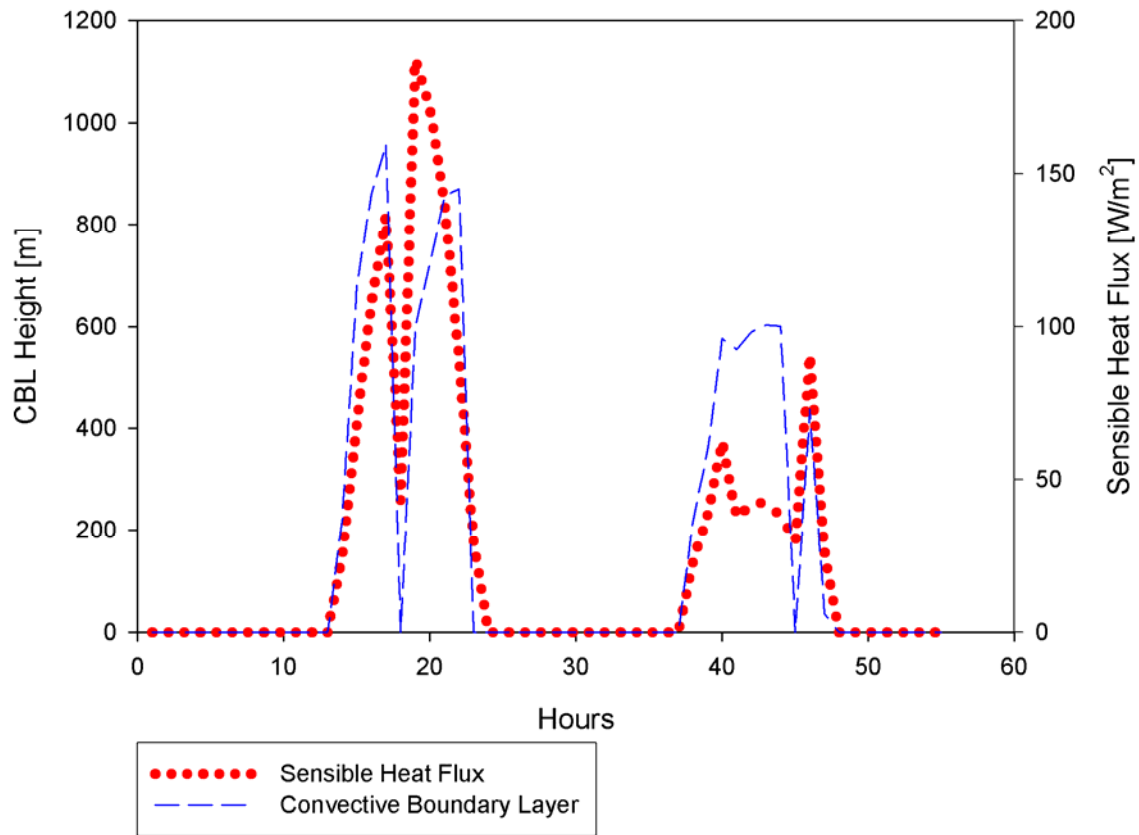

Figure 4. Time series of sensible heat flux and convective mixing height for 2 days from Figure 3.

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4.3   RESOLUTION OF ISSUES

Based on the results of the comparisons summarized above, EPA determined that insufficient documentation and justification was available to approve the VISTAS version of the CALPUFF modeling system for regulatory applications. In order to resolve this situation, TRC agreed to implement the following changes in the CALPUFF modeling system code:

1. Incorporate the non-optional technical enhancements under the optional technical enhancements, removing non-optional technical enhancements as a potential source of differences;
2. Incorporate a new regulatory default switch (MREG=1) in CALMET to allow the optional technical enhancements to be included in the model, but to require the user to override the default options to exercise these optional technical enhancements; and
3. Modify the CALPUFF model code to include the minimum sigma-v of 0.5 m/s over water as part of the regulatory default setting.

These modifications were incorporated into CALPUFF (v5.8) and CALMET (v5.8), which were then approved by EPA for regulatory modeling. These actions effectively isolated bug fixes as the only source of differences between the previous EPA-approved version and the new versions of CALMET and CALPUFF (v5.8), when applied in the regulatory default mode. Table 5 includes a summary of the final comparisons between the previous EPA-approved version (CALPUFF, v5.711a) and the new EPA-approved version (CALPUFF, v5.8), identified as Test 8. Comparison results for Tests 5, 6, and 7 are also presented for reference. Table 5 confirms that comparison results for Test 8 are nearly identical to results for Test 5, which was intended to isolate impacts due solely to bug fixes. The minor differences noted between Tests 5 and 8 for Scenarios 2 and 3, both of which include the use of MM5 data, were attributable to additional bug fixes incorporated into version 5.8 that were identified by TRC as part of this assessment. A more detailed summary of maximum absolute differences in high ranked values by source and scenario are presented in Table 6 for Scenarios 1 through 5 and in Table 7 for Scenarios 6 through 10.

5.0 REFERENCES

1. EPA, 2005. *Guideline on Air Quality Models*. 40 CFR Part 51 Appendix W.

2. EPA, 2008. Protocol for Updating the CALPUFF Modeling System.

3. EPA, 2005. EPA 8th Modeling Conference CALPUFF presentation, (http://www.epa.gov/ttn/scram/8thmodconf/presentations/day2morning/calpuffanalysisto olrevised.ppt)

4. EPA, 2006. CALPUFF Modeling System Update #1 (version 5.711a).

5. TRC, 2007. Summary of Model Tests Conducted with the VISTAS-Approved CALMET and CALPUFF Model Codes vs. EPA-Approved Versions of the Models, prepared for VISTAS.

6. Earth Tech, 2006. Development of the Next Generation Air Quality Models for Outer Continental Shelf (OCS) Applications, Final Report: Volume 1, MMS 2006-006, prepared for U.S. Department of the Interior, Minerals Management Service.

	Test 5 – Bug Fixes	Test 6 – Non-Optional Technical Enhancements	Test 7 – New Default Parameters	Test 8 – Base 5.711a vs. Beta 5.8 (Final Test)[a]
Scenario 1	-1.0 to +22.6	-18.6 to +1.9	-22.0 to +24.4	-1.1 to +22.6
Scenario 2	-15.4 to +27.8	-30.5 to +0.7	-21.8 to +118.3	-21.8 to +29.2
Scenario 3	-5.1 to +6.0	-0.8 to +1.7	-19.3 to +60.8	-4.0 to +7.3
Scenario 4	-18.4 to +8.4	-0.7 to +4.2	-3.2 to +30.5	-18.4 to +8.4
Scenario 5	-32.4 to +9.5	-9.2 to +0.6	-41.8 to +20.9	-32.4 to +9.5
Scenario 6	-1.4 to +0.6	-2.0 to +6.3	-12.6 to +5.5	-1.4 to +0.6
Scenario 7	No differences > |0.01|	-1.7 to +1.0	0.0 to +0.4	No differences > |0.01|
Scenario 8	-1.4 to +0.6	-2.0 to +3.1	-12.1 to +5.5	-1.4 to +0.6
Scenario 9	No differences > |0.01|	-1.2 to +1.0	No differences > |0.01|	No differences > |0.01|
Scenario 10	No differences	No differences	No differences	No differences

Table 5: Range of Maximum Absolute Percent Differences by Scenario

[a] Test 8 differences are due to bug fixes, but include some additional bug fixes compared to Test 5.

Table 6. CALPUFF Comparison Results for Scenarios 1 - 5 for Base v5.711a vs. Beta v5.8

Scenario	Source Type					
	Area Source	Volume Source	30 m Point Source	65 m Point Source	99 m Point Source	Buoyant Area Source
1	✕ 0.12	✕ 0.20	✕ 0.48	✕ 7.59		
	✕ 0.41	✕ 1.07	✕ 0.28	✕ 22.63		
2	✕ -21.78	✕ -6.71	✕ -2.84	✕ 29.24		
	✕ 0.68	✕ 2.35	✕ 0.58	✕ 25.24		
3	✕ -0.02	✕ 0.00	✕ -0.05	✕ 7.26	✕ -3.98	
4	✕ 8.40	✕ -4.55	✕ -4.95	✕ -18.37		✕ -13.02
5	✕ 0.02	✕ -0.30	✕ -0.88	✕ -32.43		
	✕ 0.32	✕ 0.12	✕ -5.10	✕ -7.36		

✓ No differences in highest ranked (design) values

✕ Differences in one or more design values

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Figure 7. CALPUFF Comparison Results for Scenarios 6 - 10 for Base v5.711a vs. Beta v5.8

	Area			Volume			30 m stack			65 m stack			Downwash from 35 m capped stack		Downwash from 35 m non-capped stack			Downwash from 50 m non-capped stack		
Stable	0.002	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓			-0.824			✓		
	0.002	0.002		✓	✓		✓	✓		✓	✓		✓			✓			✓		
Neutral	-0.003	-0.003	✓	0.005	0.005	✓	0.006	0.006	✓	0.018	0.018	✓	-0.001			0.003			0.022		
	-0.003	-0.003		✓	✓		✓	✓		✓	✓		✓			✓			✓		
Unstable	0.137	0.137		0.565	0.565		0.626	0.626		-1.419	-1.419		0.541			-0.068			-1.282		
	0.005	0.005		✓	✓		✓	✓		✓	✓		✓			✓			✓		

Key to results for Scenarios 6 - 10

	Simulated Hill	Flat Terrain	Simulated Hill (with wind shear)
Similarity	6	8	10
PG	7	9	

✓ No differences found
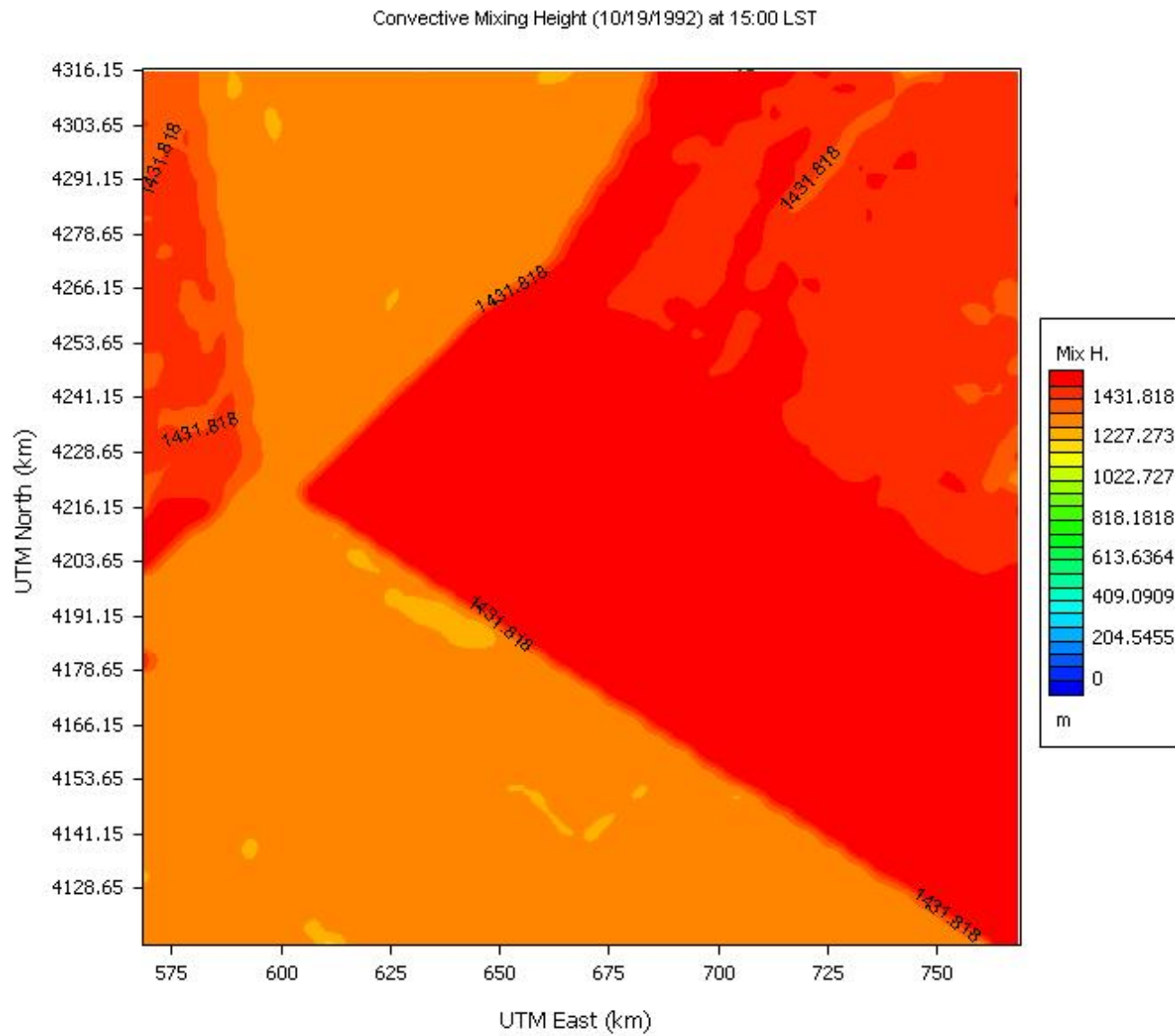
✗ Differences found

Figure 5a. Contour plot of convective mixing heights (m) with default THRESHL for Scenario 4, 10/19/92, 15:00 LST
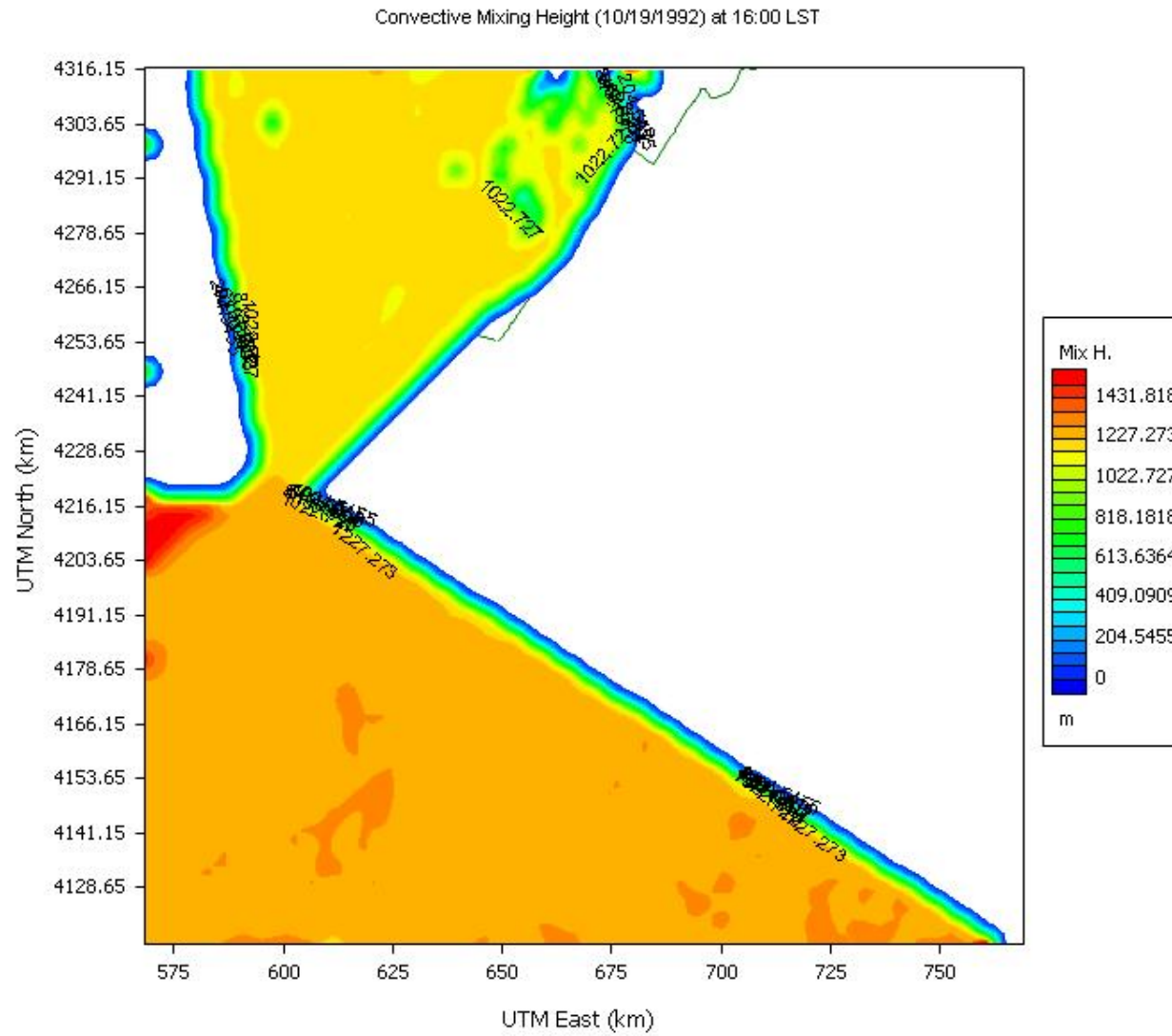
Figure 5b. Contour plot of convective mixing heights (m) with default THRESHL for Scenario 4, 10/19/92, 16:00 LST
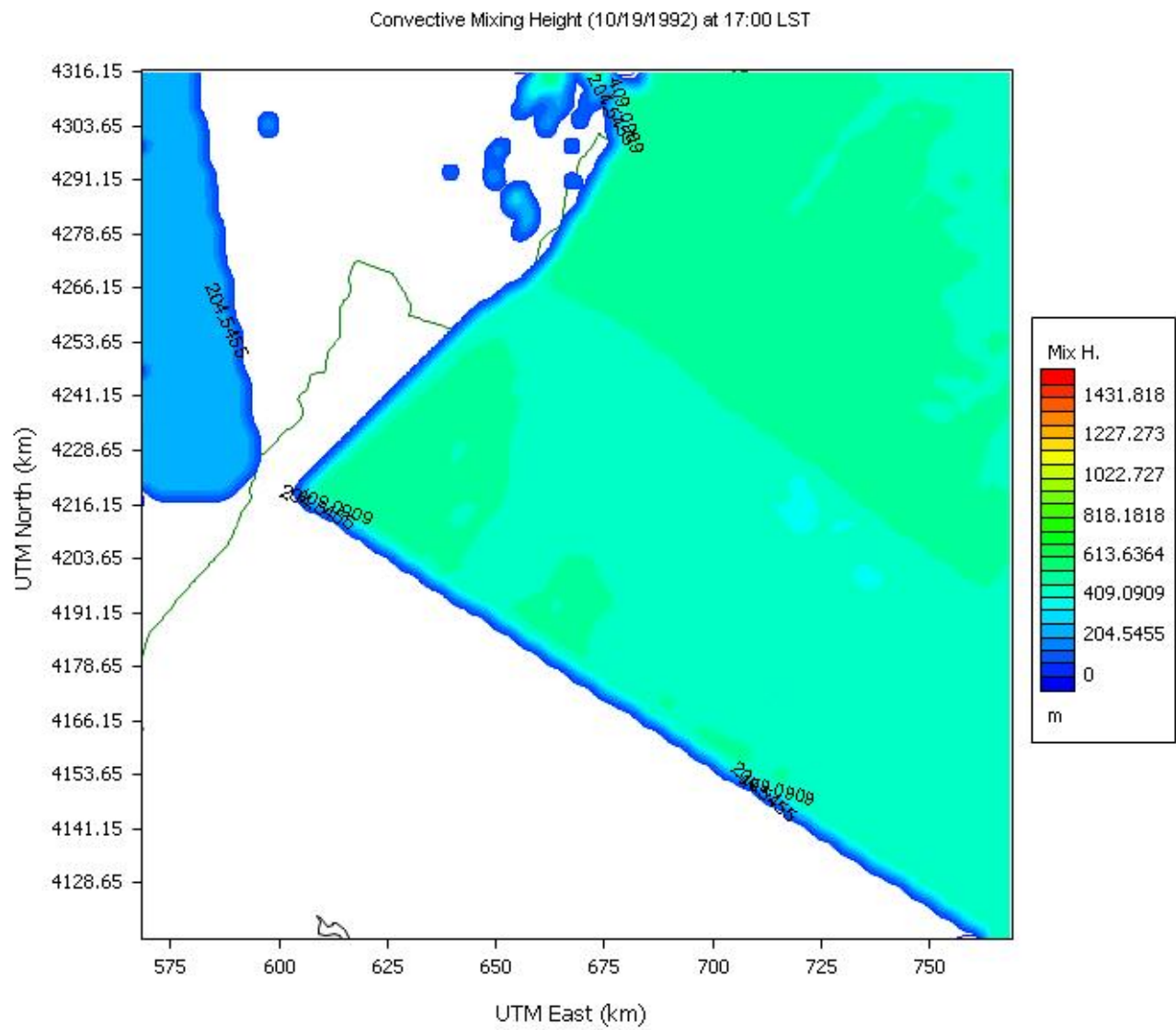
Figure 5c. Contour plot of convective mixing heights (m) with default THRESHL for Scenario 4, 10/19/92, 17:00 LST