CALPUFF Modeling System: Science and Implementation Issues

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Outline

- Assessment of VISTAS version of CALPUFF
- Unresolved technical issues with v5.8
- Near-field Clarification Memo
- Some examples of complex wind situations
- Discussion of technical issues and concerns related to CALPUFF near-field applications
- Other CALPUFF implementation and science issues
- Summary and conclusions

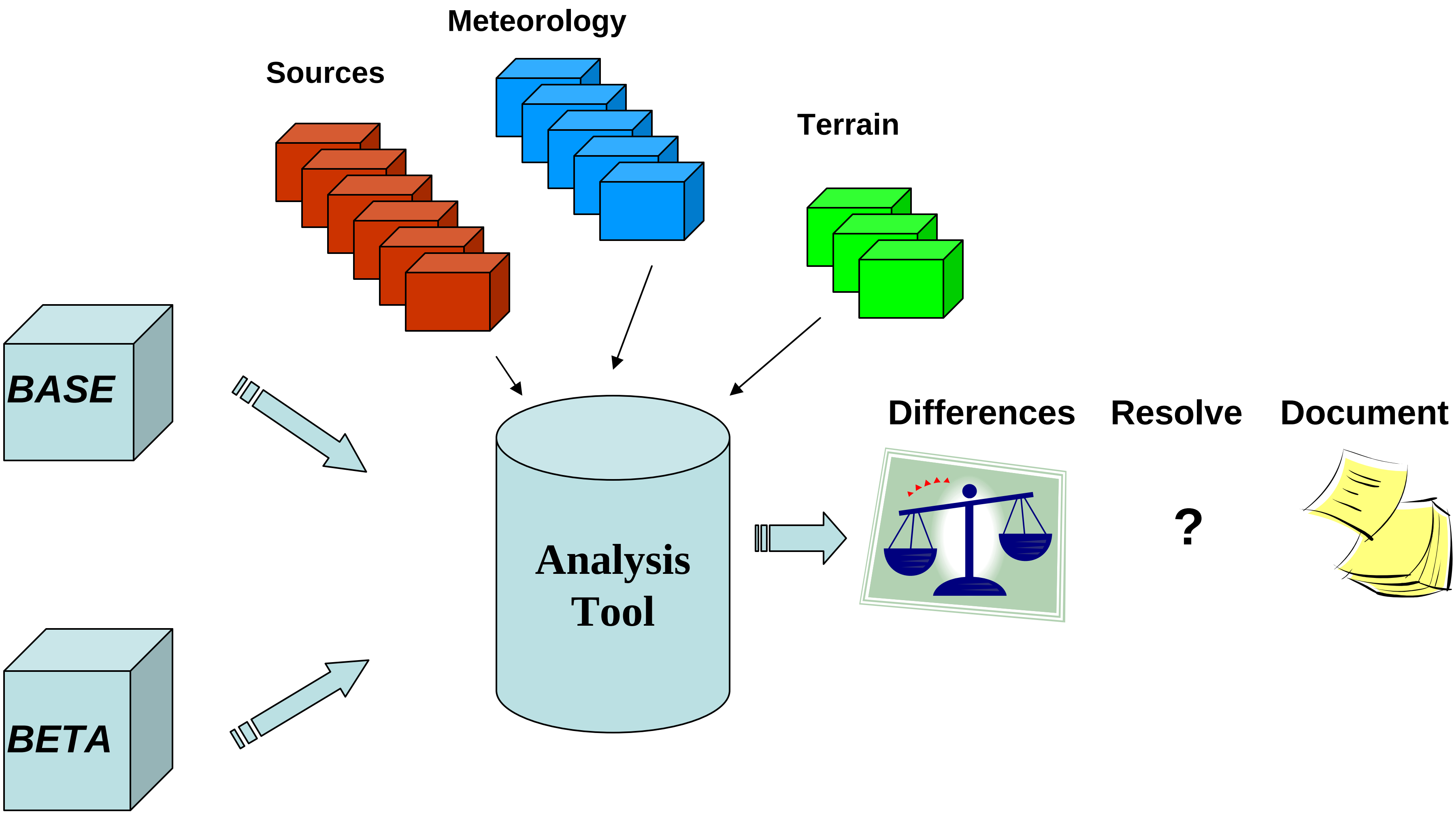
CALPUFF Update Process

- Incumbent upon EPA to perform an independent assessment of CALPUFF when updating to new versions
- CALPUFF requires extensive assessment and understanding of changes made; approvals made by EPA, not developer
- CALPUFF Update Tool – Introduced at 8th Modeling Conference in Sept 2005

CALPUFF Update Tool

- Compares 2 CALPUFF versions; proposed (beta) vs. current version (base)
- Determines code changes and differences in results across 10 scenarios
- Provides a standardized methodology for evaluating changes in model codes

CALPUFF Update Tool



CALPUFF Update Process: Initial Assessments of v5.756

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

EPA, 2008: Assessment of the "VISTAS" Version of the CALPUFF Modeling System, EPA-454/R-08-007, available on SCRAM website.

CALPUFF Update Process: Additional Assessments of v5.756

- TRC provided the following interim versions, to facilitate isolating impacts due to (1) bug fixes and (2) non-optional technical enhancements:
  - CALMET v5.53c = CALMET v5.53a + bug fixes
  - CALMET v5.53c2 = CALMET v5.53c + non-optional technical enhancements
  - CALPUFF v5.711c = CALPUFF v5.711a + bug fixes

CALPUFF Update Process: Additional Assessments of v5.756

- EPA conducted several tests in order to compare and isolate affects of the following categories of changes:
  - Bug fixes
  - Non-optional technical enhancements
  - New default parameters for optional technical enhancements

CALPUFF Update Process: Summary of Significant Findings

- Significant differences attributed to each of the three known factors:
  - Bug Fixes
  - Non-optional Technical Enhancements
  - New Default Parameters for Optional Technical Enhancements
- Of the three known factors, the New Default Parameters for Optional Technical Enhancements caused the largest differences overall
- Differences varied significantly across different scenarios and source types, with no significant overall bias evident

CALPUFF Update Process: Summary of Differences – v5.8 Final

Range of Maximum Absolute Percent Differences by Scenario				
	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)[1]
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

[1]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

CALPUFF Assessment Results from Previous Update – v5.7 to 5.711a

CALPUFF Base/Beta Comparison - Results for Scenarios 1 - 5

Scenario	Area Source	Volume Source	30 m Point Source	65 m Point Source	99 m Point Source	Buoyant Area Source
1	✓	✗ -0.001 %	✗ -0.008 %	✗ -0.295 %		
	✗ -0.011 %	✗ -0.008 %	✗ -0.008 %	✗ -0.201 %		
2	✓	✗ +0.005 %	✓	✗ +0.091 %		
	✓	✓	✓	✓		
3	✓	✓	✓	✓	✗ +0.006 %	
4	✗ -0.037 %	✗ -5.254 %	✗ +0.239 %	✗ +0.006 %		✗ -0.003 %
5	✗ -0.015 %	✗ +0.011 %	✗ -0.004 %	✗ -0.003 %		
	✗ +0.002 %	✗ -0.003 %	✗ +0.006 %	✗ -0.003 %		

✓ No differences in highest ranked (design) values

✗ Differences in one or more design values

Scenario 2 - 65m Point Source, Salem Location
Percent Difference - 1st Highest, 1-Hour Averages

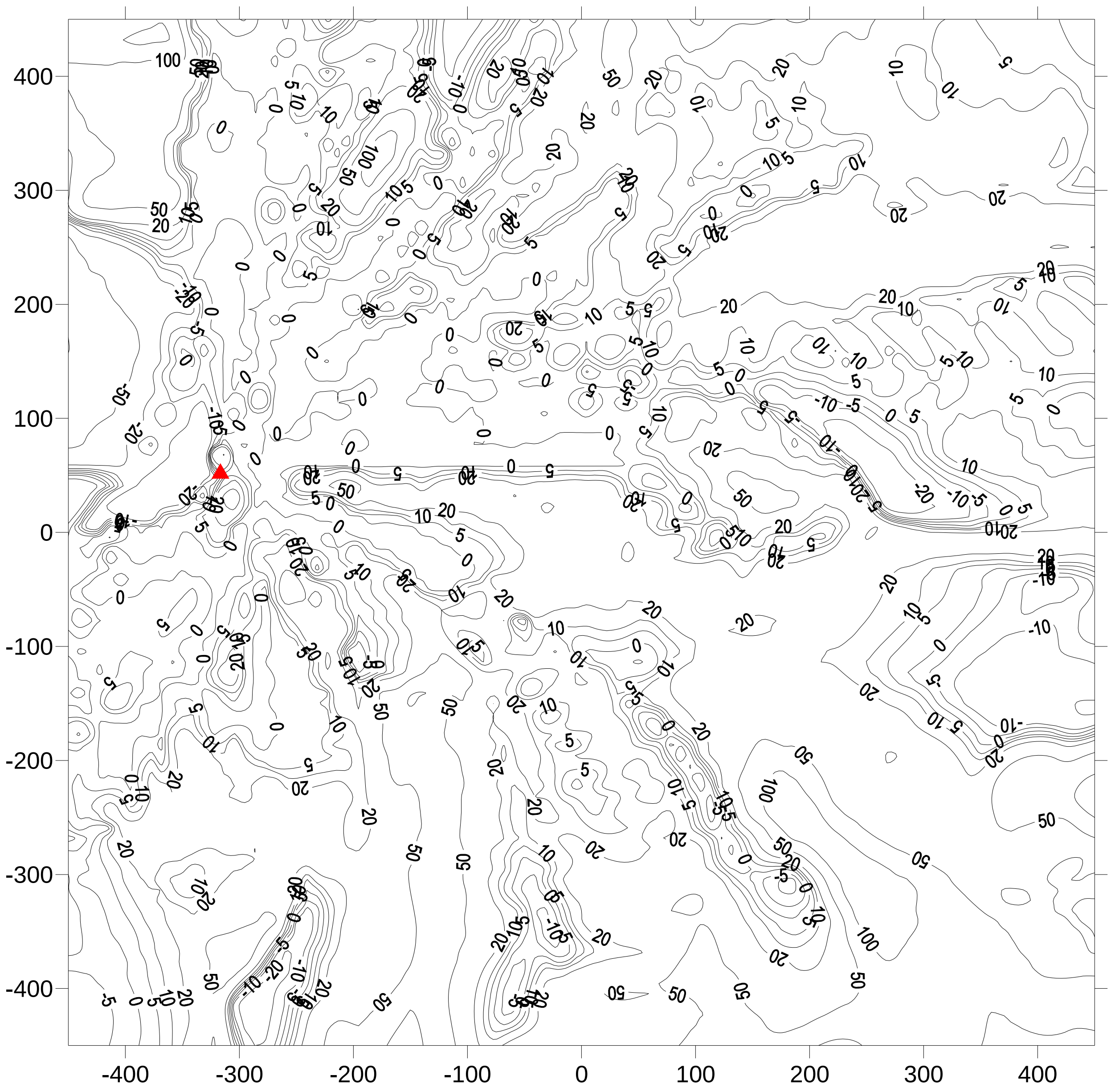
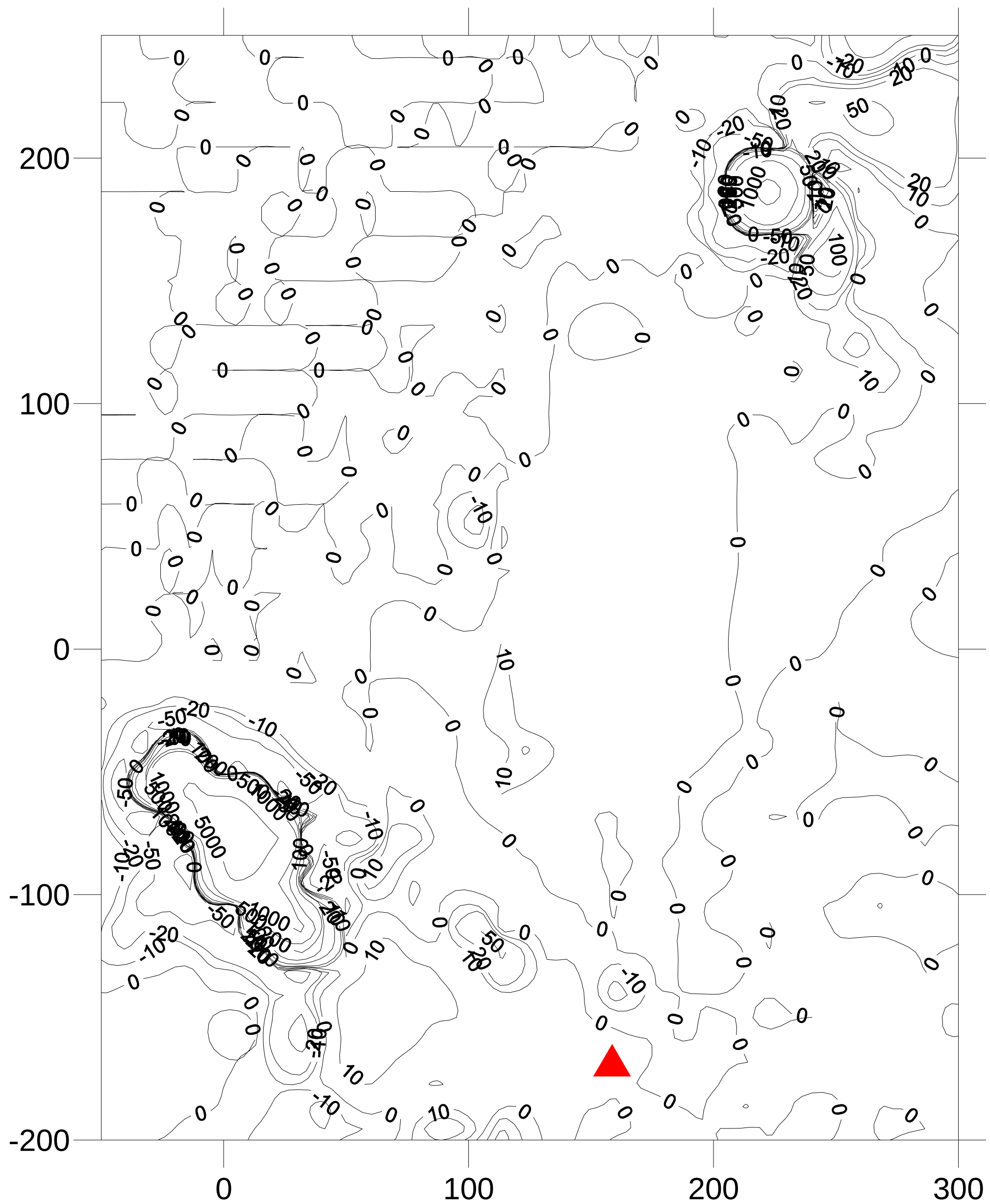


Figure 1: Contour Plot of Percent Differences for Scenario 2
Jordan Valley 65m Point Source; 4th-Highest 24-Hour Averages

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



CALPUFF Update Process: Unresolved Issues with v5.8

- EPA has unresolved technical concerns regarding how the optional technical enhancements for mixing height have been implemented in CALMET
- These concerns are related to the new default parameters THRESHL and THRESHW for the threshold buoyancy energy flux over land and water, respectively
- These new thresholds were implemented as part of the MMS-sponsored enhancements, to prevent unlimited growth of the convective boundary layer over water

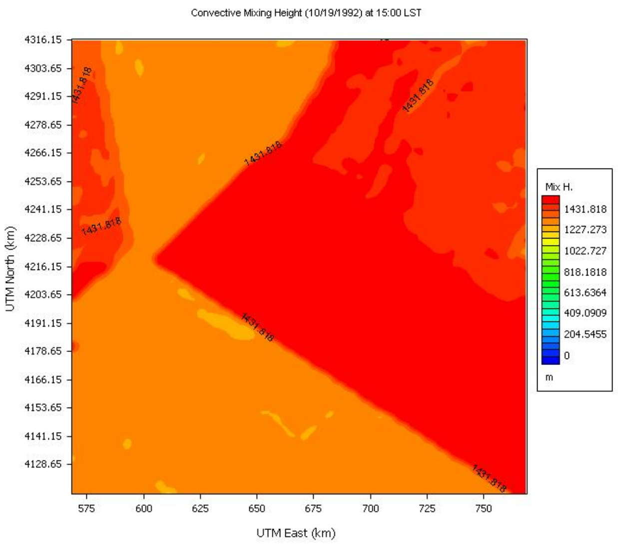
CALPUFF Update Process: Unresolved Issues with v5.8

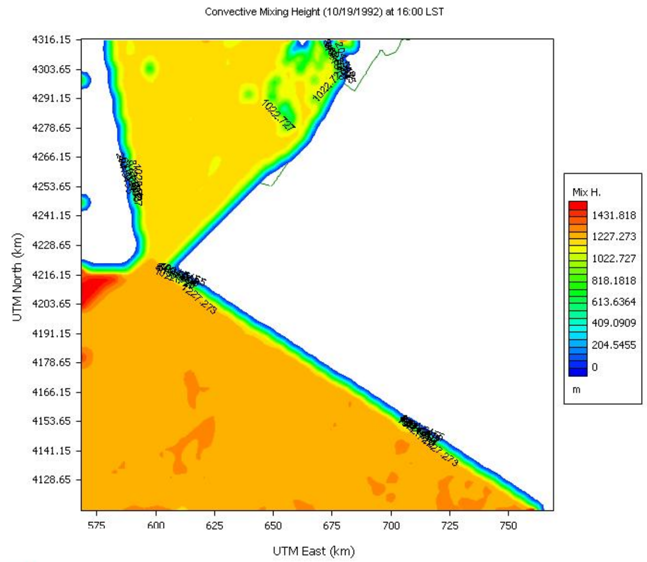
- These new thresholds are defined (in the limited documentation available) as the “threshold buoyancy flux required to sustain convective mixing height growth”
- However, the code indicates that when the sensible heat flux falls below the threshold, the convective mixing height is immediately assigned to 0m for that grid cell, eliminating convective turbulence
- A new convective boundary layer may form on subsequent hours

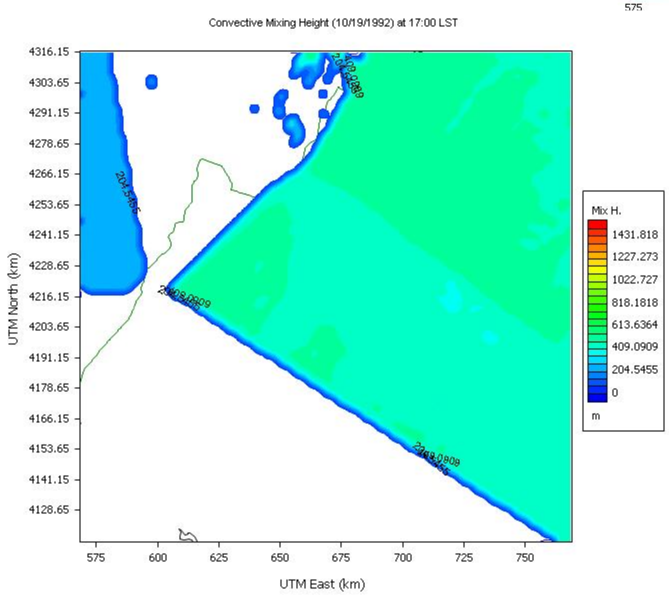
CALPUFF Update Process: Unresolved Issues with v5.8

- This behavior is masked somewhat by other defaults within CALMET, including the default minimum mixing height of 50m, the use of the maximum of convective and mechanical mixing heights as the overall mixing height, and the default option for upwind averaging of mixing heights
- The default threshold is 0.05 $W/m^2/m$.
  - For example, if Zic = 3000m at 2pm, and H = 149 W/m^2 at 3pm, then Zic = 0m at 3pm. A new CBL will likely form at 4pm.
- The following figures from Scenario 4 illustrate this behavior

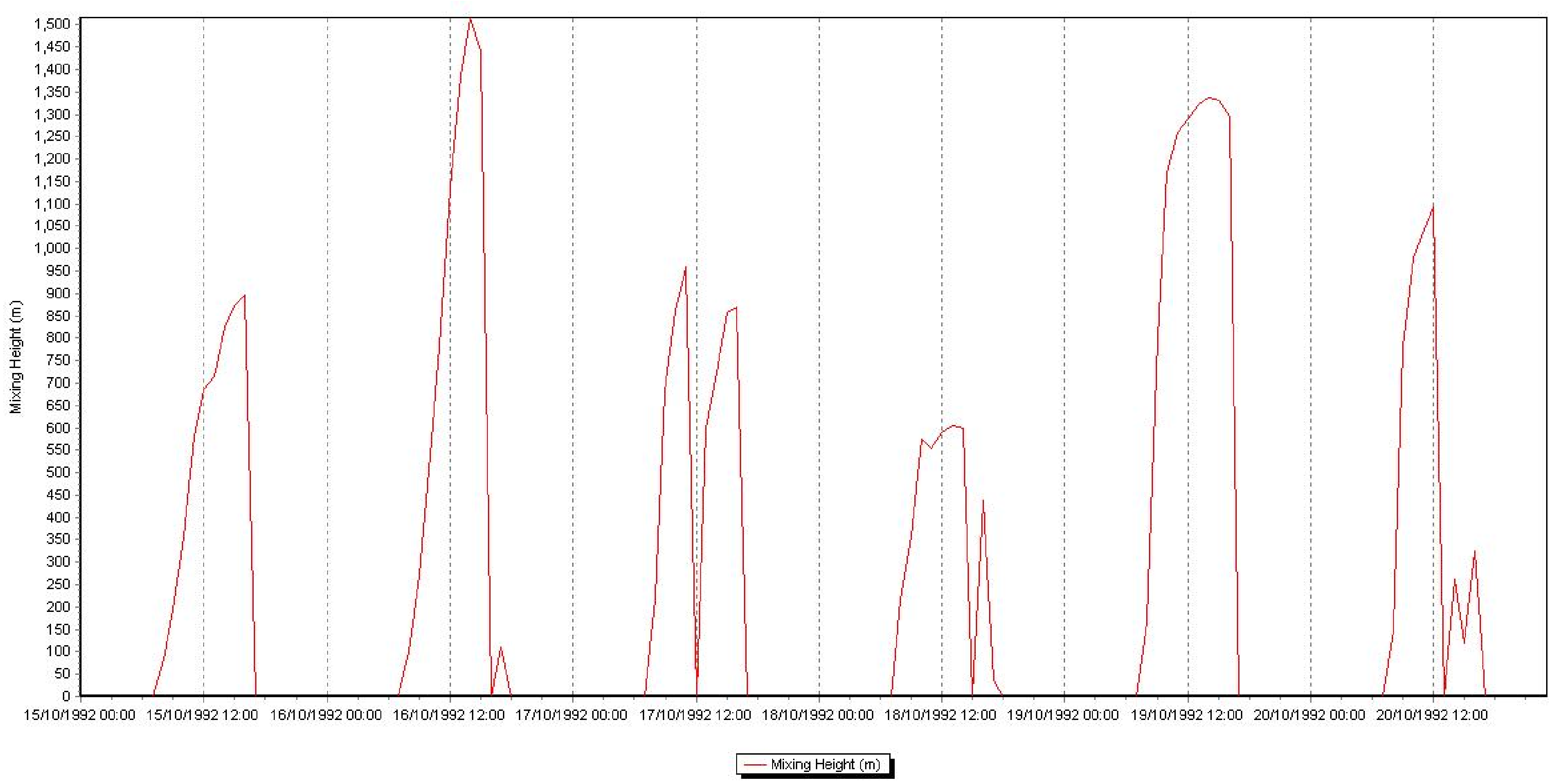
CALMET v5.8 Convective Boundary Layer Heights (THRESHL = 0.05)







Time series of convective mixing height from CALMET



CALPUFF Update Process: Resolution of Issues (Partial)

- TRC agreed to implement the following changes in the CALPUFF modeling system code, allowing EPA to approve v5.8:
  - Incorporate the non-optional technical enhancements under the optional technical enhancements, removing non-optional technical enhancements as a potential source of differences;
  - 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
  - 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.

CALPUFF Update Process: Summary of Differences – v5.8 Final

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CALPUFF Implementation Issues

- Lack of adequate documentation
  - New MREG option in CALMET not well-documented; CALMET.INP sample input file indicates “no default” and assigns value of MREG = 0, i.e., don’t enforce regulatory defaults
  - Many important technical details are not documented, except in the code
- Magnitude of differences between v5.8 of CALPUFF and previous version raises questions regarding “validity” of original model evaluations for CALPUFF
- PG vs. turbulence dispersion option in CALPUFF
  - Addressed in March 2006 Model Clearinghouse Memo: not an automatic switch with promulgation of AERMOD, requires separate assessment
  - Assessment is underway, but has uncovered other PG-class dependencies with turbulence option
- Pending assessment of v5.8’n’ and v6 updates
  - Currently “on hold” due to need to address broader issues
- CALPUFF near-field Clarification Memo

CALPUFF Near-field Clarification Memorandum

- Summary of Key Points:
  - **The EPA-preferred model for near-field regulatory applications (less than 50 kilometers) for simple and complex terrain is AERMOD.** The AERMOD model should be used for all near-field regulatory applications, unless an adequate determination is made that AERMOD is not appropriate for that application or is clearly less appropriate than an alternative model. *[See paragraph 4.2.2(b) of Appendix W – "For a wide range of regulatory applications in all types of terrain, the recommended model is AERMOD."]*
  - **CALPUFF is <u>not</u> the EPA-preferred model for near-field applications, but may be considered as an alternative model on a case-by-case basis for near-field applications involving "complex winds," subject to approval by the reviewing authority.** The approval of CALPUFF for near-field regulatory applications should be based on case-specific justification, including necessary documentation and an adequate determination that AERMOD is not appropriate or clearly less appropriate than CALPUFF. Generalized approval of CALPUFF for near-field applications based on reference to other cases where CALPUFF has been approved for near-field use is not acceptable, unless such cases are similar enough to the application under review to be applicable, and are adequately documented to support that determination. *[See paragraph 7.2.8(a) of Appendix W – "the CALPUFF modeling system (described in Appendix A) may be applied on a case-by-case basis for air quality estimates in such complex non-steady-state meteorological conditions."]*

CALPUFF Near-field Clarification Memorandum

- From Preamble to April 2003 FR Notice promulgating CALPUFF:
  - *“We will require approval to be obtained prior to accepting CALPUFF for complex wind situations, as this will ensure that a protocol is agreed to between the parties involved, and that all are willing to accept the results as binding. As experience is gained in using CALPUFF for complex wind situations, acceptance will become clear and those cases that are problematic will be better identified.” (pp. 18441-2)*

CALPUFF Near-field Clarification Memorandum

- From Section 7.2.8 of Appendix W:
  - *“The setup and application of the model should be determined in consultation with the appropriate reviewing authority (paragraph 3.0(b)) consistent with limitations of paragraph 3.2.2(e).”*
  - *Reference to paragraph 3.2.2(e) places CALPUFF in the status of an alternative model.*

CALPUFF Near-field Clarification Memorandum

- Paragraph 3.2.2(e) of Appendix W:

"e. Finally, for condition (3) in paragraph (b) of this subsection [preferred model is less appropriate for the specific application, or there is no preferred model], an alternative refined model may be used provided that:

i. The model has received a scientific peer review;

ii. The model can be demonstrated to be applicable to the problem on a theoretical basis;

iii. The data bases which are necessary to perform the analysis are available and adequate;

iv. Appropriate performance evaluations of the model have shown that the model is not biased toward underestimates; and

v. A protocol on methods and procedures to be followed has been established."

CALPUFF Near-field Clarification Memorandum

- Summary of main steps:
  1) *a determination that treatment of complex winds is critical to estimating design concentrations;*
  2) *a determination that the preferred model is not appropriate or less appropriate than CALPUFF; and*
  3) *a demonstration that the five criteria listed in paragraph 3.2.2(e) for use of an alternative model are adequately addressed.*
- Each of these steps involves case-specific considerations

CALPUFF Near-field Clarification Memorandum

- Importance of consistency, spelled out in paragraph 1(b) of the Guideline:

  “The model that most accurately estimates concentrations in the area of interest is always sought. However, it is clear from the needs expressed by the States and EPA Regional Offices, by many industries and trade associations, and also by the deliberations of Congress, that **consistency in the selection and application of models and data bases should also be sought, even in case-by-case analyses**. Consistency ensures that air quality control agencies and the general public have a common basis for estimating pollutant concentrations, assessing control strategies and specifying emission limits. Such consistency is not, however, promoted at the expense of model and data base accuracy. The *Guideline* provides a consistent basis for selection of the most accurate models and data bases for use in air quality assessments.”

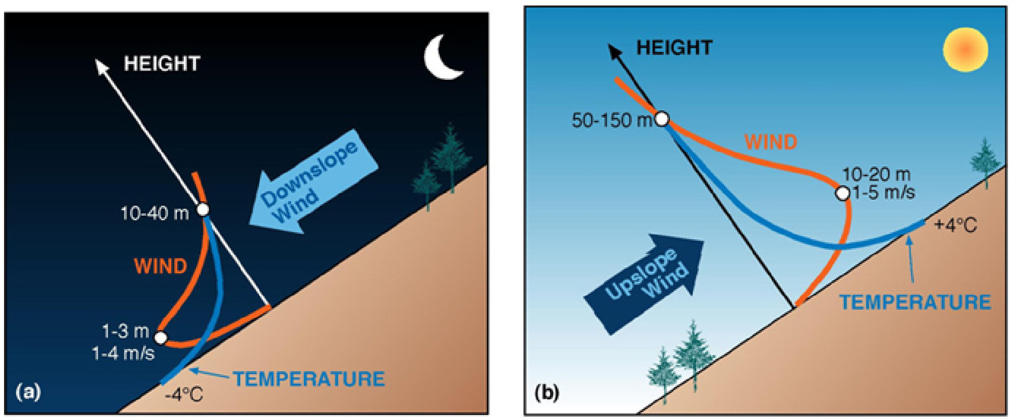
Examples of Complex Winds

- Examples of complex winds are described in paragraph 7.2.8(a) of Appendix W:
  - “a. *Inhomogeneous Local Winds.* In many parts of the United States, the ground is neither flat nor is the ground cover (or land use) uniform. These geographical variations can generate local winds and circulations, and modify the prevailing ambient winds and circulations. Geographic effects are most apparent when the ambient winds are light or calm. In general these geographically induced wind circulation effects are named after the source location of the winds, e.g., lake and sea breezes, and mountain and valley winds. In very rugged hilly or mountainous terrain, along coastlines, or near large land use variations, the characterization of the winds is a balance of various forces, such that the assumptions of steady-state straight-line transport both in time and space are inappropriate.”

Examples of Complex Winds

- Valley flows
  - Down-slope/down-valley flows under light wind stable conditions
  - Cross-valley circulations due to differential heating under convective conditions
  - Valley channeling, may be driven by different conditions
  - Stagnation conditions
  - Significant horizontal and vertical discontinuities in wind, temperature, etc.
  - Grid resolution and availability of representative met data may be significant issues

Slope Flows

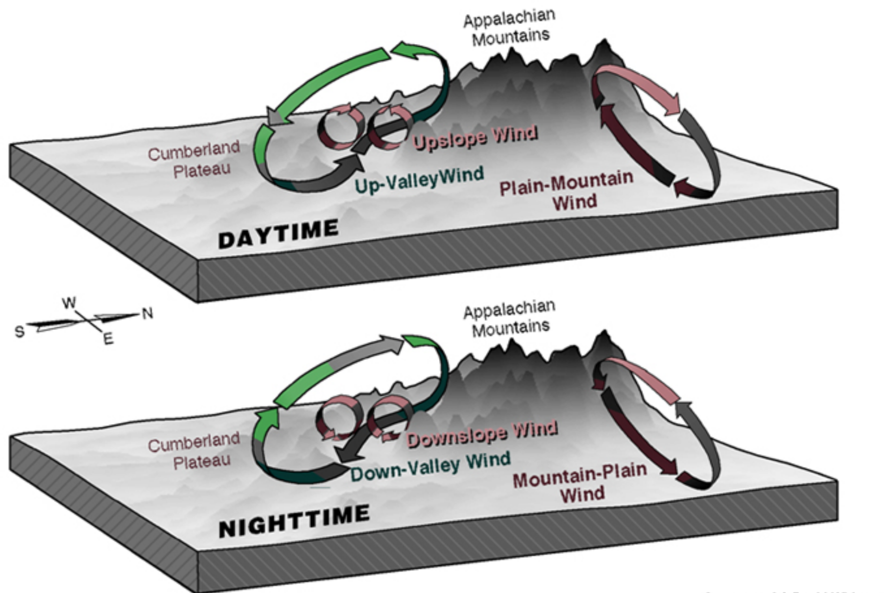


Courtesy of C.David Whiteman

- Part of local diurnal wind pattern that is thermally induced.
- Formation is favored under weak synoptic pressure gradients.
- Depends upon surface temperature contrasts due to daytime heating and nighttime cooling.

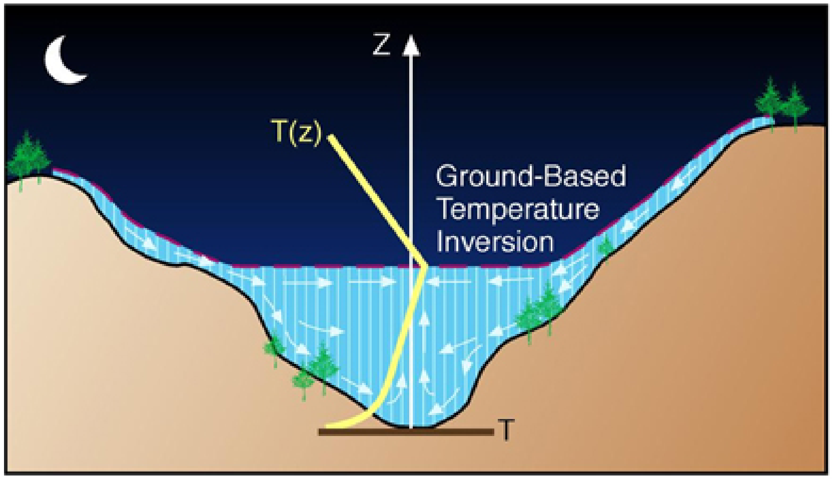
Mountain-Plain Circulations

- Mountain-Plain circulations also develop due to thermal effects.
- Rising air over mountains as upslope winds develop create a weak pressure gradient which causes air from the plains to flow toward the mountain to compensate for the rising
- At night, the circulation reverses, and the winds flow from the mountains onto the plains.



Courtesy of C.David Whiteman

Nocturnal Thermal Structure



Courtesy of C.David Whiteman

- As air over mountain slopes cools, it becomes more dense than its surrounding environment and begins to drain down the gradient of the terrain slopes.
- Cold air accumulates in the valley basin and creates a temperature inversion at the top of the valley.
- Air within valley is stably stratified and pollution can become trapped and accumulate.

Examples of Complex Winds

- Coastal influences
  - Land/sea-breeze (lake-breeze) circulations driven by differential heating between land and water
  - Thermal internal boundary layer (TIBL) near coast during daytime onshore flow
  - Grid resolution and representative met data may be significant issues
  - TIBL effects most important for elevated releases near the coast, and may be addressed through subgrid-scale modules

Complex Winds - Issues

- General issues
  - Complex wind influences will vary significantly based on source characteristics and location
  - Plume recirculation may occur under various conditions, such as cross-valley and coastal circulations and stagnation
  - Availability of representative meteorological inputs to “inform” the system
  - Ability of modeling system to effectively utilize site-specific information
  - Model performance/uncertainty for spatiotemporal pairing of model results is not well documented or understood

Complex Winds - Issues

- More specific issues
  - Near-field, localized plume terrain interactions may be significantly misrepresented due to grid resolution limitations
  - Ability of modeling system to effectively utilize site-specific information appears to be significantly lacking – important information may be effectively destroyed or misrepresented
  - Recent Staff Memorandum, dated September 26, 2008, provides additional details regarding these issues

Complex Winds – Performance Evaluations

- CALPUFF modeling system performance for near-field complex wind applications is not well-documented
- IWAQM Phase 2 report includes some CALPUFF evaluation results for Kincaid (flat terrain) and Lovett (complex terrain)
- Evaluation results for Lovett show good performance

CALPUFF Lovett Evaluation Results from IWAQM Phase 2 Report

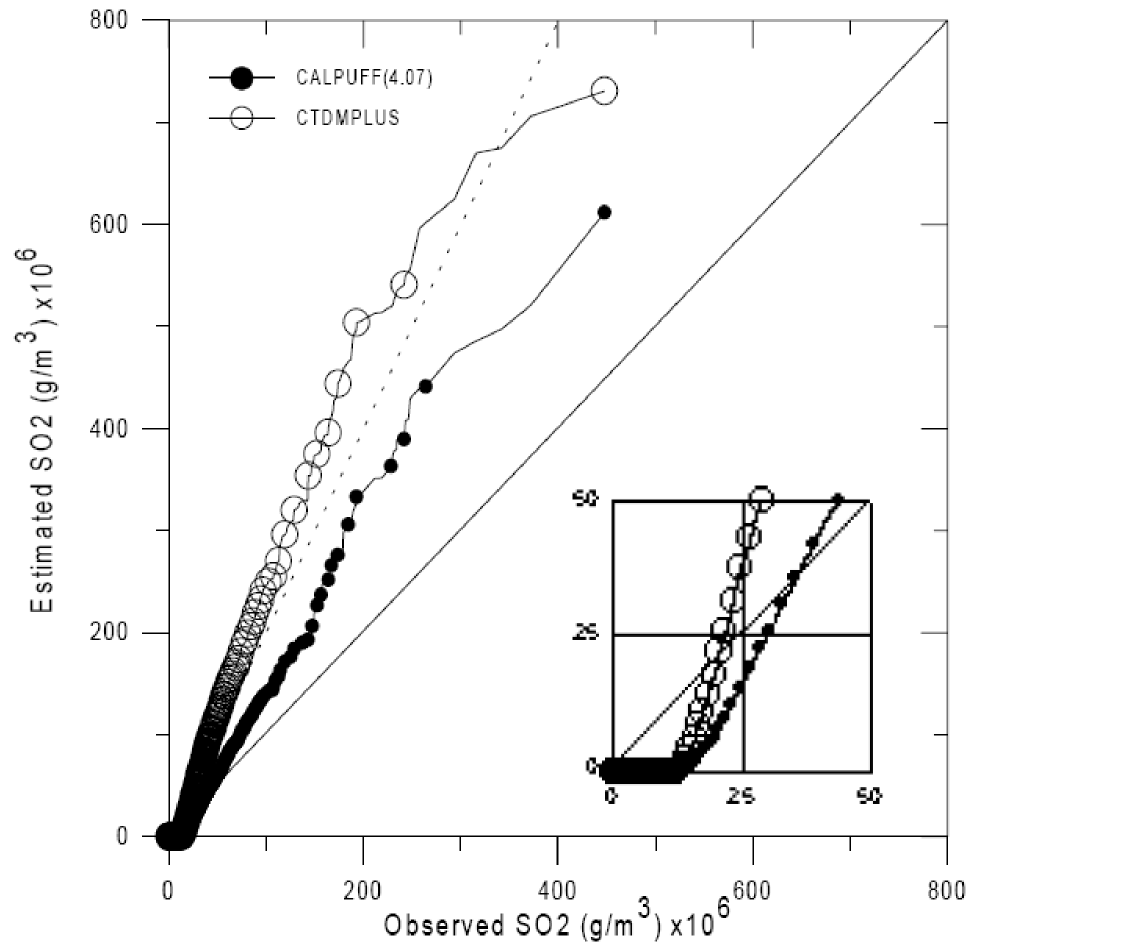


Figure 28. Q-Q plots for Lovett, comparing observed surface concentration values of SO_2 with simulation results CALPUFF(4.07) and CTDMPLUS

Complex Winds – Performance Evaluations

- However, CALPUFF was applied with CTDMPLUS met inputs, bypassing CALMET
- This is not consistent with motivation for CALPUFF near-field applications under paragraph 7.2.8 of Appendix W, which is to “fully treat the time and space variations of meteorology effects on transport and dispersion.”
- Therefore, these evaluation results are not relevant to near-field applications under paragraph 7.2.8 of Appendix W

CALPUFF/CALMET Evaluations for Lovett

- Various methods, including graphical and statistical measures, are used for evaluating model performance for near-field regulatory models, such as AERMOD or the Industrial Source Complex (ISC) models.
- The Cox-Tikvart method uses the Fractional Bias (FB) as the statistical measure of agreement between the observed and predicted concentration;
  - The FB is bounded between -2 and +2, with a value of 0 (zero) indicating perfect agreement. An absolute value of less than 0.667 for FB indicates agreement within a factor of 2

Near-Field Evaluation Procedure Cont'd

- Fractional bias calculated from Robust Highest Concentration (RHC):

$$RHC = X(N) + \left[\overline{X} - X(N) \right] \ln \left[\frac{3N - 1}{2} \right] ,$$

- Model comparisons based on Composite Performance Measure (CPM) and Model Comparison Measure (MCM)

$$CPM = \frac{1}{3} \overline{(AFB)_{r,s}} + \frac{2}{3} \left[\frac{(AFB)_3 + (AFB)_{24}}{2} \right] ,$$

$$MCM = CPM(1) - CPM(2) ,$$

Lovett Near-Field Complex Terrain

- CALMET 3-D Windfields Developed
  - 3 Level Tower (10m, 50m, 100m) simulated as 3 surface stations with corresponding anemometer heights
  - Upper air data from Albany, NY
  - 125 meter grid spacing using SRTM-1 (terrain) and NLCD92 (landuse).
- Various CALPUFF configurations tested
  - P-G
  - AERMOD turbulence
  - Plume Half-Height Adjustment
  - CALPUFF Strain Based Adjustment
  - AERMOD surface and profile data

Model Configurations Evaluated

- CALPUFF1:
  - P-G Dispersion
  - Plume Half Height Adjustment
- CALPUFF2:
  - AERMOD Turbulence
  - Plume Half Height Adjustment
- CALPUFF3:
  - P-G Dispersion
  - CALPUFF Strain Based Adjustment
- CALPUFF4:
  - AERMOD Turbulence
  - CALPUFF Strain Based Adjustment
- CALPUFF5:
  - AERMOD Profile Data
  - Plume Half Height Adjustment
- AERMOD (Version 07026)

Robust Highest Concentrations

3-Hour

MODEL	RHC	FB
OBSERVED	186.63	
CALPUFF1	270.83	-0.3681
CALPUFF2	331.69	-0.5597
CALPUFF3	215.26	-0.1424
CALPUFF4	498.73	-0.9107
CALPUFF5	170.94	8.778E-02
AERMOD	190.79	-2.202E-02

24-Hour

MODEL	RHC	FB
OBSERVED	51.77	
CALPUFF1	79.98	-0.4282
CALPUFF2	50.03	3.42E-02
CALPUFF3	80.19	-0.4307
CALPUFF4	88.91	-0.5280
CALPUFF5	45.20	0.1356
AERMOD	52.19	-8.16E-03

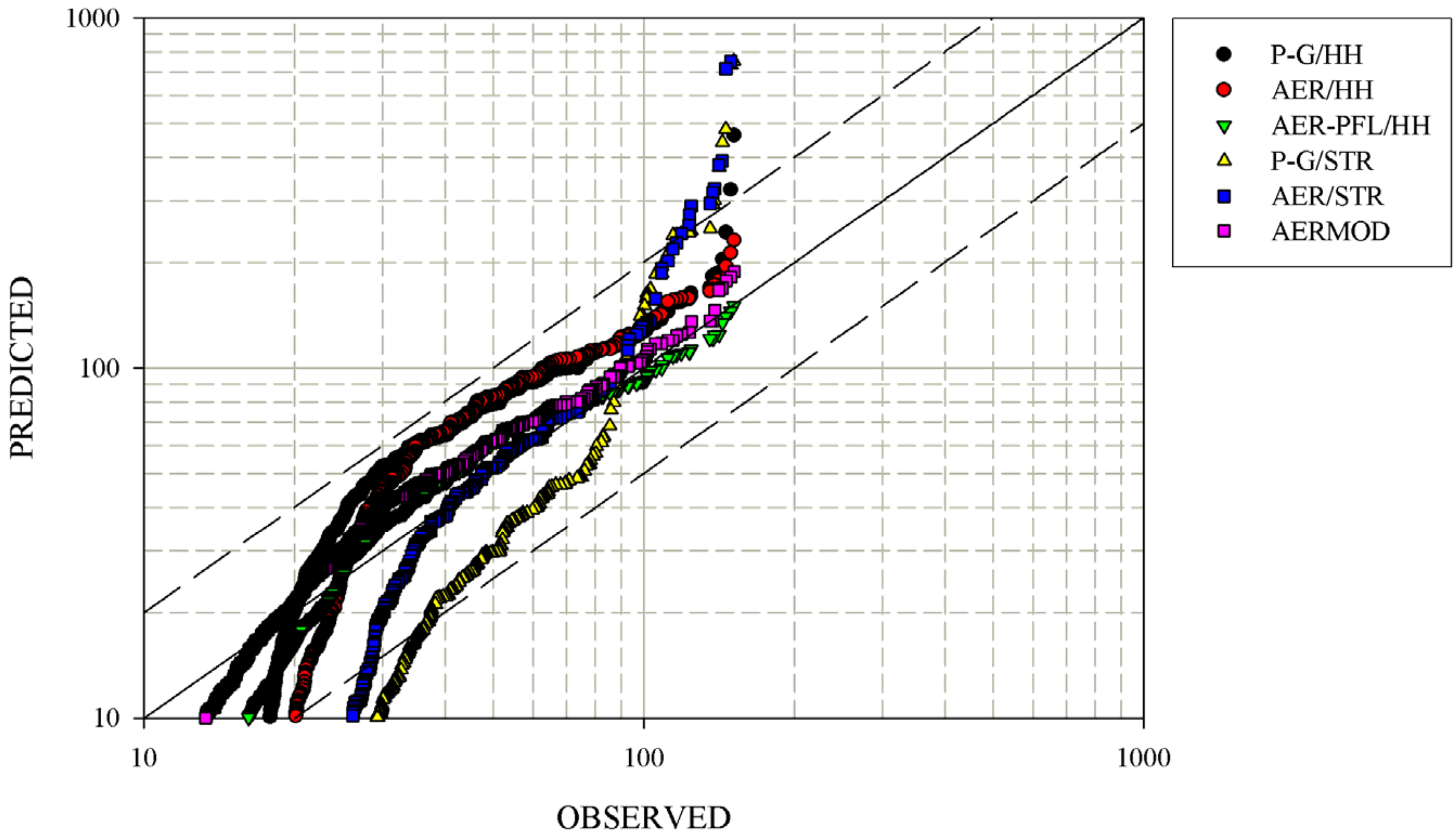
Composite Performance Measure (CPM)

Model	CPM	+/- C.I. 90%	+/- C.I. 95%
CALPUFF1	0.5956	0.1280	0.1526
CALPUFF2	0.6005	0.1708	0.2036
CALPUFF3	0.4763	0.1210	0.1442
CALPUFF4	0.7884	0.2349	0.2800
CALPUFF5	0.4382	0.1008	0.1202
AERMOD	0.4234	0.0980	0.1168

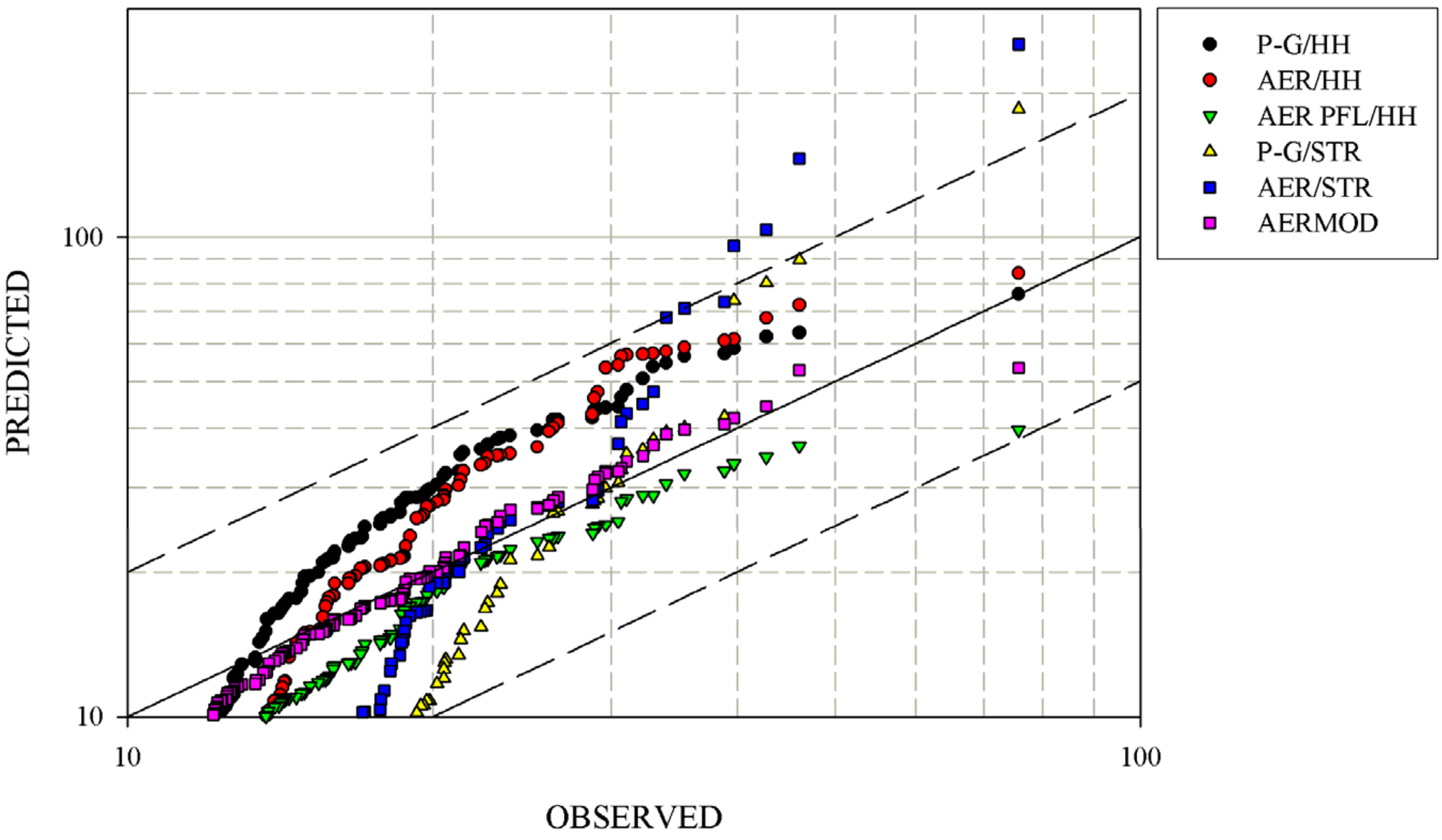
Model Comparison Measure (MCM)

Model - Model	MCM	+/- C.I. 90%
CALPUFF1-CALPUFF2	-4.943E-03	0.3247
CALPUFF1-CALPUFF3	0.1192	0.1709
CALPUFF1-CALPUFF4	-0.1928	0.3939
CALPUFF1-CALPUFF5	0.1574	0.3377
CALPUFF1-AERMOD	0.1722	0.2679
CALPUFF2-CALPUFF3	0.1242	0.3195
CALPUFF2-CALPUFF4	0.1879	0.4114
CALPUFF2-CALPUFF5	0.1624	0.3563
CALPUFF2-AERMOD	0.1771	0.3353
CALPUFF3-CALPUFF4	-0.3120	0.3897
CALPUFF3-CALPUFF5	3.819E-02	0.3319
CALPUFF3-AERMOD	5.295E-02	0.2619
CALPUFF4-CALPUFF5	0.3503	0.4839
CALPUFF4-AERMOD	0.3650	0.4344
CALPUFF5-AERMOD	1.476E-02	0.2107

3-Hour Q-Q Plot - Lovett



24-Hour Q-Q Plot - Lovett



Observations – Near Field Evaluation

- CALPUFF model performance exhibits significant sensitivity to dispersion and terrain options.
- More "advanced" options (turbulence and strain-based terrain adjustment) exhibited poorest performance.
- CALPUFF with AERMOD profiles (i.e. no CALMET) performed best of CALPUFF configurations.
- <u>CAVEAT</u>: These evaluation results are very preliminary and will be updated based on additional insights into treatment of tower data in CALMET

Questions?