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RESULTS OF THE INDEPENDENT VERIFICATION AND VALIDATION STUDY FOR THE D2-PUFF MODEL

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The D2-Puff atmospheric dispersion model was developed for use in estimating the downwind hazards resulting from accidental releases of toxic chemicals at U.S. Army chemical munitions storage depots. D2PC, the only model currently accredited for that purpose, assumes flat terrain and steady-state meteorological conditions. D2-Puff is intended to extend the D2PC methodology to complex terrain and variable meteorology in a user-friendly computer code. The independent verification and validation (IV&V) study of D2-Puff Version 2.0.6 focused on these accreditation requirements and the implicit requirement that the model provide safe-sided hazard estimates. The conclusion of the independent verification is that D2-Puff correctly implements the D2PC methodology in a convenient and easy-to-use computerized model that fully satisfies all of the specified operational requirements. The conclusion of the independent validation is that D2-Puff is unlikely to underestimate downwind hazards in terrain typical of that found in the vicinity of chemical depots. However, D2-Puff is likely to overestimate the time that it will take for a toxic cloud to travel more than a few kilometers downwind because the model does not consider the height variation of wind speed.

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SECTION 1. EXECUTIVE SUMMARY

The D2-Puff atmospheric dispersion model was developed by Innovative Emergency Management, Inc. (IEM) under contract to the Product Manager for Chemical Stockpile Emergency Preparedness (PM CSEP) for use in estimating the downwind hazards resulting from accidental releases of toxic chemicals at U.S. Army chemical munitions storage depots. D2PC, the only model currently accredited for that purpose, uses a methodology originally developed in the late 1970s and outlined in Department of Defense Explosives Safety Board Technical Paper No. 10. D2PC currently is supplemented by the Partial Dosage (PARDOS) model, which uses the D2PC methodology to predict cloud arrival and departure times and dosage accumulation times. The D2PC/PARDOS models assume flat terrain and steady-state meteorological conditions (i.e., conditions that do not vary in space or time over the duration and downwind transport of the simulated release). However, many storage depots are in regions of complex terrain, and the steady-state assumption is realistic only for small, short-term releases. D2-Puff is intended to replace D2PC/PARDOS by extending the Technical Paper No. 10 methodology to complex terrain and variable meteorology.

This report summarizes the results of the independent verification and validation (IV&V) study of the D2-Puff model Version 2.0.6 that was performed for PM CSEP by the Meteorology & Obscurants Division at Dugway Proving Ground's West Desert Test Center (WDTC). The D2-Puff Accreditation Plan developed by PM CSEP (Myirski, 1999) specifies that D2-Puff must reproduce D2PC/PARDOS results to within 10 percent for the flat-terrain, steady-state scenarios considered by D2PC. The Accreditation Plan also requires that D2-Puff have a user-friendly graphical user interface (GUI) with a number of specific features. Although not a requirement of the Accreditation Plan, a requirement that D2-Puff provide conservative (safe-sided) estimates of hazard areas is implicit in the model's intended use for chemical hazard prediction. The emphasis of the WDTC Meteorology & Obscurants Division's IV&V study was on determining if the requirements in the D2-Puff Accreditation Plan had been met.

The major tasks of the IV&V study consisted of a review of all D2-Puff model documentation provided by IEM, independent comparisons of D2-Puff and D2PC/PARDOS predictions for 79 test cases, technical evaluation of the methodology incorporated in D2-Puff and D2PC/PARDOS, and quantitative comparisons of D2-Puff predictions with field data. The technical evaluation and the majority of the validation results are applicable to both D2-Puff and D2PC/PARDOS.

The results of the verification tasks indicate that the D2-Puff code is well designed, accurately coded, and correctly implements the D2PC methodology. The D2-Puff GUI is convenient and easy to use, and the graphical and tabular output capabilities are excellent. The authors know of no computerized dispersion model of comparable complexity that is more user-friendly than D2-Puff. Although the user documentation is also good, the technical documentation probably would be incomprehensible to anyone who is not a subject matter expert in Gaussian dispersion modeling.

The D2-Puff and D2PC/PARDOS model comparison tests demonstrated that D2-Puff accurately implements the basic D2PC/PARDOS methodology, although there were several cases in which the D2-Puff results differed by more than 10 percent from the corresponding D2PC/PARDOS results. All of these cases are explained by intentional methodology differences between models or round-off in D2-Puff's fixed-decimal tabular output when the predicted value is very small. D2-Puff's methodology differences with D2PC include a different treatment of dispersion with wind speeds less than 1 m/s and termination of the concentration and dosage (time-integrated concentration) calculations at the distance where the concentration or dosage has decreased to 1 percent of the peak value. D2-Puff's method of modeling dispersion during periods with very light winds is more realistic than the D2PC approach, but cannot be implemented in a steady-state Gaussian dispersion model such as D2PC. Because D2-Puff terminates calculations when the concentration or dosage decreases to 1 percent of the peak value, the model can underestimate the width of hazard areas within a few hundred meters of a very large release made under stable atmospheric conditions. However, this limitation is not of practical importance because storage depots establish a circular exclusion zone within a 500-m radius of an accidental release. Also, the modification needed to remove this minor D2-Puff limitation would increase the model execution time, which would be undesirable in a model intended to provide answers in near real time.

The technical evaluation revealed that D2-Puff and D2PC are based on Gaussian puff/plume dispersion modeling techniques that are representative of the state of the art in the late 1970s when Technical Paper No. 10 was prepared. Although most operational dispersion models still are based on the Gaussian modeling approach, the D2-Puff/D2PC methodology cannot still be considered as representative of the state of the art. Model improvements over the last 20 years include better parameterizations of atmospheric turbulence, boundary layer structure, and the dispersion process. However, the fact that the modeling methodology employed in D2-Puff is not representative of the current state of the art does not necessarily mean that D2-Puff should not be used for its intended purpose as a safe-sided hazard prediction tool.

Perhaps the most serious limitation of the D2-Puff/D2PC methodology for chemical hazard prediction arises from the neglect of the variation of wind speed with height. Because both the D2-Puff and D2PC models assume that the wind speed at 10 m is representative of the transport wind speed at all downwind distances, they will tend to overestimate transport speeds for low-level releases at short range and underestimate transport wind speeds for all release heights at longer downwind distances. Thus, the toxic cloud produced by a large accident will arrive in areas more than 1 to 2 km from the release sooner than predicted by the models. The neglect of the wind speed height dependence in the Technical Paper No. 10 methodology is probably explained by the computer constraints of the era and the additional complexity that this dependence would have introduced in the 2-min equivalent dosage correction. This correction is omitted in D2-Puff because it is computationally complex and acts to decrease rather than increase hazard distances.

The authors of D2-Puff used unique and innovative procedures to extend the D2-Puff methodology to variable meteorology while minimizing the required computer resources and model execution time. These innovations included effectively combining the puffs normally used to represent a quasi-continuous release into a smaller number of plume segments and reducing the number of receptors needed to resolve peak concentrations and dosages by using a "plume finder" to search the area around each receptor. These innovations are suitable in a safe-sided hazard model, but could be inappropriate in other applications. For example, the plume finder can result in apparent hazard areas that are much wider than the actual hazard areas. Also, there are several instances in which D2-Puff can predict an unrealistic increase in concentration with downwind distance (mixing depth decrease between time steps, wind speed decrease along puff/plume trajectory, and shallow mixing depths in complex terrain), but this conceptual limitation does not affect the model's usefulness as a safe-sided hazard prediction tool.

D2-Puff satisfies the requirement of providing a complex terrain vapor dispersion modeling capability. However, it should be recognized that there is no generally accepted or validated complex terrain dispersion modeling methodology. D2-Puff uses one of several approaches that have been tried by other model developers. When applied in complex terrain, D2-Puff can use time-varying three-dimensional gridded wind fields provided by any prognostic or diagnostic wind field model, including its own mass-consistent diagnostic wind field model. The use of full-physics prognostic mesoscale models with high resolution is becoming more practical, and these models may eventually eliminate the need for diagnostic wind field models.

The D2-Puff validation effort included comparisons of model predictions with field data from the Prairie Grass, Green Glow, Ocean Breeze, Defense Special Weapons Agency (DSWA) Model Validation Phase I, and DSWA Model Validation Phase II (Dipole Pride 26) experiments. The results indicate that the model generally provides conservative estimates of concentrations and dosages. However, the model showed a bias toward underestimation of concentrations for the DSWA I puff ensembles and the Prairie Grass trials conducted under stable conditions. The DSWA

I trials were conducted over extremely smooth salt flats, which are not representative of surface roughness in the vicinity of chemical storage depots. Also, the Prairie Grass data appear to be rather unique because most dispersion models that have not been specifically tuned to the Prairie Grass results show a similar bias toward underestimation for the stable trials. The validation results also illustrate that the D2-Puff/D2PC assumption that the 10-m wind speed is representative of the cloud transport speed at all downwind distances is unrealistic. It should not be difficult to correct this deficiency in D2-Puff.

In summary, D2-Puff correctly implements the D2PC/PARDOS methodology and extends it to variable meteorology and complex terrain, which should allow D2-Puff to provide more realistic hazard predictions than D2PC/PARDOS. D2-Puff also generally satisfies the requirement that it provide safe-sided hazard estimates, although the model's assumption that the wind speed at 10 m represents the cloud transport speed at all downwind distances can be expected to cause the model to overestimate how long it will take for the toxic cloud from a large release to arrive at downwind distances of more than a few kilometers. Although D2PC and its predecessors have served their intended purpose well and form the basis of many current plans, more recent modeling techniques could improve the hazard information available to planners and emergency responders. For example, a recently available Department of Defense (DoD) dispersion model, which is based on a second-order closure solution of the advection-diffusion equation, can quantify the effects on its predictions of stochastic atmospheric variability and uncertainties in meteorological inputs. In addition to the ensemble mean results (i.e., what happens on average) provided by D2-Puff and other conventional models, this model can define the hazard area for any specified dosage with any desired degree of confidence (e.g., 99 percent).

SECTION 2. OVERVIEW OF THE VERIFICATION AND VALIDATION PLAN

Appendix A contains the Verification and Validation (V&V) Implementation Plan for the D2-Puff model that the WDTC Meteorology & Obscurants Division prepared at the beginning of this study. To the extent possible, the V&V Plan and the independent verification and validation (IV&V) process followed during this study adhered to the guidance provided in U.S. Army Test and Evaluation Command (TECOM) Pamphlet 73-4 (Modeling and Simulation Verification, Validation, and Accreditation Methodology), dated 7 May 1998. (This pamphlet is in turn based on Department of Defense and Department of the Army guidelines and suggested practices for V&V.) The format used in this report also follows the format specified in TECOM Pamphlet 73-4.

Table 2-1 lists the acceptability criteria for the D2-PC model, which are taken from the D2-Puff Accreditation Plan (Myirski, 1999). We established the verification and validation tasks respectively listed in Tables 1 and 2 of the V&V Plan in order to assess whether each of these criteria had been met, partially met, or not met. Note that there are two types of acceptability criteria in Table 2-1. The verification tasks primarily considered the operational criteria, while the validation tasks primarily considered the fidelity (accuracy) criteria. Criterion 1.5 is not explicitly contained in the accreditation plan, but is implicit in the intended use of D2-Puff as a conservative (safe-sided) hazard prediction tool. In general, the fidelity criteria relate D2-Puff's predictions to those of D2PC and the supplemental Partial Dosage (PARDOS) model, which gives cloud arrival and departure times and dosage accumulation versus time values which are consistent with the D2PC methodology and predictions. Although D2PC is the only model accredited for chemical hazard prediction at CSEPP sites, it has never been subjected to a formal V&V review. This study therefore serves as the IV&V for both the D2PC and D2-Puff models.

There are two possible approaches for interactions between an independent model reviewer and the model's developer. The first approach is for the reviewer to restrict communications to the submission of questions and the second is to provide the developer with both questions and feedback on major findings. As noted in the Accreditation Plan, the second approach was followed throughout this study in the interests of fielding the best possible model in the shortest time. Consequently, IEM corrected some of the problems identified early in our study and is working on solutions to some of the other problems identified in this report.

The D2-Puff IV&V study was performed by the WDTC Meteorology & Obscurants Division at U.S. Army Dugway Proving Ground. The three authors of this report have a combined total of over 60 years of experience in the

Table 2-1
Acceptability Criteria for D2-Puff

Criterion	Criterion Type[a]
1. Able to reproduce D2PC/PARDOS results for spatially invariant meteorological conditions	
1.1 Centerline total dosages must agree within 10% (2% desired)	F
1.2 Dosage widths at 3 σ_y must agree within 10% (2% desired) or ±1 m, whichever is greater	F
1.3 Centerline dosage accumulation times must agree within 10% (2% desired) or ±0.1 min, whichever is greater	F
1.4 Centerline concentrations must agree within 10% (2% desired)	F
1.5 Conservative (safe-sided) for hazard prediction	F
2. Provides same capabilities as D2PC/PARDOS	
2.1 Supports all D2PC/PARDOS release types except buoyant sources	O
2.2 Uses D2PC/PARDOS default constants and coefficients unless documented technical justification for a change	O
2.3 Calculates vapor concentration/dosage calculations for meteorological conditions that vary in space and time	O
2.4 Able to compute concentration/dosage at any point over any time interval	O
2.5 Able to account for the effects of sheltering	O
2.6 Able to account for the effects of terrain on vapor transport and diffusion	O
3. Graphical user interface (GUI) capabilities	
3.1 User-friendly	O
3.2 Source screen with predefined and user-defined munition/agent/release specification options	O
3.3 Meteorology screen with user-defined and real-time input options	O
3.4 Receptor screen with predefined and user-defined receptor, dosage/concentration of interest, and output display	O
3.5 Map screen for viewing predicted agent cloud/plume on a Geographical Information System (GIS)	O
3.6 Review screen from which the user can review all inputs in narrative form	O
3.7 Summary of source and meteorological inputs available from all screens	O

[a] F = fidelity requirement; O = operational requirement.

development, validation, and application of atmospheric transport and diffusion models for the U.S. Army, U.S. Environmental Protection Agency (EPA), National Aeronautics and Space Administration (NASA), and others. One of the authors (JFB) was also a contributor to the preparation of Department of Defense Explosives Safety Board Technical Paper No. 10, which established the hazard prediction methodology implemented by D2PC and D2-Puff, and currently chairs an international working group on chemical/biological hazard modeling.

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SECTION 3. DESCRIPTION OF THE VERIFICATION PROCESS

3.1 REQUIREMENTS VERIFICATION

Army Regulation (AR) 50-6 requires the U.S. Army to plan for a potential accident involving the chemical munitions it stores at eight sites: (1) Aberdeen Proving Ground, Maryland; (2) Anniston Army Depot, Alabama; (3) Blue-Grass Army Depot, Kentucky; (4) Newport Chemical Depot, Indiana; (5) Pine Bluff Arsenal, Arkansas; (6) Pueblo Chemical Depot, Colorado; (7) Desert Chemical Depot, Utah; and (8) Umatilla Chemical Depot, Oregon. Since the 1970s, the Army has used various forms of the D2 atmospheric dispersion model to assist in planning for such an accident. D2PC, the current version of the D2 model, is used daily in planning for chemical munition operations. In the event of an actual release of chemical agent, the model would also be used to identify the areas that would be at risk. Department of the Army (DA) Pamphlet 385-61 accredits use of the D2 model and designates Headquarters DA as the accrediting authority for the use at chemical stockpile sites of hazard prediction models other than D2. No model other than D2 currently has been accredited for hazard prediction at any storage site.

Most current atmospheric dispersion models predict the ensemble mean concentrations and dosages (time-integrated concentrations) that would be expected for a given release under specified meteorological conditions. To illustrate this point, assume that an identical explosive release of agent from a chemical munition occurs 100 times under the same meteorological conditions. Because of the stochastic variability of the atmospheric dispersion process, the 100 individual events would result in a distribution of outcomes rather than a single outcome. A state-of-the-art dispersion model should predict what happens on average for this ensemble. However, the results for any single event could differ significantly from the ensemble mean. Because D2 is one of the tools that is used to protect human health, it is more important that D2 place an upper bound on what might happen during any single event than that it accurately predict the ensemble mean results.

The D2 model is a steady-state Gaussian dispersion model which assumes that meteorological conditions do not vary in space or time over the transport distance and time of concern for the accidental chemical agent release. (The model has a limited capability to consider variations in meteorological conditions in time for the special case of the transition from stable nighttime conditions to unstable daytime conditions.) The model also assumes flat terrain with straight-line trajectories for all chemical agent clouds and plumes. However, most of the storage depots are located in complex terrain, and the assumption that meteorological conditions are constant in space and time generally is reasonable only for small releases with short downwind hazard distances. PM CSEP is aware of these limitations and decided in 1996 to extend the D2 methodology to complex terrain with provision for spatially and temporally varying meteorological conditions. As a result of that decision, the D2-Puff model was developed by IEM under contract to PM CSEP.

Table 3-1 lists the documentation that the WDTC Meteorology & Obscurants Division reviewed as part of the D2-Puff verification. (Note that earlier versions of some of the reports listed in Table 3-1 were also reviewed.) Based on our review of these documents and other information provided by PM CSEP, including the D2-Puff Accreditation Plan (Myirski, 1999), we believe that the intended uses of D2-Puff are clearly documented and that the requirements for the model are clear and consistent with each other.

3.2 DESIGN VERIFICATION

Based on our review of the documentation listed in Table 3-1, we believe that the design of the D2-Puff software is clear and consistent and that it is traceable to and conforms with the model's documented requirements.

3.3 IMPLEMENTATION VERIFICATION

The D2-Puff documentation listed in Table 3-1 includes a two-volume report entitled "D2-Puff Model Software Test Description." Volume II of this report includes approximately 89 test cases developed by IEM to demonstrate that D2-Puff correctly implements the D2PC/PARDOS methodology. As part of our D2-Puff implementation verification, we independently repeated 79 of these tests. Each test represented a different scenario of chemical agent type, release type, number of munitions or source amount, meteorological inputs, and receptor parameters (e.g., breathing rate). The D2-Puff run for each test case was made using the input file (*.pmi) provided by IEM. We then compared the D2-Puff tabular output with the expected (i.e., D2PC/PARDOS) results listed by IEM for that case. We also independently verified the expected results provided by IEM by running D2PC/PARDOS with the inputs specified by IEM. The test cases not included in our independent verification were those in which D2-Puff was used in a manner that could not be duplicated by D2PC/PARDOS. We did not attempt to duplicate IEM's manual computations of the expected results for these cases.

Table 3-2 summarizes the results of our independent tests of D2-Puff. As noted in Table 2-1, it is required that D2-Puff reproduce D2PC/PARDOS centerline concentrations, centerline dosages, and dosage widths to within 10 percent and desired that these results agree to within 2 percent. Additionally, it is required that D2-Puff reproduce D2PC/PARDOS centerline dosage accumulation times to within

Table 3-1
List of Documentation Reviewed as Part of D2-Puff Verification

IEM, 12 November 1996: Puff Model Requirements Specification. IEM, Inc., Baton Rouge, LA.
Weltman, J., 30 June 1997: Puff Model 1.2 Design Document. IEM, Inc., Baton Rouge, LA.
Asmus, G., B. Boyle, and L. Morgan, 5 October 1998: D2-Puff Software Requirements Specification. IEM, Inc., Baton Rouge, LA.
Prater, E., S. Stage, and J. Weltman, 30 November 1998: D2-Puff Technical Manual. IEM, Inc., Baton Rouge, LA.
IEM, 1998: D2-Puff User Guide, Version 2.02 (Draft). IEM, Inc., Baton Rouge, LA.
Morgan, L., E. Prater, S. Stage, and J. Weltman, 30 November 1998: D2-Puff Version 2.05 Reference Manual. IEM, Inc., Baton Rouge LA.
IEM, 1998: D2-Puff User Guide, Version 2.05. IEM, Inc., Baton Rouge, LA.
Asmus, G., K. Baggett, B. Boyle, and L. Morgan, 30 November 1998: D2-Puff Model Software Test Description, Volumes I & II. IEM, Inc., Baton Rouge, LA.
Boyle, B. and E. Prater, 15 January 1999: Addenda to Version 2.05 D2-Puff Documents. IEM, Inc., Baton Rouge, LA.
IEM, January 1998: D2-Puff User Guide, Version 2.06. IEM, Inc., Baton Rouge, LA.
Boyle, B., 15 January 1999: D2-Puff Model Version 2.06 Software Test Report.
Stage, S.A., Z. Wu, N. Mainkar, J. Weltman, and M. Myirski, 3 May 1999: The Mixing Layer Terrain Wind Adjustment Model (MILTWAM) for Airflow Over Complex Terrain. IEM, Inc., Baton Rouge, LA and PM CSEP, Aberdeen Proving Ground, MD.

Table 3-2
Summary of Independent Comparisons of D2-Puff and D2PC/PARDOS Predictions

Parameter(s) Compared	Difference Between Models	IEM Test Cases
Centerline Dosages and Concentrations	0-2%	1.1, 1.2, 1.3, 1.4, 1.6, 1.7, 1.11, 1.12, 1.13, 1.14, 2.1, 2.2, 3, 3.1, 5, 8, 9, 10, 12, Met. 1a, Met. 1b, Met. 2a, Met. 2b, Met. 3b, Met. 3c, Met. 4a, Met. 4b, Met. 5, Met. 8, Multisource 1, 14.1, 14.2, 14.3, 14.4, 14.5, 14.6, 14.7, 14.12, 14.11, 14.15, 14.16, 14.17, ERDEC1, ERDEC2, ERDEC3, ERDEC4, ERDEC5, ERDEC7, ERDEC8, ERDEC9, ERDEC12, ERDEC16, ERDEC17, ERDEC24, 4-2-77
	2-10%	6.7, 11, Met. 13, 14.8, 14.9, ERDEC6
	>10%	ERDEC13, 4-2-78, 4-2-79, 1.5, Met. 7, Met. 10, Met. 11
Plume Widths	0-2%	10, 14.3, 14.6
	2-10%	1.1, 1.3, 1.4, 1.7, 1.11, 1.14, 5, Met. 8, 14.5, 14.11, 4-2-78, 4-2-79, 4-2-80
	>10%	1.2, 2, 3, Met. 6, 8, Met. 7, 14.1, 4-2-77
Dosage Accumulation Time	0-2%	8, 10
	2-10 %	1.1, 1.11, 1.14, 2.1, 2.22, 3.1, 5, Multisource 1
	>10%	None

10 percent (2 percent required) or ±0.1 minute, whichever is greater. As shown by Table 3-2, the majority of test cases resulted in D2-Puff centerline concentrations and dosages that agreed to within 2 percent of the D2PC results. The 10-percent agreement requirement was slightly exceeded (differences of 11 to 15 percent) for Test Cases ERDEC13, 4-2-78, and 4-2-79. These cases were characterized by low concentrations and dosages, and the differences between models are probably attributable to round-off in D2-Puff's fixed-decimal output for these low values when compared with D2PC's output in scientific notation. The other test cases with differences in predicted dosages of more than 10 percent were wooded stability cases in which extrapolation of the above canopy wind speed to below the canopy resulted in a below canopy speed less than 1 m/s. As discussed in Section 4.2.3.5, D2-Puff and D2PC use different procedures to account for winds less than 1 m/s. The differences in model predictions for these cases result from methodology differences. Many of the cases in which the D2-Puff and D2PC plume widths differed by more than 10 percent (Test Cases 1.2, 2, Met. 6, and 4-2-77) were very large releases at short downwind distances, and the differences are explained by the fact that D2-Puff does not make concentration and dosage calculations more than $3\sigma_y$ from the centerline, where σ_y is the lateral dispersion coefficient (see Section 4.2.3.2). The dosage isopleth half-widths (i.e., distances from the centerline to the specified dosage) for the other cases differed by only 1 m. All of the dosage accumulation times agreed to within the required 10 percent.

3.4 DEVELOPMENTAL PROCESS REVIEW

The WDTC Meteorology & Obscurants Division began its D2-Puff IV&V study relatively late in the D2-Puff developmental effort and thus had little opportunity to review and comment on the developmental process. However, we reviewed many of the interim IEM reports prepared during the model's development (see Table 3-1), and two of the authors met with the IEM developers in Baton Rouge, Louisiana on 16 December 1998 to discuss the development process, model architecture, IEM's tests of the model, and WDTC's IV&V plans.

3.5 RESULTS AND UNRESOLVED ISSUES

Table 2-1 in Section 2 lists the acceptability criteria for the D2-Puff model, which consist of operational and fidelity (accuracy) requirements. The operational requirements specify that D2-Puff must extend the D2PC/PARDOS methodology to complex terrain and variable meteorological conditions in a user-friendly software package. The verification portion of our IV&V study focused on these operational requirements. However, because the majority of the fidelity requirements are related to ensuring the correct implementation of the D2PC/PARDOS methodology in D2-Puff, there was an overlap between the verification and validation tasks. D2-Puff's performance in meeting all of the operational requirements is discussed below, while the model's performance in meeting all of the fidelity requirements is summarized in the discussion of validation results in Section 4.3.

Table 3-3 is a traceability matrix for the D2-Puff model's operational requirements. These requirements, which are also shown in Table 2-1, are based on the D2-Puff Accreditation Plan (Myirski, 1999). The status of each item is shown as met, partially met, or not met. Based on the results of our verification tasks, it is our opinion that D2-Puff fully satisfies all of the operational requirements specified for the model. It is also our opinion that D2-Puff exceeds the minimum requirements for the graphical user interface. Our verification and validation tasks required that we execute D2-Puff many times using different model options and capabilities. In the process, we found D2-Puff's graphical user interface to be one of the most convenient and user-friendly interfaces that we have encountered. We believe that it would be easier for a novice user to execute D2-Puff correctly than any other dispersion model with which we are familiar.

Table 3-3
Traceability Matrix for D2-Puff Operational Requirements

Acceptability Criterion	Status[a]
2. Provides same capabilities as D2PC/PARDOS	
2.1 Supports all D2PC/PARDOS release types except buoyant sources	M
2.2 Uses D2PC/PARDOS default constants and coefficients unless documented technical justification for a change	M
2.3 Calculates vapor concentration/dosage calculations for meteorological conditions that vary in space and time	M
2.4 Able to compute concentration/dosage at any point over any time interval	M
2.5 Able to account for the effects of sheltering	M
2.6 Able to account for the effects of terrain on vapor transport and diffusion	M
3. Graphical user interface (GUI) capabilities	
3.1 User-friendly	M
3.2 Source screen with predefined and user-defined munition/agent/release specification options	M
3.3 Meteorology screen with user-defined and real-time input options	M
3.4 Receptor screen with predefined and user-defined receptor, dosage/concentration of interest, and output display	M
3.5 Map screen for viewing predicted agent cloud/plume on a Geographical Information System (GIS)	M
3.6 Review screen from which the user can review all inputs in narrative form	M
3.7 Summary of source and meteorological inputs available from all screens	M

[a] M = met; P = Partially met; N = not met.

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SECTION 4. DESCRIPTION OF THE VALIDATION PROCESS

4.1 VALIDATION CRITERIA

Acceptability criteria 1.1 through 1.5 in Table 2-1 are the fidelity (accuracy) requirements for the D2-Puff model. All but one of these requirements relate to the model's ability to reproduce D2PC/PARDOS model results when executed in the steady-state, flat terrain mode assumed by D2PC/PARDOS. The remaining requirement is that the model be conservative (safe-sided) in its hazard predictions. The results of the D2-Puff and D2PC/PARDOS quantitative comparisons are discussed in Section 3.3. The focus of this section is on validation of the D2PC/PARDOS methodology used by D2-Puff.

The validation approaches suggested by TECOM Pamphlet 73-4 include "face validation" and quantitative comparisons of model predictions with real world measurements. Face validation is a technical evaluation and assessment by subject matter experts of the extent to which a model is likely to represent real word behavior. Section 4.2.3 provides our technical evaluation of the general methodology used by the D2PC/PARDOS and D2-Puff models, and Section 4.2.4 summarizes our quantitative comparisons of model predictions with field data.

A number of different measures of performance have been suggested to quantify dispersion model performance. In cases where there are large variations in the magnitudes of the predicted and observed variables, either within the same data set or between data sets, Hanna (1993) suggests

$$MG = \exp\left[\overline{\ln x_p} - \overline{\ln x_o}\right] \tag{4-1}$$

and

$$VG = \exp\left[\overline{(\ln x_o - \ln x_p)^2}\right] \tag{4-2}$$

where x_o and x_p respectively represent the observed and predicted quantity, MG is the geometric mean bias (geometric mean of the individual x_p/x_o ratios), and VG is the geometric mean variance. (Note that MG is sometimes written as the geometric mean of the x_o/x_p ratios.) If there were perfect agreement between predictions and measurements, MG and VG would both equal unity. We used Equations (4-1) and (4-2) to quantify the correspondence between D2-Puff model predictions and observations.

4.2 VALIDATION TASKS

4.2.1 Review of Model Developer's Tests

IEM did not make any quantitative comparisons of D2-Puff predictions with field data. However, IEM made numerous comparisons of D2-Puff predictions with D2PC/PARDOS model predictions. Section 3.3 discusses our review and independent checks of IEM's tests.

4.2.2 Comparisons of D2-Puff With D2PC

Section 3.3 summarizes our comparisons of D2-Puff predictions with D2PC/ PARDOS model predictions.

4.2.3 Technical Evaluation

4.2.3.1 General

D2-Puff and D2PC are based on the methodology outlined in Department of Defense Explosives Safety Board Technical Paper No. 10 (Change 3, June 1980). This technology reflects both the state of the art of Gaussian puff/plume modeling techniques in the late 1970s and the computer constraints of that era. In the late 1990s, the Gaussian model continues to be the most widely used approach for operational dispersion models because of both its relative simplicity and the fact that Gaussian models often agree with experimental data as well as or better than far more complex models. Gaussian models are highly dependent on empiricism, as are all other dispersion modeling approaches, and there can be significant differences between the predictions of different Gaussian models with different empirical bases. To the best of the authors' knowledge, this study is the first to compare D2PC/D2-Puff predictions with experimental data.

D2-Puff implements all of the capabilities found in D2PC except the buoyant cloud/plume rise capability and the 2-min equivalent dosage capability. The cloud/plume rise capability may not be of critical importance for hazard prediction at storage depots, but it is routinely used to predict cloud touchdown distances and sampling locations during emergency destructions of range recovered chemical rounds at Dugway Proving Ground. The omission of the 2-min equivalent dosages in D2-PUFF will, in some cases, lead to D2-Puff hazard distances that are longer than the D2PC hazard distances for the same scenario. We believe that the additional degree of conservatism given by the omission of the 2-min equivalent dosage correction is reasonable given the computational complexity of the correction and the current uncertainty about its suitability, which is discussed below. We also point out that the version of D2PC currently used at storage depots does not use the 2-min equivalent dosage correction in its default mode.

Virtually all current hazard assessment models assume that there is a linear physiological response to exposure to a toxic chemical. For example, consider the case of exposure to a constant concentration c for time t. The total dosage D, which is given by

$$D = ct, \tag{4-3}$$

can be correlated with different physiological responses. However, as early as World War II some toxicologists concluded that the response to some chemicals is nonlinear. The Technical Paper No. 10 methodology implemented in D2PC attempts to account for nonlinear response through a relationship of the form

$$D_{2e} = D_2 \left(\frac{t}{2}\right)^{0.274} ; t \geq 2 \text{ min} \tag{4-4}$$

where D_2 is the dosage that produces a specified response in a specified fraction of the population if received over an exposure time of 2 min and D_{2e} is the dosage that produces the same response if received over time t. The details of the empirical basis for Equation (4-4) were never published and appear to have been lost to history. More recently, toxicologists have begun to relate physiological response to the toxic load L, which is given by

$$L = ct^n \tag{4-5}$$

where n is an empirical coefficient that ranges from about 1 (linear response) to 3. Yee (1996) recently found that Equation (4-5) provides a good fit to the data available for the nerve agent GB (sarin).

The basic components of any modern Gaussian dispersion model include the dispersion coefficients, transport wind speed, and mixing depth. Other components of the D2-Puff methodology include the VX and HD impaction algorithms, the forested terrain option, and the shelter infiltration/exfiltration algorithm. The following subsections review the technical bases for these components. Because the numerical techniques used in a variable meteorology Gaussian puff/plume model are as important as the model's individual components, D2-Puff's numerical techniques and unique puff/plume sampling methodology are also discussed below.

4.2.3.2 Dispersion Coefficients

D2-Puff and D2PC define the longitudinal or alongwind (σ_x), lateral or crosswind (σ_y), and vertical (σ_z) dispersion coefficients by equations of the form

$$\sigma_x = 0.1522\,x^{0.9294} \tag{4-6}$$

$$\sigma_y = \sigma_{yR}\left(\frac{x + B}{x_R}\right)^{\alpha} \tag{4-7}$$

$$\sigma_z = \sigma_{zR}\left(\frac{x + C}{x_R}\right)^{\beta} \tag{4-8}$$

where x is the distance downwind from the source, x_R is a reference distance (assumed to be 100 m), σ_{yR} is the lateral dispersion coefficient for a point source at downwind distance x_R, B is the lateral virtual distance, and α is the lateral expansion coefficient. (Note that D2PC and D2-Puff use different σ_{yR} values for instantaneous and quasi-continuous releases.) The lateral virtual distance is given by

$$B = x_R\left(\frac{\sigma_{ys}}{\sigma_{yR}}\right)^{1/\alpha} \tag{4-9}$$

where σ_{ys} is the initial ($x=0$) value of σ_y. The parameters σ_{zR}, C, β, and σ_{zs} are similarly defined for the vertical dispersion coefficient.

Historically, little attention has been placed on alongwind cloud growth for two reasons. First, it can be neglected in a steady-state Gaussian dispersion model when calculating concentrations for continuous sources or total dosages for instantaneous or short-term releases. Second, sampling techniques capable of providing the concentration time histories required to determine alongwind cloud growth have not been available at an affordable cost until fairly recently. Consequently, relatively little is known about how σ_x varies with distance (or time) and stability. Many instantaneous source dispersion models therefore assume that σ_x and σ_y are equal. However, even in the 1970s there was empirical evidence that σ_x and σ_y are not necessarily the same (for example, see Nickola, 1971).

Equation (4-6) is based on an unpublished analysis by Halvey (1973) of the then available data on alongwind dispersion. All of the field tests and experiments considered by Halvey consisted of crosswind line source releases which Halvey analyzed under the assumption that the releases formed instantaneous line sources. However, the ship releases (and possibly some of the truck releases) probably did not form quasi-instantaneous line sources, which could have resulted in overestimates of σ_x. On the other hand, Halvey may have obtained underestimates of σ_x by assuming that the surface wind speed at the sampling station represented the cloud transport speed. (Halvey multiplied the σ_t derived from the concentration time history by the surface wind speed to estimate σ_x.) Halvey did not find a strong dependence of σ_x on stability, although the limited sample size and data uncertainties could have contributed to this result.

Equation (4-6) is consistent with other published findings that σ_x varies approximately linearly with transport distance or time (see Bowers, 1992 or Hanna and Franzeze, 1999). Although more recent σ_x algorithms (e.g., Wilson, 1981 and Dumbauld and Bowers, 1983) relate alongwind expansion to the combined effects of atmospheric turbulence and vertical wind-speed shear, there is as yet no conclusive evidence that they provide a better overall fit to the available data. Also, it is likely that the empirical coefficients in Equation (4-6) implicitly account for both effects.

Technical Paper No. 10 does not document the source of the recommended values of either the reference dimensions σ_{yR} and σ_{zR} or the expansion coefficients α and β. However, we believe that the σ_{yR} and σ_{zR} values were selected to yield an approximate match with the widely used Pasquill-Gifford σ_y and σ_z curves (Turner, 1970) at a downwind distance of 100 m. In the case of an instantaneous release, the σ_{yR} values recommended by Technical Paper No. 10 are the recommended quasi-continuous source values divided by a factor ranging from 3 for very stable conditions to 2 for stable conditions. This adjustment is similar to the empirical corrections recommended by several Gaussian model developers for quasi-instantaneous sources (see Barr and Clements, 1984).

The recommended (and D2-Puff default) values of α and β vary with stability (but not transport time or distance) and are the same for both instantaneous and quasi-continuous releases. As noted above, the empirical basis of the recommended values of α and β has never been documented. At the time when Technical Paper No. 10 was prepared, a number of power-law coefficients for lateral and vertical expansion could be found in the literature, and the D2-Puff default values generally fall within the range of published values. Some of the differences in the published values are explained by differences between source type (instantaneous and quasi-continuous), release height (surface or elevated), and assumptions made to derive α and β.

It should be recognized that, because σ_z is almost always inferred from surface measurements at distances beyond about 100m, empirical σ_z values depend in part on the assumptions made about puff/plume behavior. For example, if the plume centroid for a surface release lifted off the surface in a convective updraft, the resulting rapid decrease of concentration with downwind distance would lead to a very rapid increase in σ_z with distance if σ_z was inferred under the assumption that the plume centroid remained at the surface. Plume liftoff under very unstable conditions is now generally recognized as the reason for the rapid increase of β with distance implicit in the Pasquill-Gifford σ_z curve for A stability.

Most modern Gaussian dispersion models relate the lateral and vertical dispersion coefficients directly to atmospheric turbulence. For example, the lateral dispersion coefficient at downwind distance x or transport time t is given by

$$\sigma_y = I_y \; x \; f_y(x) \tag{4-10}$$

or

$$\sigma_y = \sigma_v \; t \; f_y(t) \tag{4-11}$$

where I_y is the lateral turbulence intensity (standard deviation of the lateral wind component σ_v divided by the mean wind speed) and $f_y(x)$ or $f_y(t)$ is an empirical or semi-empirical "universal function." Similar relationships are defined between σ_z and the vertical turbulence intensity I_z or vertical velocity standard deviation σ_w. (Note that, for small angles, I_y and I_z are respectively equal to the standard deviations of the wind azimuth and elevation angles in radians.) The turbulence inputs for the more modern dispersion coefficient algorithms are either obtained from direct measurements or estimated from Monin-Obukhov similarity theory. Equations (4-7) and (4-8) could be used to approximate some of the more recent σ_y and σ_z algorithms in order to incorporate onsite turbulence measurements into D2PC and D2-Puff without any significant recoding.

The D2-Puff and D2PC default expansion rates are the same for both instantaneous and quasi-instantaneous releases. Although it is not uncommon to assume that the vertical expansion rates are the same for both release types, the assumption that the lateral expansion rates are the same is rather unusual.

Batchelor's (1952) classical theoretical analysis of instantaneous puff dispersion in homogeneous turbulence indicates that

$$\sigma \propto \begin{Bmatrix} t & ; \text{ short } t \\ t^{3/2} & ; \text{ intermediate } t \\ t^{1/2} & ; \text{ long } t \end{Bmatrix} \tag{4-12}$$

where t is transport time. (In contrast, Taylor's (1921) theorem for a continuous source indicates that σ is proportional to t at short transport times and to $t^{1/2}$ at long times.) Assuming a constant transport wind speed, Equation (4-12) implies that

$$\sigma \propto \begin{Bmatrix} x & ; \text{ short } x \\ x^{3/2} & ; \text{ intermediate } x \\ x^{1/2} & ; \text{ long } x \end{Bmatrix} \tag{4-13}$$

Although there is limited evidence for an accelerated growth regime for an instantaneous puff, the $\sigma_y \propto t^{1/2}$ regime generally is not apparent at long transport times, a result that Hanna et al. (1982) attribute to the presence of mesoscale and synoptic scale eddies. A $\sigma_y \propto t$ relationship gives a good overall fit to the available data for t less than 30 hours (Hanna et al., 1982 and Gifford, 1984), which is longer than the longest travel time of concern for accidents at storage depots. With the exception of β for A stability, the D2-Puff default values for α and β are all less than or equal to 1.0. Thus, the D2-Puff default values could possibly lead to a bias toward overestimation of concentrations and dosages at longer range. This bias is not necessarily inappropriate in a hazard prediction model.

D2-Puff does not consider any wind shear effects on dispersion. Some σ_y algorithms (e.g., Cramer et al., 1972 and Pasquill, 1976) explicitly consider the effects of vertical wind-direction shear on crosswind cloud or plume growth. Similarly, some σ_x algorithms (e.g., Wilson, 1981 and Dumbauld and Bowers, 1983) explicitly consider the effects of vertical wind-speed shear on alongwind cloud growth. Unfortunately, little data exist to validate these algorithms. Also, many empirical σ_x and σ_y algorithms may implicitly include wind shear effects. Consequently, we do not view the neglect of explicit wind shear effects in D2-Puff as a significant deficiency, especially for the model's intended purpose of downwind hazard estimation.

4.2.3.3 Transport Wind Speed

D2-Puff and D2PC assume that the wind speed 10 m above the surface is representative of the transport wind speed at all downwind distances. In reality, the effective transport wind speed of a cloud released near the surface increases with downwind distance as the cloud expands vertically and encounters the higher wind speeds above the surface. (The cloud attains its final transport wind speed when it becomes uniformly mixed within the surface mixing layer.) The fact that the low-level wind speed is an underestimate of the actual cloud transport speed is consistently demonstrated by field data (e.g., Drivas and Shair, 1974 and Hanna and Franzeze, 1999). Because D2-Puff uses the 10-m wind speed as the transport speed at all downwind distances, the model will tend to overestimate the transport wind speed at short distances downwind of a surface release and underestimate the transport wind speed at longer distances. Consequently, the model will tend to overestimate cloud transport times and dosages at downwind distances of more than a few hundred meters. A bias toward overestimation of dosages is not a serious deficiency in a hazard prediction model. However, cloud arrival at a given location sooner than predicted by D2-Puff could present a problem.

Virtually all current Gaussian dispersion models consider the height variation of wind speed using either the power law or logarithmic wind profile. Different models use different assumptions to relate these wind speed profiles to transport wind speed. For example, Bjorklund et al. (1998) define the transport wind speed as

$$U(x) = \frac{1}{(z_2 - z_1)} \int_{z_1}^{z_2} u(z)\,dz \tag{4-14}$$

where u(z) is the mean wind speed at height z, and z_2 and z_1 are the heights of the upper and lower cloud boundaries at downwind distance x. Another approach (Smith and Singer, 1966) is to use the vertical concentration distribution as a weighting function, which yields

$$U(x) = \frac{\int_{o}^{\infty} \chi(x,o,z)\, u(z)\,dz}{\int_{o}^{\infty} \chi(x,o,z)\,dz} \tag{4-15}$$

where $\chi(x,o,z)$ is the centerline concentration at distance x and height z. The simplest assumption for a surface release is that the transport wind speed is approximately equal to the wind speed at $0.6\sigma_z$ (Hanna and Franzeze, 1999).

D2-Puff has the capability of using wind data from multiple towers to derive its wind inputs. In flat terrain, the wind components at any grid point are obtained using a simple $1/r^2$ weighting of the winds at the various towers, where r is the distance from a tower to the grid point. In complex terrain, the wind field obtained from the $1/r^2$ weighting is adjusted so that it is mass consistent (non-divergent) using a variational analysis technique. In complex terrain with stable conditions, D2-Puff's Mixing Layer Terrain Wind Adjustment Model (MILTWAM) predicts highly channeled two-dimensional flows with no winds predicted for terrain elevations above the top of the surface mixing layer (see Section 4.2.4.5).

4.2.3.4 Mixing Depth

The mixing depth (height) is a critical parameter in Gaussian dispersion models because it provides a lid on vertical mixing for releases made within the surface mixing layer. At longer downwind distances, concentrations and dosages are inversely proportional to the mixing depth. The mixing depth can range from tens of meters on clear nights with light winds to several kilometers on clear days with strong solar heating and light winds. The site-specific default mixing depths used by D2-Puff and D2PC are based on analyses of upper-air soundings from the nearest airports with routine, twice-daily soundings. The afternoon mixing depths, which are assumed to apply to the unstable Pasquill categories, probably are reasonably representative of conditions at the storage depots. However, the early morning mixing depths, which are assumed to apply to the stable Pasquill categories, may tend to be higher than the mixing depths at some of the depots because of the effects of urban roughness elements and heat sources in the vicinity of the airports.

The alternatives to the use of the D2-Puff climatological (default) mixing depths are: (1) use a model to predict the mixing depth and (2) have the user specify the mixing depth. There are a number of different models for the convective and/or mechanical components of the mixing depth. Although some of these models work reasonably well in describing average conditions, they often perform poorly when used to estimate mixing depths for specific events. On the other hand, a meteorologist with experience in dispersion modeling usually can estimate the mixing depth from discontinuities in observed wind, temperature, and humidity profiles, where available. Sources of these profiles can include multilevel meteorological towers, Doppler acoustic sounder wind profiles, radar wind profiler wind profiles (and virtual temperature profiles if equipped with a radio acoustic sounding system (RASS)), and radiosonde or tethersonde soundings. Although there have been attempts to automate the estimation of mixing depths, these efforts have met with little success to date. The professional judgment of an experienced meteorologist probably is the best source of mixing depth estimates at storage depots for the foreseeable future.

There are no generally accepted or validated procedures for modeling dispersion in complex terrain, and a number of different approaches have been used over the years. D2-Puff uses a complex terrain methodology that is similar to that of the SHORTZ/LONGZ models (Bjorklund and Bowers, 1982). When D2-Puff is used in complex terrain, the mixing depth is assumed to remain at a constant elevation above mean sea level over the entire computational domain. This elevation is given by the sum of the mixing depth and the elevation of the center of the Chemical Limited Area (CLA). Thus, the depth of the mixing layer varies over the computational domain, which can lead to unrealistic results in some cases. For example, assume that a cloud has become uniformly mixed within the mixing layer and that the mixing depth decreases as the cloud continues to travel downwind toward high terrain. D2-Puff will predict an increase in concentration that will not occur in the real world, where the decrease in the vertical cloud extent will be compensated by changes in the horizontal dimensions.

4.2.3.5 Other D2-Puff Components

<u>VX and HD Impaction</u>

The methodology used by D2-Puff to predict hazards for VX and HD impaction from explosive releases is derived from empiricism rather than generalized Gaussian dispersion model concepts. D2PC uses empirical fits by Solomon et al. (1970) and Whitacre (1979) to data from VX and HD weapons tests to estimate the peak agent impaction on a vertical surface as a function of downwind distance. The only meteorological predictor for the VX munitions is the wind speed. However, the empirical relationship for the HD munitions considers the wind speed, air temperature, and stability. D2-Puff uses Gaussian dispersion model concepts to generalize these empirical relationships so that the model can calculate concentration/deposition time histories and off-axis hazards.

It is possible to use Gaussian dispersion concepts to develop a generalized model capable of predicting VX and HD impaction hazards for any weapon (for example, Bjorklund, 1990). However, the generalized model will still require weapon-specific source information (e.g., initial drop size distribution), and it is not clear that the advantages of a generalized model offset the disadvantage of greater complexity for the special purpose of predicting downwind hazards for accidental functioning of specific weapons at Army storage depots.

<u>Shelter Infiltration/Exfiltration</u>

D2-Puff provides a capability not available in D2PC, the capability to predict concentration and dosage time histories within a building. The D2-Puff shelter methodology implicitly assumes that the agent concentration in the ambient air is uniform over the shelter's exterior and explicitly assumes that mixing within the shelter is so rapid that the concentration within the shelter is uniform. This uniform mixing assumption, which is widely used in indoor air quality modeling, can be extended to multiple well-mixed zones (e.g., inner rooms which receive much or all of their air from outer rooms). However, this multizonal capability is not available in D2-Puff.

The uniform mixing approximation often works well for concentration averaging times of a few minutes or longer. For example, the multizonal models applied to the interior tracer releases made during the 911-Bio Advanced Concept Technology Demonstration (ACTD) at Dugway Proving Ground generally worked as well as or better than the much more complex computational fluid dynamics (CFD) models after about the first minute (Ponikvar, 1998). However, the assumption of a uniform concentration over the building's exterior is unrealistic except at longer downwind distances where the dimensions of the cloud or plume are large in comparison with those of the structure. Also, the effective air exchange rate, which is required for input to the infiltration/exfiltration model, is hard to estimate with accuracy without performing tracer studies in the building to be modeled as was done prior to the 911-Bio model simulations. Consequently, the D2-Puff building infiltration/exfiltration option should be used with caution.

Forest Terrain

D2PC uses lateral and vertical reference dimensions and expansion coefficients (see Equations (4-7) and (4-8)) within forest canopies that differ from the open terrain values. These forest parameters vary with canopy type and above canopy wind speed. The D2PC forest parameters come from the unpublished recommendations of the late H.E. Cramer based on his review of the data available in the spring of 1967. The table which summarizes Dr. Cramer's recommendations also includes estimates of the below canopy wind speed as a function of forest type and above canopy wind speed.

D2-Puff adopts the D2PC "woods stability" methodology with several modifications. First, D2-Puff interpolates between or extrapolates from the forest parameters in the Cramer table to estimate below canopy parameters for above canopy wind speeds other than the four wind speeds listed in the table. Second, unlike D2PC, D2-Puff allows the below canopy wind speed to be less than 1 m/s. As the wind speed decreases below this threshold, D2-Puff allows the cloud or plume to become stationary. However, the cloud or plume continues to expand at the same rate as if it were being transported at 1 m/s. (D2-Puff uses an identical approach for calm and very light winds in open terrain.) D2PC must define a minimum nonzero wind speed because the predicted dosages would otherwise approach infinity as the wind speed approached zero.

Dumbauld and Bowers (1983) summarize a review of forest dispersion studies, several of which were conducted after Cramer's 1967 literature review. They point out that virtually all of the studies indicate that below-canopy lateral dispersion rates are slower and vertical dispersion rates are faster than the corresponding open terrain rates. The values of α and β tabulated by Dumbauld and Bowers are generally consistent with the D2PC values. However, Dumbauld and Bowers caution that the field results were complicated by unquantified losses of the particulate tracer by deposition and impaction on vegetation. Consequently, the empirical α and β values are subject to considerable uncertainty.

One phenomenon not considered by the D2PC/D2-Puff forest methodology is the limitation on vertical mixing that tends to occur at the top of the canopy (see Bowers et al., 1994). On sunny days, strong solar heating of the canopy top forms an unstable thermal stratification above the canopy with a stable stratification below the canopy top. Consequently, clouds or plumes released below the canopy top during the day tend to remain within the canopy except in clearings where "thermal chimneys" transport the material upwards. On the other hand, clouds or plumes released above a canopy on sunny days mix upward, but generally do not penetrate down into the canopy. The situation is reversed on clear nights when strong radiative cooling at the canopy top results in a stable thermal stratification above the canopy top and a relatively unstable stratification below it. Clouds or plumes released below the canopy top on clear nights tend to mix rapidly to the canopy top where they are trapped, while clouds or plumes released above the canopy generally do not penetrate down into the canopy. Thus, it would be appropriate to set the mixing height equal to the canopy height in D2PC or D2-Puff model runs for below canopy releases.

Numerical Implementation

Traditional Gaussian puff dispersion models account for the effects of spatial and/or temporal variations in meteorological conditions on the transport and diffusion of a quasi-continuous release by representing the cloud or plume segment by a series of overlapping puffs, each of which must be tracked as long as it remains within the computational domain. In some cases, this traditional approach can require computation for a very large number of individual puffs, which can result in relatively long model execution times. Because D2-Puff is intended to provide operational hazard predictions in near real time, IEM developed a unique methodology to increase the model's computational efficiency. In the D2-Puff approach, the location of a cloud or plume with respect to a fixed receptor is used to determine how many "plume segments" are needed to resolve its effects at the receptor. That is, many of the discrete puffs that would be used by a traditional puff model are grouped into plume segments, with the motion of these puffs entirely determined by the two ends of the segment. When the variation in flow over the segment becomes significant, the segment is split to allow independent motion of its components. Several current steady-state Gaussian dispersion models (e.g., Bjorklund et al, 1998) predict concentrations for a quasi-continuous release by using an analytic solution to the integral of the Gaussian puff equation over the duration of the release. D2-Puff calculates concentrations for a plume segment in a similar manner, which further reduces the model's computation time over that of the traditional Gaussian puff approach.

One of the practical problems in developing a variable trajectory Gaussian puff dispersion model is how to provide a sufficient density of receptors to resolve concentration patterns, especially under stable meteorological conditions when puff dimensions are small. If a density of fixed receptors sufficient to resolve puffs at short downwind distances under any meteorological conditions is used, the computational cost can be prohibitive. On the other hand, a computationally practical spacing of fixed receptors may allow puffs to pass undetected between receptors. Many current Gaussian puff models resolve this problem through the use of some type of adaptive grid in which a dense receptor spacing is used in the vicinity of puffs. D2-Puff addresses this problem with a unique "plume finder." If the plume finder is off, the model calculates the concentration and dosage at the location of each receptor. If the plume finder is on, the model assigns to each receptor the maximum concentration and dosage that could be computed for any point in a region surrounding the receptor. In the case of a regular polar or Cartesian receptor grid, the dimensions of the surrounding region are based on the grid spacing. In the case of a discrete receptor, the surrounding region is a circle with a specified radius (currently 15 m).

The authors of D2-Puff caution that the plume finder option can result in hazard area plots that are wider than the actual hazard area, a phenomenon that is clearly preferable to missing a hazard area altogether. However, many D2-Puff users will still not appreciate the extent to which hazard area plots depend on the combination of receptor grid and plume finder on/off. For example, Figures 1 through 4 show four different simulations made using the same source and meteorological inputs. All four simulations assume the detonation of 15 155 mm GB projectiles, and all four simulations assume the same meteorological conditions at the locations of Dugway Proving Ground's remote automated weather stations. (In each case, the meteorological inputs were updated every 15 min during the 2-hour simulation.) Figures 1 and 2 respectively show the simulations made using the D2-Puff default polar grid with and without the plume finder. Similarly, Figures 3 and 4 respectively show the simulations made using the D2-Puff default Cartesian grid with and without the plume finder. Comparisons of Figures 1 with Figure 2 and Figure 3 with Figure 4 illustrate the value of the plume finder. If this option is not used, the downwind extent of the hazard area for a given effect (e.g., No Deaths) can be underestimated or the hazard area can be entirely missed. Even with the plume finder on, a comparison of Figure 1 with Figure 3 shows that there can be differences in both the width and downwind extent of the hazard area, depending on the receptor system used.

The most accurate estimates of hazard areas can be obtained using a high resolution receptor array without the plume finder. For example, Figures 5 and 6 show the hazard areas calculated for the same scenario as considered in Figures 1 through 4 using high resolution polar and Cartesian receptor grids. The high resolution polar grid used to generate Figure 5 consisted of a 1-degree angular spacing of receptors placed at the default radial distances, while the high resolution Cartesian grid used to generate Figure 6 had a 200-m resolution for both the east-west and north-south coordinates. The plume finder was turned off for both simulations. Comparison of Figures 5 and 6 shows good agreement between the simulations for the two high resolution receptor grids. In operational settings where a high resolution receptor grid is not practical, Figures 1 through 6 demonstrate why use of the plume finder is strongly recommended.

There are several situations in which the current D2-Puff methodology causes the model to produce a physically unrealistic increase in concentration with downwind distance. First, as discussed above, an artificial compression of a cloud or plume segment can occur in complex terrain when the terrain elevation increases with distance along the cloud or segment's trajectory. Also, if the mixing depth decreases between time steps in flat or complex terrain, an artificial compression can occur because D2-Puff assumes that all of the material within the mixing layer during one time step is confined within the mixing layer during the next time step, even if the second mixing depth is shallower than the first mixing depth. In reality, material that remains above the shallower mixing layer is decoupled from the surface layer and does not affect concentrations at the surface until the mixing layer again increases to its height. D2PC shares this artificial compression problem when the mixing depth decreases with time. However, although not explicitly stated in their report, we believe that the authors of Technical Paper No. 10 only intended that the methodology used by D2PC be applied to the transition from stable nighttime conditions to unstable daytime conditions. The final situation in which D2-Puff can yield an artificial increase in concentration with downwind distance is the case of a plume segment when there is a decrease of wind speed with distance along the segment's trajectory. Traditional Gaussian puff models share this problem unless they explicitly account for distortions of the puffs by nonuniform wind fields.

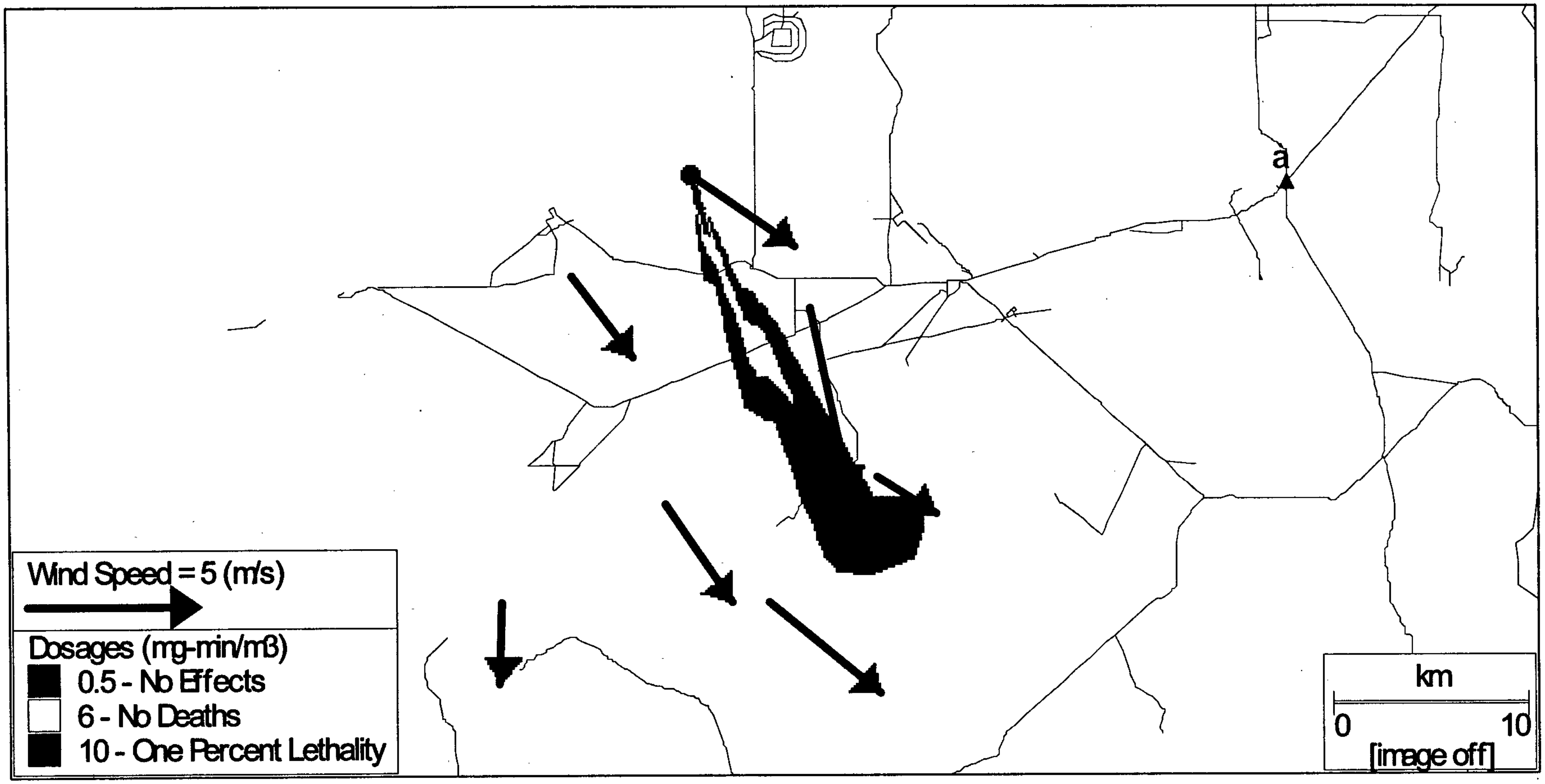

Figure 1. Hazard area calculated for detonation of 15 155 mm GB projectiles using the default polar receptor grid with the plume finder on.

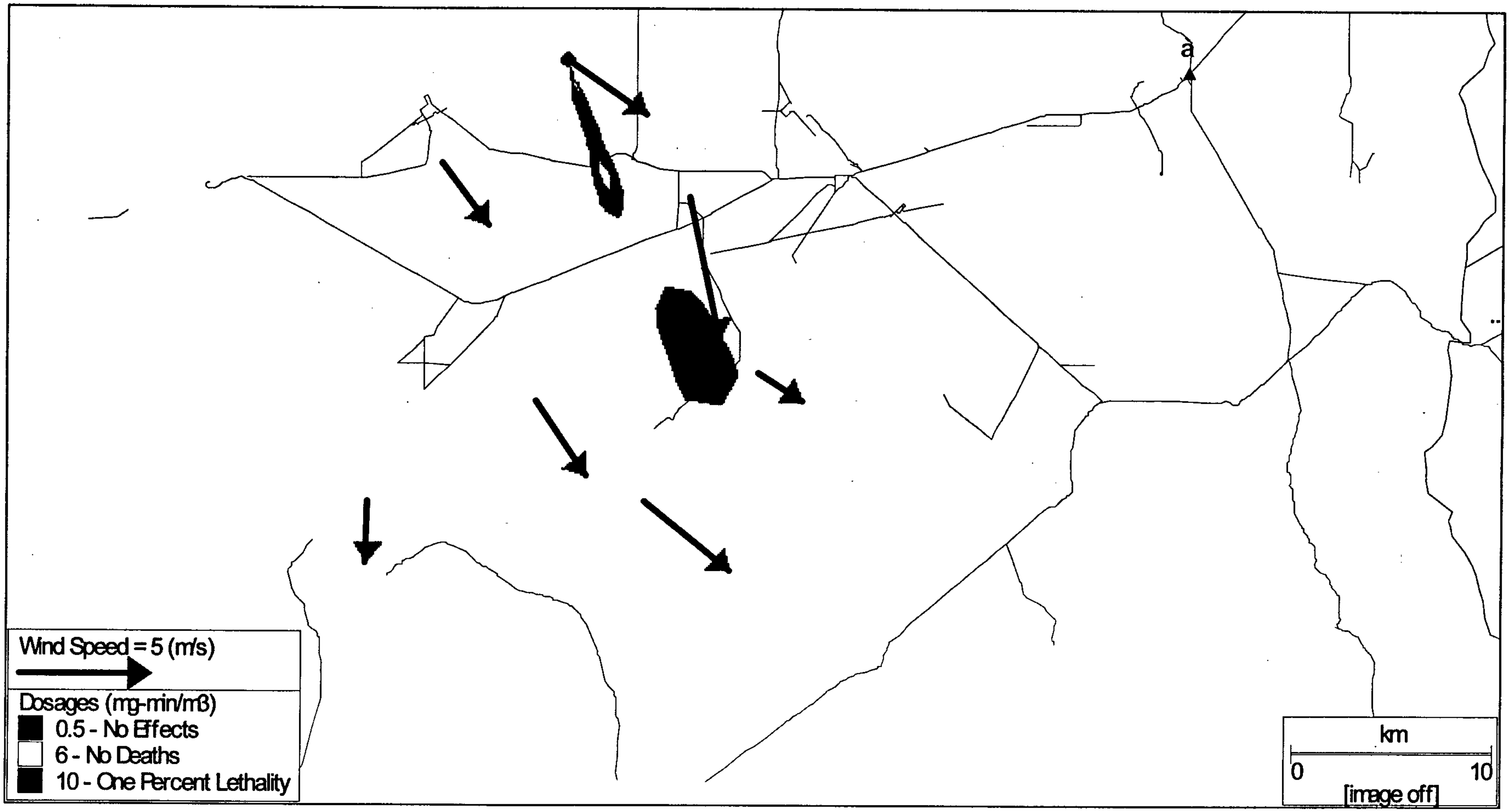

Figure 2. Hazard area calculated for detonation of 15 155 mm GB projectiles using the default polar receptor grid with the plume finder off.

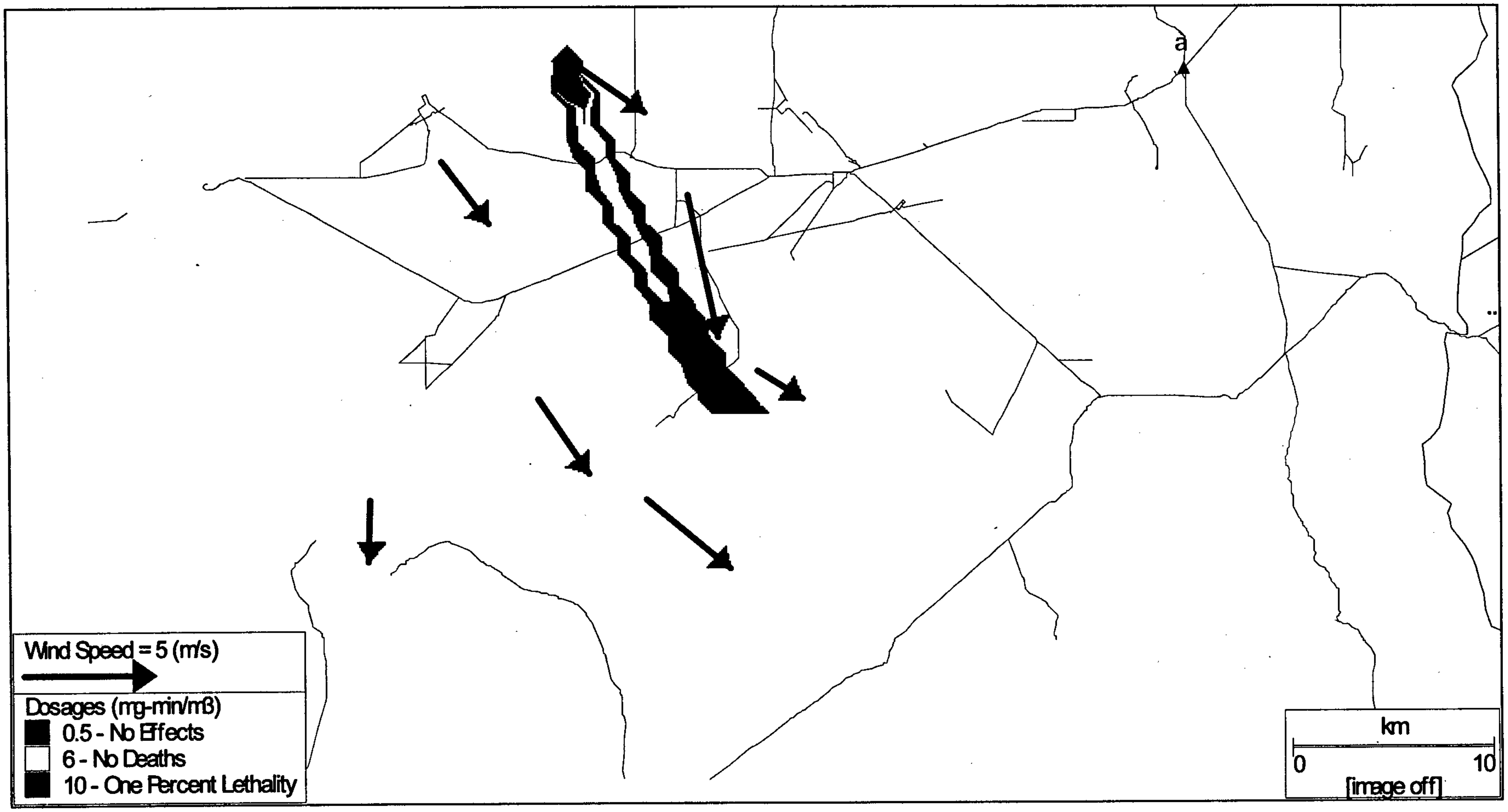

Figure 3. Hazard area calculated for detonation of 15 155 mm GB projectiles using the default Cartesian receptor grid with the plume finder on.

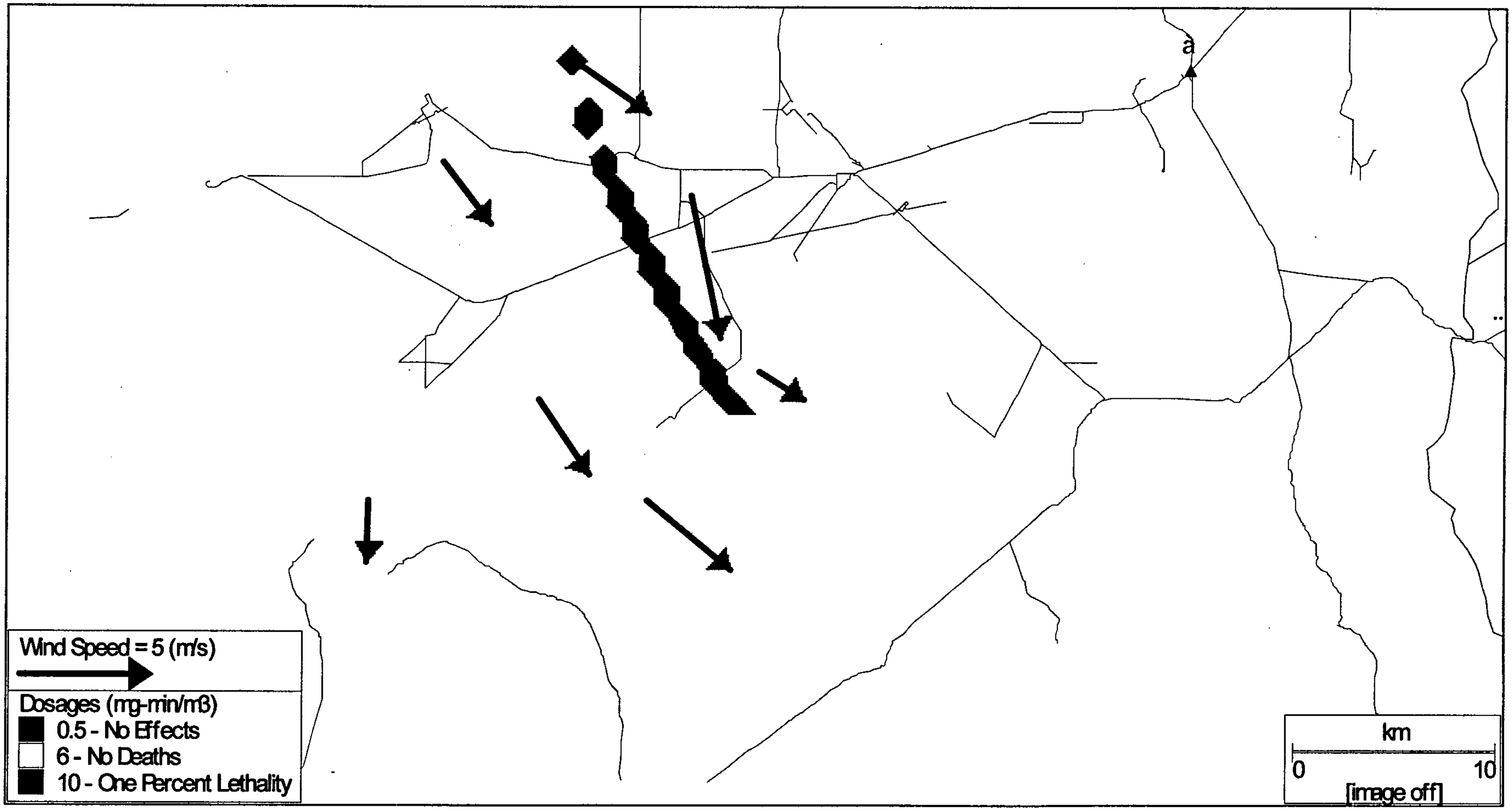

Figure 4. Hazard area calculated for detonation of 15 155 mm GB projectiles using the default Cartesian receptor grid with the plume finder off.

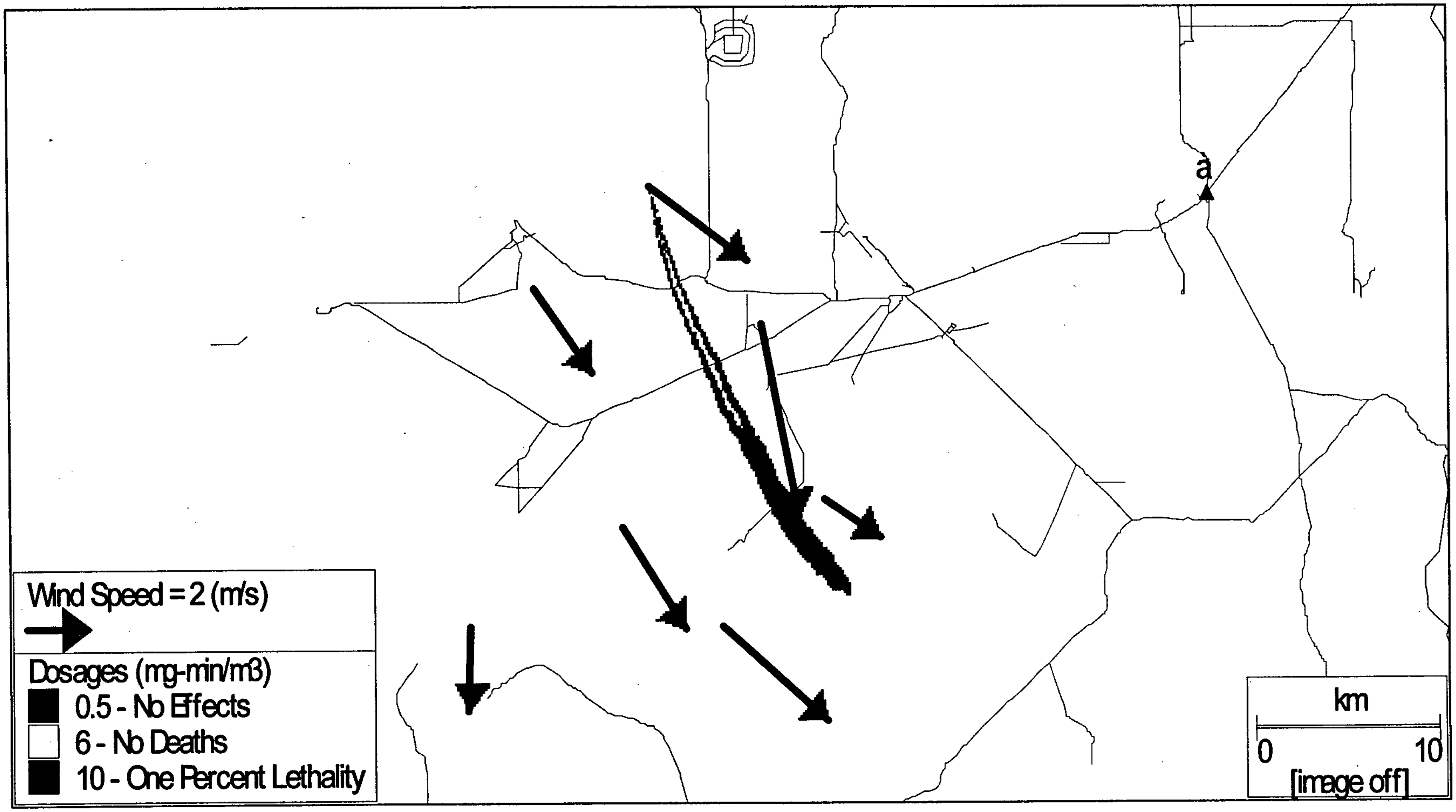

Figure 5. Hazard area calculated for detonation of 15 155 mm GB projectiles using a high resolution polar receptor grid with the plume finder off.

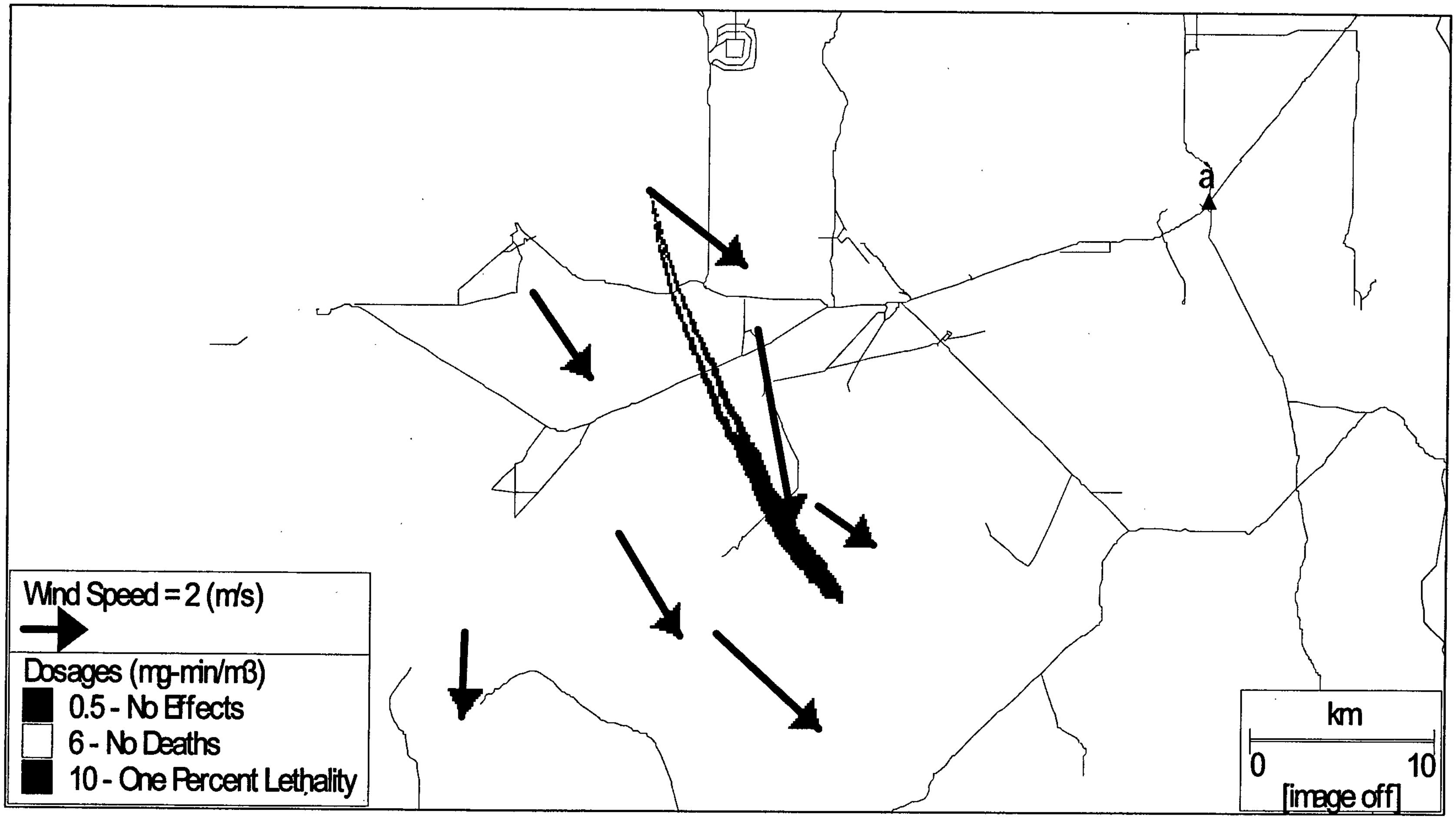

Figure 6. Hazard area calculated for detonation of 15 155 mm GB projectiles using a high resolution Cartesian Receptor grid with the plume finder off.

The artificial compression problems described above represent violations of the Second Law of Thermodynamics in that they all effectively result in a reconstitution of material that has been dispersed in the atmosphere. However, because these conceptual problems all result in overestimates of concentrations, they are not serious impediments to D2-Puff's use as a hazard prediction tool. IEM is aware of these problems and is working on solutions to several, which may be included in a future D2-Puff release.

4.2.4 Validation Using Field Data

4.2.4.1 Introduction

We compared the results of D2-Puff model predictions with measurements made during the Prairie Grass, Green Glow, Ocean Breeze, DSWA Model Validation Phase I, and DSWA Model Validation Phase II field dispersion experiments. Brief descriptions of these experiments are given below:

> Prairie Grass (Barad, 1958) is perhaps the best known dispersion experiment of all time. The intent of the Prairie Grass trials, which were conducted near O'Neill, Nebraska during July and August 1956, was to study dispersion over an idealized flat, grassy surface without any complicating factors such as complex terrain or surface inhomogenieties. Sulfur dioxide (SO_2) gas was released near the surface over 10-min periods and sampled on concentric arcs at 50, 100, 200, 400, and 800 m downwind from the source.
>
> The Green Glow trials (Barad and Fuquay, 1962) were conducted during June through August 1959 at Hanford, Washington in an area covered with desert grasses interspersed with sagebrush. Fluorescent particles (FP) were released near the surface over 30-min periods and sampled on concentric arcs at 0.2, 0.8, 1.6, 3.2, 12.8, and 25.6-m downwind from the source.
>
> The Ocean Breeze trials (Haugen and Fuquay, 1963) were conducted during May and June 1961 and January through March 1962 at Cape Canaveral, Florida in an area with rolling sand dunes (3 to 6 m in height) which were covered with dense palmetto growth (1 to 2 m) and brushwood (2 to 4 m). All trials were conducted with onshore flow from the Atlantic Ocean. During each trial, the FP tracer was released over a 30-min period, and total dosage was measured on sampling arcs at 1.2, 2.4, and 4.8 km downwind.
>
> The DSWA I trials (Biltoft, 1997) were conducted on an area of salt flats at Dugway Proving Ground during September 1996. The purpose of this unique field experiment was to disseminate a sufficient number of instantaneous puffs under the "same" meteorological conditions to form

ensembles that could be used to validate the probabilistic prediction capability of the next generation of dispersion models. Instantaneous puffs of the tracer gas propylene were released near the surface and sampled at a rate of 50 Hz by photoionization detectors (PIDs) on sampling lines ranging from 200 to 1200 m downwind. The typical puff ensemble contained approximately 20 puffs.

The DSWA II experiment (also known as Dipole Pride 26) (Biltoft, 1998) was conducted at the Nevada Test Site (NTS) during November 1996 in an area of desert scrub on a dry lake bed. Instantaneous puffs of the tracer gas sulfur hexafluoride (SF_6) were released near the surface and measured using sequential 15-min whole-air (bag) samplers on three crosswind sampling lines ranging from 2 to 20 km downwind. Six SF_6 continuous analyzers located on the middle sampling line measured concentration time histories at a rate of 4 Hz.

4.2.4.2 Prairie Grass

Under contract to Dugway Proving Ground, Hanna et al. (1991) developed a "modeler's data base" of source, meteorological, and tracer concentration data for several historical data sets, including Prairie Grass. We used the Prairie Grass data summarized by Hanna et al. (1991) in the D2-Puff validation.

During the Prairie Grass trials, SO_2 was continuously released for 10-min periods at a height of 0.45 m above ground level (AGL) and sampled at a height of 1.5 m AGL. Consequently, our D2-Puff runs predicted dosages at 1.5 m AGL for 10-min releases made at 0.45 m AGL. Barad (1958) provides the sampling results as "10-min average" concentrations, which were obtained by dividing the total dosages by the 10-min release time. We converted these average concentrations back to dosages by multiplying by 10 for comparison with the D2-Puff dosage predictions. Because Hanna et al. (1991) provide only the 2-m wind speeds for the Prairie Grass trials, we obtained the 8-m wind speeds from Barad (1958) for use in the D2-Puff calculations. (The 8-m level is the Prairie Grass measurement height closest to the 10-m measurement height assumed by D2-Puff.) The Pasquill stability categories provided by Hanna et al. (1991) were estimated from Obukhov lengths derived from the onsite meteorological measurements. To the best of our knowledge, the storage depots do not use the Obukhov length as a stability index. Consequently, we used the Turner (1964) method to estimate the Pasquill stability categories from the 10-m wind speed (8-m speed in this case), cloud cover, and solar elevation angle. For the Prairie Grass trials for which no mixing depths are provided in the Hanna et al. (1991) data base (all of the stable and some of the neutral trials), we assumed that the D2-Puff default mixing depths for Deseret

Chemical Depot are representative of O'Neill, Nebraska. The assumed mixing depths did not affect the dosages calculated by D2-Puff for these trials.

Table 4-1 summarizes the performance of the D2-Puff model in predicting centerline dosages for the Prairie Grass trials. If all stabilities are considered, the MG shows that D2-Puff closely matches the observed centerline dosages at short range and has a bias toward overestimation at longer range. Hanna (1993) concludes from the results of a number of different dispersion model validation studies that the better models have MGs that range from about 0.5 to 2.0 and VGs that range from about 1 to 3. D2-Puff exhibits this state-of-the-art performance at very short range, but the variability in its predictions as indicated by the VG exceeds that of the better models beyond about 200 m. The sample sizes for the unstable and stable trials are so small that firm conclusions about model performance under these conditions may not be warranted. However, the D2-Puff predictions for the unstable trials exhibit a bias toward overestimation that increases rapidly with downwind distance, which is consistent with the expected plume lift off in convective updrafts. On the other hand, the D2-Puff predictions for the stable trials exhibit an apparent bias toward underestimation that is of concern in a model intended for use as a safe-sided hazard prediction tool. The Prairie Grass data appear to be fairly unique because most dispersion models not specifically tuned to the Prairie Grass data show a similar bias for the stable trials at downwind distances beyond 200 m (for example, see Figure 6 of Hanna, 1993).

4.2.4.3 Green Glow

We also used the Green Glow data tabulated by Hanna et al. (1991) for D2-Puff validation. Our D2-Puff runs assumed that the FP tracer was released over 30-min periods at 2.5 m AGL. Barad and Fuquay (1962) report the FP tracer measurements as total dosages divided by the 30-min dissemination time. As in the case of the Prairie Grass concentration measurements, we converted the Green Glow mean concentrations back to dosages for comparison with the D2-Puff dosage predictions at 1.5 m AGL. The wind speeds measured at 12.2 m AGL were used to approximate 10-m wind speeds in the D2-Puff runs. We used the Turner (1964) method to estimate the Pasquill stability categories with the 10-m wind speed approximated by the 12.2-m wind speed. Because all of the Green Glow trials were conducted at night, only stable and neutral conditions occurred during the trials. In the absence of any mixing depths reported for the Green Glow trials, we assumed that the D2-Puff default mixing depths for Umatilla Chemical Depot are representative of conditions at the nearby Hanford, Washington site where the Green Glow trials were conducted.

Table 4-1
Summary of D2-Puff Performance in
Predicting Prairie Grass Centerline Dosages

Downwind Distance (m)	Pasquill Stability Category (Number of Trials)						
	All (43)[a]	A (0)	B (2)	C (3)	D (31)[b]	E (4)[c]	F (3)[d]
			(a) Geometric Mean MG				
50	0.88	--	0.98	0.84	0.94	0.56	0.70
100	0.91	--	1.20	0.91	0.99	0.50	0.60
200	0.89	--	1.61	1.03	1.03	0.39	0.62
400	1.02	--	3.19	1.46	1.19	0.36	0.71
800	1.17	--	8.58	2.45	1.40	0.30	0.42
			(b) Geometric Variance VG				
50	1.27	--	1.02	1.04	1.29	1.49	--
100	1.62	--	1.04	1.02	1.72	1.88	--
200	2.25	--	1.25	1.00	2.21	3.73	5.13
400	3.41	--	4.11	1.18	3.46	5.08	3.92
800	9.25	--	120.32	2.39	8.88	8.38	11.48

[a] Data for only 39 trials are available at 50 m, 40 trials for 100 m, and 42 trials for 200 m.

[b] Data for only 30 trials are available at 50 m.

[c] Data for only 3 trials are available at 50 and 100 m.

[d] Data for only 1 trial are available at 50 and 100 m and data for only 2 trials are available at 200 m.

Table 4-2 summarizes D2-Puff's performance in predicting centerline dosages for the Green Glow trials. Both the MG and VG for the neutral trials fall within Hanna's (1993) limits for the better models at all downwind distances, although there is a consistent bias toward overestimation. However, in contrast to the results for the stable Prairie Grass trials, the D2-Puff results for the stable Green Glow trials show a bias toward overestimation that increases with downwind distance. One possible explanation for this result is that the assumed mixing depths are too low. However, when we increased the mixing depth from

160 to 5,000 m for several of the trials conducted under F stability, the overprediction was only reduced by about one-third, which indicates that other factors account for most of the bias toward overestimation for the stable trials. It is important to note that the D2-Puff predictions do not consider losses of the FP tracer due to deposition at the surface and impaction on vegetation. These losses are believed to have been significant during the stable trials, especially at the longer distances. Consequently, the neglect of FP depletion in the D2-Puff predictions helps to account for the increase in the model's bias toward overestimation as the stability and/or downwind distance increase. If all stabilities are considered, the D2-Puff bias toward overestimation monotonically increases with downwind distance. We believe that the Green Glow results in Table 4-2 are of particular interest for D2-Puff validation because surface conditions at the Hanford site are far more representative of conditions in the vicinity of the chemical storage depots than the idealized conditions at the Prairie Grass site.

Fuquay et al. (1963) compare the Prairie Grass results with data from the Green Glow and "30 series" experiments. The "30 series" was conducted at the Green Glow site using the same methodology as used in the Green Glow trials. However, in contrast to the Green Glow trials, all of the "30 series" trials were conducted under unstable conditions. Fuquay et al. compare normalized crosswind-integrated dosages (CWIDs) for the three experiments to remove the effects of the different dissemination times. They conclude that the Prairie Grass and "30 series" CWIDs are in close agreement for unstable conditions, but that the CWIDs for the stable Prairie Grass trials are about double those of the Green Glow trials at 200 and 800 m. (Note that, because CWIDs reflect only the effects of vertical disperison, even larger differences would be expected for centerline dosages.) Fuquay et al. speculate that the differences in surface roughness (and hence mechanical turbulence) between the Hanford and O'Neill sites may account for much of these differences. They also cite FP depletion as a possible contributing factor.

4.2.4.4 Ocean Breeze

We used the Ocean Breeze data tabulated by Hanna et al. (1991) for D2-Puff validation. Our D2-Puff runs assumed 30-min FP releases at 2.5 m AGL. Because the highest wind measurement height during the Ocean Breeze trials was 3.7 m AGL, we used the 3.7-m wind speeds both as the D2-Puff transport wind speeds and in the Turner (1964) method to estimate Pasquill stability categories. In some cases, the use of a 3.7-m rather than a 10-m wind speed can affect the Pasquill stability category yielded by the Turner (1964) scheme. As a check on the effects of using the lower-level wind speeds to estimate stability, we used the open-terrain power-law coefficients suggested by Bowers et al. (1994) to estimate 10-m wind

Table 4-2
Summary of D2-Puff Performance in Predicting
Green Glow Centerline Dosages

Downwind Distance (km)	Pasquill Stability Category (Number of Trials)						
	All (24)[a]	A (0)	B (0)	C (0)	D (14)[b]	E (5)[c]	F (5)
				(a) Geometric Mean MG			
0.2	1.80	--	--	--	1.29	1.85	4.48
0.8	2.01	--	--	--	1.22	1.79	9.14
1.6	2.74	--	--	--	1.58	2.27	15.47
3.2	3.39	--	--	--	1.90	3.30	17.51
12.8	3.70	--	--	--	1.58	7.36	25.19
25.6	4.80	--	--	--	1.70	10.89	49.97
				(b) Geometric Variance VG			
0.2	2.10	--	--	--	1.23	1.68	11.58
0.8	4.24	--	--	--	1.51	2.04	159.85
1.6	8.41	--	--	--	1.69	3.29	1.94×10^3
3.2	13.03	--	--	--	2.28	4.96	4.51×10^3
12.8	29.93	--	--	--	2.27	69.59	4.56×10^4
25.6	128.68	--	--	--	3.12	394.26	5.63×10^6

[a] Data for only 22 trials are available at 12.8 and 25.6 km.

[b] Data for only 13 trials are available at 12.8 and 25.6 km.

[c] Data for only 4 trials are available at 12.8 and 25.6 km.

speeds and recomputed stabilities. The resulting stability category estimates agreed with the original estimates for 66 of the 69 trials. Because no mixing depths are available for the Ocean Breeze trials, we used the Johnston Island default mixing depths in our D2-Puff runs. However, these mixing depths did not affect the calculated dosages. Hanna et al. report the FP tracer measurements as mean concentrations, which were obtained by dividing the total dosages by the 30-min dissemination time. We converted these mean concentrations back to total dosages for comparison with the dosages predicted by D2-Puff for a sampling height of 4.6 m AGL.

Table 4-3 summarizes D2-Puff's performance in predicting centerline dosages for the Ocean Breeze trials. In contrast to the Prairie Grass results, D2-Puff underestimates centerline dosages for the very unstable trials. The model's best overall performance is for the trials when the estimated stability category is the slightly unstable Pasquill C category. The MG is very close to the ideal value of unity at all downwind distances for the C stability trials, although the VG at distances of more than 1.2 km exceeds the limit found by Hanna (1993) for the better models. The Ocean Breeze trials were designed to take advantage of onshore sea breezes, and it is reasonable to hypothesize that slightly unstable conditions existed during all of the trials no matter what the stability category indicated by the objective Turner (1964) method. Under this hypothesis, D2-Puff should overestimate dispersion (underestimate dosages) for the unstable trials and underestimate dispersion (overestimate dosages) for the neutral and stable trials. The results given in Table 4-3 are consistent with this hypothesis.

Table 4-3
Summary of D2-Puff Performance in Predicting
Ocean Breeze Centerline Dosages

Downwind Distance (km)	Pasquill Stability Category (Number of Trials)						
	All (69)	A (1)[a]	B (8)[b]	C (18)[c]	D (34)[d]	E (2)	F (6)[a]
	(a) Geometric Mean MG						
1.2	2.05	0.408	0.85	1.10	2.59	3.62	12.15
2.4	2.43	0.394	0.65	1.02	3.62	5.28	20.46
4.8	2.11	---	0.29	1.11	2.99	4.46	---
	(b) Geometric Mean Variance VG						
1.2	4.97	---	1.58	2.32	4.20	6.46	651.81
2.4	12.72	---	1.73	4.08	11.60	22.38	1.11×10^4
4.8	5.31	---	4.77	4.34	5.29	9.62	---

[a] No data available at 4.8 km.

[b] Data for only 3 trials are available at 4.8 km.

[c] Data for only 4 trials are available at 4.8 km.

[d] Data for only 20 trials are available at 4.8 km.

4.2.4.5 DSWA I Puff Trials

Yee et al. (1998) summarize the processing and analysis of the meteorological and tracer concentration data from the DSWA I experiment. The tracer data from the multiple puff releases were combined into 17 ensembles and analyzed in the relative (puff-centered) frame of reference. That is, the centers of mass of the individual puffs in each ensemble were superimposed, and the alongwind and crosswind concentration distributions were averaged to obtain the ensemble mean puff. For each ensemble, Yee et al. provide the ensemble mean peak dosage, peak concentration, crosswind puff dimension σ_y, alongwind puff dimension (in time units) σ_t, and transport speed of the puff centroid to the sampling line. However, the results presented by Yee et al. do not exactly correspond to what is predicted by D2-Puff. For example, their peak concentrations are actually the concentrations at the puff centers of mass. Because the puffs are skewed in time, the actual peak concentrations are higher than the concentrations at the centers of mass. (Each puff concentration time history is skewed about the arrival time of the puff's center of mass because of puff growth during passage over the sampling line.) Consequently, we used the actual ensemble mean peak concentrations and total dosages, which were determined by Technical Panel 9 (1998) in a similar study. Under the assumption of a Gaussian distribution, we graphically estimated σ_y for each ensemble from the crosswind dosage plots given by Chandler (1997) by dividing the distance between the points at which the ensemble mean dosage decreased to 10 percent of the peak dosage by 4.3. We estimated σ_t in a similar manner.

The D2-Puff predictions for the DSWA I trials assumed instantaneous puff releases at 1.3 m AGL. The initial alongwind (σ_{xo}), crosswind (σ_{yo}), and vertical (σ_{zo}) puff dimensions ranged from 1 to 2 m, depending on the values estimated for each trial by Biltoft (1997) from an analysis of infrared imagery of the initial puffs. Dosages, peak concentrations, and concentration time histories were computed for the sampling height of 1.6 m AGL. The mean wind speed measured at 8 m was used to approximate the 10-m wind speed for each ensemble, and the Turner (1964) method was used to estimate the Pasquill stability category. In some cases, the stability category indicated by the Turner (1964) scheme changed during the trial. In these cases, the D2-Puff predictions assumed the stability category at the start of the trial. (Note that Yee et al. concluded from visual examination of sonic anemometer and PID concentration data that the actual stability was essentially constant during these trials.) Although Biltoft (1997) provides mixing depths for the DSWA I ensembles, we used the D2-Puff default values for nearby Deseret Chemical Depot. Because of the relatively short downwind distances to the sampling line and the absence of very stable conditions, the assumed mixing depths had little or no effect on the D2-Puff predictions.

Tables 4-4 and 4-5 summarize the D2-Puff model's performance in predicting DSWA I peak (centerline) dosages and peak concentrations, respectively. Because only a few ensembles are available for each combination of stability and downwind distance, it is perhaps most informative to consider the results for all stabilities combined or all downwind distances combined. When all downwind distances are considered, D2-Puff shows an apparent tendency to change from a bias toward overestimation of dosages to a bias toward underestimation of dosages as the stability category changes from unstable to stable. The model underestimates peak concentrations for all stabilities. However, there are so few unstable and stable ensembles that firm conclusions about stability-dependent biases are not warranted. When all stabilities are considered, D2-Puff shows a bias toward underestimation of peak concentrations and dosages at all downwind distances except 300-350 m, where a large overprediction for a single ensemble results in a bias toward overestimation. Although D2-Puff's bias toward underestimation of concentrations and dosages is a source of concern in a hazard model, it should be remembered that the DSWA I site is even smoother (surface roughness length z_o <0.001 m) and more idealized than the Prairie Grass site ($z_o = 0.006$ m). Because many of the more modern dispersion models explicitly consider the effects of surface roughness in their predictions, they do not necessarily share D2-Puff's bias toward underestimation for smooth surfaces. For example, the model evaluated by Technical Panel 9 (1998) showed an overall bias toward overestimation rather than underestimation of the DSWA I dosages and concentrations.

The overall D2-Puff dosage and concentration MG and VG values given in Tables 4-4 and 4-5 are within the ranges given by Hanna (1993) for the better models. However, Hanna's (1993) conclusions about limits on model performance are based on comparisons of model predictions of ensemble means with observations that represent single realizations. Because Tables 4-4 and 4-5 compare predicted and observed ensemble means, it would be reasonable to expect that the MGs and VGs would be somewhat closer to their ideal value of unity than found by Hanna.

Tables 4-6 and 4-7 respectively summarize D2-Puff's performance in predicting the lateral (σ_y) and alongwind (σ_t) Gaussian dispersion coefficients for the DSWA I ensembles. The D2-Puff σ_y values were obtained from the crosswind dosage profiles under the assumption of a Gaussian distribution and the σ_t values were computed from the 1-s concentrations predicted at the centerline of each puff trajectory. As shown by Table 4-6, D2-Puff may have a bias toward overestimation of σ_y that increases with downwind distance. In contrast, inspection of Table 4-7 indicates that D2-Puff's bias toward overestimation of σ_t is essentially independent of downwind distance. D2-Puff's biases toward overestimation of σ_y and σ_t readily account for the model's biases toward underestimation of peak dosages and concentrations, including a greater bias toward underestimation of concentrations than dosages. As noted above, D2-Puff's biases toward overestimation of σ_y and σ_t probably result from its empirical σ_y and σ_t algorithms, which almost certainly represent larger surface roughness lengths than found at the site where the DSWA I trials were conducted.

Table 4-4
Summary of D2-Puff Performance in Predicting
DSWA I Peak Dosages

Downwind Distance (m)	Pasquill Stability Category						
	All	A	B	C	D	E	F
			(a) Number of Ensembles				
200	3	0	0	0	3	0	0
300-350	7	0	1	1	3	2	0
800	5	0	0	0	5	0	0
1200	2	0	0	0	2	0	0
All	17	0	1	1	13	2	0
			(b) Geometric Mean MG				
200	0.53	---	---	---	0.53	---	---
300-350	1.61	---	1.99	1.36	3.07	0.59	---
800	0.71	---	---	---	0.71	---	---
1200	0.41	---	---	---	0.41	---	---
All	0.88	---	1.99	1.36	0.85	0.59	---
			(c) Geometric Variance VG				
200	1.60	---	---	---	1.60	---	---
300-350	4.35	---	---	---	21.14	1.33	---
800	2.02	---	---	---	2.02	---	---
1200	---	---	---	---	5.18	---	---
All	2.97	---	---	---	3.80	1.33	---

Table 4-5
Summary of D2-Puff Performance in Predicting
DSWA I Peak Concentrations

Downwind Distance (m)	Pasquill Stability Category						
	All	A	B	C	D	E	F
				(a) Number of Ensembles			
200	3	0	0	0	3	0	0
300-350	7	0	1	1	3	2	0
800	5	0	0	0	5	0	0
1200	2	0	0	0	2	0	0
All	17	0	1	1	13	2	0
				(b) Geometric Mean MG			
200	0.36	---	---	---	0.36	---	---
300-350	1.10	---	0.78	0.73	2.03	0.64	---
800	0.53	---	---	---	0.53	---	---
1200	0.32	---	---	---	0.32	---	---
All	0.63	---	0.78	0.73	0.69	0.64	---
				(c) Geometric Variance VG			
200	2.88	---	---	---	2.88	---	---
300-350	2.19	---	---	---	5.15	1.22	---
800	2.21	---	---	---	2.21	---	---
1200	6.23	---	---	---	6.23	---	---
All	2.60	---	---	---	3.35	1.22	---

Table 4-6
Summary of D2-Puff Performance in Predicting
DSWA I Lateral Dispersion Coefficients

Downwind Distance (m)	Pasquill Stability Category						
	All	A	B	C	D	E	F
(a) Number of Ensembles							
200	3	0	0	0	3	0	0
300-350	7	0	1	1	3	2	0
800	5	0	0	0	5	0	0
1200	2	0	0	0	2	0	0
All	17	0	1	1	13	2	0
(b) Geometric Mean MG							
200	1.04	---	---	---	1.04	---	---
300-350	1.07	---	0.81	1.51	1.08	1.04	---
800	1.16	---	---	---	1.16	---	---
1200	1.47	---	---	---	1.47	---	---
All	1.13	---	0.81	1.51	1.15	1.04	---
(c) Geometric Variance VG							
200	1.02	---	---	---	1.02	---	---
300-350	1.05	---	---	---	1.04	1.00	---
800	1.06	---	---	---	1.06	---	---
1200	1.20	---	---	---	1.20	---	---
All	1.06	---	---	---	1.07	1.00	---

Table 4-7
Summary of D2-Puff Performance in Predicting
DSWA I Alongwind Dispersion Coefficients

Downwind Distance (m)	Pasquill Stability Category						
	All	A	B	C	D	E	F
			(a) Number of Ensembles				
200	3	0	0	0	3	0	0
300-350	7	0	1	1	3	2	0
800	5	0	0	0	5	0	0
1200	2	0	0	0	2	0	0
All	17	0	1	1	13	2	0
			(b) Geometric Mean MG				
200	1.36	---	---	---	1.36	---	---
300-350	1.38	---	1.75	1.80	1.49	0.95	---
800	1.25	---	---	---	1.25	---	---
1200	1.25	---	---	---	1.25	---	---
All	1.32	---	1.75	1.80	1.33	0.95	---
			(c) Geometric Variance VG				
200	1.10	---	---	---	1.10	---	---
300-350	1.21	---	---	---	1.24	1.00	---
800	1.07	---	---	---	1.07	---	---
1200	1.09	---	---	---	1.09	---	---
All	1.13	---	---	---	1.12	1.00	---

Table 4-8 summarizes D2-Puff performance in predicting the transport time of the puff centroid to the sampling line. MGs less than unity in Table 4-8 indicate that the predicted transport time is too short, and hence that the assumed transport speed is too high. As discussed in Section 4.2.3.3, this result is expected for a surface release at short range because of D2-Puff's assumption that the 10-m wind speed represents the transport speed to all downwind distances. At longer range, the model can be expected to underestimate transport speeds and hence to overestimate transport times.

Table 4-8
Summary of D2-Puff Performance in Predicting
DSWA I Cloud Transport Times

Downwind Distance (m)	Pasquill Stability Category						
	All	A	B	C	D	E	F
(a) Number of Ensembles							
200	3	0	0	0	3	0	0
300-350	7	0	1	1	3	2	0
800	5	0	0	0	5	0	0
1200	2	0	0	0	2	0	0
All	17	0	1	1	13	2	0
(b) Geometric Mean MG							
200	1.05	---	---	---	1.05	---	---
300-350	0.88	---	1.03	0.93	0.89	0.80	---
800	0.89	---	---	---	0.89	---	---
1200	0.90	---	---	---	0.91	---	---
All	0.91	---	1.03	0.93	0.93	0.80	---
(c) Geometric Variance VG							
200	1.00	---	---	---	1.00	---	---
300-350	1.02	---	---	---	1.02	1.05	---
800	1.02	---	---	---	1.02	---	---
1200	1.01	---	---	---	1.01	---	---
All	1.02	---	---	---	1.01	1.05	---

4.2.4.6 Dipole Pride 26

The objective of the Dipole Pride 26 (DSWA II) experiment was to acquire a data set for the validation of integrated mesoscale wind field and dispersion models such as D2-Puff and its MILTWAM diagnostic wind field model. The Dipole Pride 26 data set is the only one of the five data sets used in the D2-Puff validation that tested the model's ability to predict dosages in complex terrain. The Nevada Test Site's mesoscale network of remote automated weather stations measured 15-min average winds at 10 m AGL throughout the Dipole Pride 26 trials. At our request, IEM processed the automated weather station data to create wind input files for each day. IEM also created a user-defined terrain grid centered on the experiment area so that we could use D2-Puff's "grid with terrain" option.

Our D2-Puff calculations for the Dipole Pride 26 trials were made using the source data given by Biltoft (1998) for each trial, including the release date and time, quantity of SF_6 tracer instantaneously released, source location and effective release height, and initial puff dimensions. The center of the CLA was defined as the location of the automated weather station nearest the center of the experiment area (Station 17). We used the Turner (1964) method with the 10-m winds from that station to estimate the Pasquill stability category for each 15-min period. The solar elevation angle used in the stability computations was for the location of Station 17 at the midpoint of each 15-min wind averaging period.

There is no clear consensus on what mixing depth should be assumed for some of the Dipole Pride 26 trials because of the variations in winds over the experiment site as well as the large vertical wind shear observed during some trials. Consequently, we assumed that the D2-Puff default mixing depths for Deseret Chemical Depot are representative of conditions at the Dipole Pride 26 site. However, we determined through trial and error that the mixing depth assumed by D2-Puff at the center of the valley must be at least 200 m for the releases made into a stable downvalley drainage flow in order to obtain nonzero dosages at the sampling lines. This result is explained by the facts that: (1) D2-Puff assumes that the upvalley release point is above the top of the surface mixing layer with a 100-m mixing depth, and (2) MILTWAM does not compute winds above the top of the mixing layer.

The three Dipole Pride 26 sampling lines each consisted of 30 whole air (bag) samplers with a nominal spacing of 250 m. We compared the D2-Puff predictions with the total dosages derived from the sequential 15-min bag samples collected at each sampling location during the Dipole Pride 26 trials. We calculated dosages for discrete receptors placed at the sampler locations and, in order to improve the resolution of the puff and better establish the peak dosage along each sampling line, we placed discrete receptors equidistant between the samplers on each line. If D2-Puff predicted that the puff center passed outside of a sampling line, we placed additional discrete receptors at the end of the line to capture the peak predicted dosage. The D2-Puff runs were made with the plume finder off. (The model comparisons for the Prairie Grass, Green Glow, Ocean Breeze, and DSWA I trials are not affected by whether the plume finder option was on or off.)

Appendix B contains plots which compare the predicted and observed dosages for the Dipole Pride 26 trials. For each trial, the results are shown from left to right for Samplers 100-130 (the northernmost sampling line), Samplers 200-230 (the center sampling line), and Samplers 300-330 (the southernmost sampling line). However, for purposes of statistical analysis, the results were grouped in order of increasing downwind distance. For example, a trial with a puff release from the north had Samplers 100-130 as the first sampling line and Samplers 300-330 as the last sampling line. On the other hand, a trial with a puff release from the south had Samplers 300-330 as the first sampling line and Samplers 100-130 as the last sampling line. Depending on the trial, the distance from the puff release location to the peak dosage ranged from 2.0 to 6.2 km for the first sampling line, 10.1-12.9 km for the second sampling line, and 17.3 to 20.2 km for the third sampling line.

Table 4-9 summarizes the comparisons of predicted and observed peak total dosages for the Dipole Pride 26 trials. It is important to note that the peak predicted and observed dosages on each sampling line are compared in Table 4-9 even if they were not located at the same sampler position. This approach is common practice in dispersion model validation studies because slight errors in puff or plume trajectories can result in large differences in the concentrations and dosages calculated for fixed locations. In many cases, the sampler data indicated that the actual peak dosage was not contained within the sampling line or that the sampler spacing was not sufficiently dense to resolve the actual peak dosage. In other cases, data are not available for several samplers located near the apparent location of the peak dosage, which results in a large uncertainty in the magnitude of the actual peak dosage. Although Table 4-9 shows predicted to observed dosage ratios for these cases, they were not included in the computations of the geometric mean MG and geometric variance VG shown at the bottom of the table. We made no attempt to classify the results by stability because of the small sample size and the fact that the stability varied during many of the trials. However, the majority of trials were characterized by neutral or stable conditions or a combination of these stabilities.

The geometric means MG shown at the bottom of Table 4-9 show that D2-Puff has an overall bias toward overestimation of peak dosages for the Dipole Pride 26 trials by a factor of 2 to 4, depending on the downwind distance category. However, the large geometric mean variances VG indicate that there is considerable variability in the differences between predictions and observations. The fact that the highest bias toward overestimation occurs at the first sampling line is probably explained by the fact that the discrete receptor array, which had a nominal 125-m spacing, better resolved the narrow puffs than the actual samplers, which had a nominal 250-m spacing.

In addition to the whole air samplers on the middle sampling line, six continuous SF_6 analyzers were used to measure SF_6 concentrations at a 4-Hz rate during the Dipole Pride 26 trials. Biltoft (1998) used the data from the continuous analyzers to estimate the cloud transport time (time of arrival of the puff centroid) and σ_t (alongwind dispersion coefficient in time units) for each puff. For comparison, we used the concentrations predicted by D2-Puff at 10-second intervals for

Table 4-9
Summary of D2-Puff Performance in Predicting
Dipole Pride 26 Peak Dosages

Trial	Predicted/Observed Dosage Ratio		
	2.0 – 6.2 km	10.1 – 12.9 km	17.3 – 20.2 km
3	5.95[a]	5.10	29.54[a]
4A	4.34	1.52[a]	---[a]
5	9.89[a]	1.61[a]	3.55
6	10.36	0.87	2.44
7	3.99	5.03	3.77[a]
9	16.34[a]	1.38	5.71
11B	2.19[a]	0.37	0.48
13	4.80[a]	6.16	5.87
14	1.93	6.29[a]	6.79
15A	2.76	2.53	1.45[a]
16B	4.33[a]	1.93[a]	9.91[a]
17A	10.02[a]	1.64[a]	1.96[a]
Sample Size	5	7	6
Geometric Mean MG	3.95	2.11	3.14
Geometric Variance VG	9.03	4.49	8.39

[a] Excluded from statistical analysis because sampler measurements indicate that the peak dosage was not contained within the sampling line, sampler measurements were missing near the location of the peak dosage, or the sampler spacing was insufficient to resolve the peak observed dosage.

the receptor on the middle sampling line with the highest predicted peak concentration to estimate cloud arrival times and alongwind dispersion coefficients.

Table 4-10 summarizes D2-Puff's performance in predicting cloud arrival times and alongwind dispersion coefficients at the middle sampling line for the Dipole Pride 26 trials. As noted above, the middle sampling line was 10-13 km from the puff release location, depending on the trial. The MGs at the bottom of the table show that D2-Puff has an overall bias toward overestimation of both the transport time and alongwind puff dimension by about 20 percent at this distance. The bias toward overestimation of the transport time is expected because of the model's assumption that the 10-m wind defines cloud transport at all downwind distances.

4.3 RESULTS AND UNRESOLVED ISSUES

Table 4-11 is a traceability matrix for the D2-Puff model's fidelity requirements. The first four fidelity requirements in the table address the correspondence between D2-Puff and D2PC/PARDOS model predictions for the flat-terrain and steady-state meteorological conditions assumed by D2PC/PARDOS. Although the required 10-percent agreement between models was slightly exceeded in several of our test cases, Table 4-11 shows all of these requirements as being fully met because we believe that D2-Puff has satisfied the intent of these requirements. The differences in dosages and/or concentrations of more than 10 percent are explained by either different treatments of wind speeds less than 1 m/s or round-off in D2-Puff's fixed–field tabular output for very small concentrations or dosages. There is no entirely satisfactory procedure to deal with very light winds, but we consider D2-Puff's approach to be more realistic than the D2PC/PARDOS approach, which is used by virtually all steady-state models. The differences in dosage area half widths of more than 10 percent are either no more than 1 m or result from the fact that D2-Puff does not make concentration or dosage calculations more than $3\sigma_y$ from the puff or plume segment center. The $3\sigma_y$ truncation affects hazard area widths only very near the source for very large releases under stable meteorological conditions. As a practical matter, the 500-m radius safety zone that is established around any accidental release at a chemical storage depot appears sufficient to cover any D2-Puff underestimates of hazard area widths.

Table 4-10
Summary of D2-Puff Performance in Predicting
Dipole Pride 26 Cloud Transport Times
and Alongwind Dispersion Coefficients

Trial	Predicted/Observed Ratio	
	Transport Time	Alongwind Dispersion Coefficient
3	1.54	1.25
4A	1.05	1.83
5	1.20	0.41
6	1.29	0.56
7	1.05	2.10
9	---	---
11B	1.15	---
13	---	---
14	1.31	1.05
15A	---	---
16B	1.21	1.61
17A	1.12	2.41
Sample Size	9	8
Geometric Mean MG	1.20	1.21
Geometric Variance VG	1.05	1.47

Table 4-11
Traceability Matrix for D2-Puff Fidelity Requirements

Acceptability Criterion	Status[a]
1. Able to reproduce D2PC/PARDOS results for spatially invariant meteorological conditions	
1.1 Centerline total dosages must agree within 10% (2% desired)	M
1.2 Dosage widths at 3 σ_y must agree within 10% (2% desired) or ±1 m, whichever is greater	M
1.3 Centerline dosage accumulation times must agree within 10% (2% desired) or ±0.1 min, whichever is greater	M
1.4 Centerline concentrations must agree within 10% (2% desired)	M
1.5 Conservative (safe-sided) for hazard prediction	P

[a] M = met; P = partially met; N = not met.

Table 4-11 shows the requirement that D2-Puff be a safe-sided hazard prediction model as being partially met. (This same finding applies to the D2PC/PARDOS methodology in general.) Although D2-Puff provided conservative estimates of concentrations and dosages for three of the five field data sets used in the validation study, the model showed a bias toward underestimation of concentrations for the DSWA I puff ensembles and dosages for the stable Prairie Grass trials. Our experience suggests that the DSWA I and Prairie Grass data are not representative of the dispersion that could be expected in the vicinity of the chemical storage depots, and virtually all of the Gaussian dispersion models with which we are familiar show a similar bias toward underestimation for the stable Prairie Grass trials. In addition to the bias toward underestimation for the DSWA I trials, D2-Puff's neglect of the variation of wind speed with height caused it to underestimate the transport time to short downwind distances for the DSWA I trials. As expected, this bias reversed (i.e., the model overestimated transport times) at the longer downwind distances of the Dipole 26 sampling lines, which could be a problem for a large release with long hazard distances (i.e., the toxic cloud would arrive in a given area much sooner than expected). We view underestimation of the transport wind speed (overestimation of the transport time) as the more serious of the two deficiencies.

APPENDIX A. VERIFICATION AND VALIDATION IMPLEMENTATION PLAN

Meteorology & Obscurants Div.
Dugway Proving Ground
Technical Note 98-90-7R
02 December 1998

VERIFICATION & VALIDATION IMPLEMENTATION PLAN FOR THE D2-PUFF MODEL

PURPOSE

This document provides a plan for the independent verification and validation of the D2-Puff computer model.

BACKGROUND

The D2-Puff computer model has been designed to calculate the dosages that would be received during an accidental release of chemical agent to the atmosphere from a chemical munitions storage depot. The model updates the U.S. Army's D2PC dispersion model (Whitacre et al., 1987) by: (1) including the effects of varying meteorological conditions and terrain, and (2) incorporating the capabilities of the PARDOS model to predict cloud arrival and departure times. When the verification, validation, and accreditation (VV&A) is completed, D2-Puff will replace D2PC as the U.S. Army's approved model for chemical hazard prediction at chemical munitions storage depots.

The sponsor for development of D2-Puff is the Chemical Stockpile Emergency Preparedness Program (CSEPP), which is tasked with managing safety issues related to the Army's chemical weapons stockpile. Innovative Emergency Management Inc. (IEM) is the developer of the D2-Puff computer model. The West Desert Test Center (WDTC) Meteorology & Obscurants Division at U.S. Army Dugway Proving Ground has been selected to perform the independent verification and validation of the D2-Puff software.

INFORMATION SOURCES

M&S Documentation:

IEM Inc., 30 November, 1998: D2-Puff Software Requirements Specification. IEM Inc., Baton Rouge, LA.

IEM Inc., 1998: D2-Puff User Guide, Version 2.0.5. IEM Inc., Baton Rouge, LA.

IEM Inc., 30 November, 1998: D2-Puff Model Technical Manual. IEM Inc., Baton Rouge, LA.

IEM Inc., 1998: D2-Puff Reference Manual, Version 2.05. IEM Inc., Baton Rouge, LA.

Validation Data:

Barad, M. L., (Ed.). 1958: Project Prairie Grass, A field program in diffusion, Vol. I. Geophysical Research Papers No. 59, AFCRC-TR-58-235 (I), Air Force Cambridge Research Center, Bedford, MA.

Barad, M. L., and J. J. Fuquay, (Eds.), 1962: The Green Glow diffusion program, Geophysical Research Papers, 73, Vols. I and II. USAEC Report HW-71400, Air Force Cambridge Research Laboratories.

Biltoft, Christopher A., 1997: Phase I of the Defense Special Weapons Agency transport and dispersion model validation. DPG Document DPG-FR-97-058, West Desert Test Center, U.S. Army Dugway Proving Ground, Dugway, UT.

Biltoft, Christopher A., 1998: Dipole Pride 26: Phase II of the Defense Special Weapons Agency transport and dispersion model validation. DPG Document DPG- FR-98-001, West Desert Test Center, U.S. Army Dugway Proving Ground, Dugway, UT.

Hanna, Steven R., David G. Strimaitis, Joseph C. Chang, and Sharon M. McCarthy, 1991: Meteorological influences on smoke/obscurant effectiveness phase II. Sigma Research Corp., prepared under contract DAAD09-89-C-0039 for U.S. Army Dugway Proving Ground, Dugway, UT.

Haugen, D. A. and J. J. Fuquay (Eds.), 1963: The Ocean Breeze and Dry Gulch Diffusion Programs, Vol. I. USAEC Report HW-78435 [Report AFCRL-63-791 (I)], Cambridge Research Laboratories and Hanford Atomic Products Operation.

Previous Verification & Validation:

IEM Inc., 30 November 1998: D2-Puff model software Test Description, Vols 1 & 2. IEM Inc., Baton Rouge, LA.

IEM Inc., 30 November, 1998: D2-Puff model software test report (draft). IEM Inc., Baton Rouge, LA.

VERIFICATION PLAN

We will review the D2-Puff documentation cited above (and any documentation subsequently provided) and consider the questions in Table 1 in making and assessment of whether the D2-Puff model works as intended using sound system engineering techniques.

TABLE 1
Verification Questions and Schedule

Question	Date to Answer
1) Is the intended use documented?	15 Dec 98
2) Are the requirements complete, clear, testable, and consistent with each other?	15 Dec 98
3) Is the design clear, correct, and consistent?	31 Dec 98
4) Does D2-Puff conform to the documented design?	31 Dec 98
5) Does D2-Puff conform to the documented requirements?	15 Jan 99
6) How much has D2-Puff been tested and how free of problems is it?	15 Feb 99

VALIDATION PLAN

We will perform the tasks listed in Table 2 to determine whether D2-Puff is sufficiently realistic for its intended purpose. Comparison of D2-Puff and D2PC predictions will be limited to cases with flat terrain with no variation in wind direction. Measured data from some or all of the following field tests will be used in Task 6 of the validation:

1) Prairie Grass (Barad, 1958)
2) Ocean Breeze (Haugen and Fuquay, 1963)
3) Dry Gulch (Haugen and Fuquay, 1963)
4) Green Glow (Barad, 1962)
5) Phase I of DSWA Transport and Dispersion Model Validation (Biltoft, 1997)
6) Phase II of DSWA Transport and Dispersion Model Validation (Dipole Pride 26) (Biltoft, 1998)

The Defense Special Weapons Agency (DSWA) tests were specifically designed for the validation of a puff model and include the following features:

1) Instantaneous (puff) releases of tracer gas
2) Measured concentration profiles versus time that will be useful in assessing cloud arrival and departure times
3) Multiple wind measurement locations that have time resolved data
4) Terrain data is available for the sites

TABLE 2
Validation Tasks and Time Table

Task	Date to Complete
1) Review the developer's test plan to ensure it contains adequate tests for model fidelity	31 Dec 98
2) Review developer's tests to ensure model fidelity	31 Jan 99
3) Compare D2-Puff predictions with those of the accredited D2PC model	28 Feb 99
4) Conduct Face Validation – Use estimates and intuition of experts to compare model and real world behaviors subjectively (i.e. technical evaluation)	15 Mar 99
5) Validate D2-Puff using functional decomposition – Validate D2-Puff's functional components (e.g. dispersion coefficients) to validate the whole	15 Apr 99
6) Compare D2-Puff results with measured data from field tests	30 May 99

REFERENCE

Whitacre, C.G., J.H. Griner, M.M. Myirski, and D.W. Sloop, 1987: Personal computer program for chemical hazard prediction (D2PC). Report CRDEC-TR-87021, Chemical Research Development and Engineering Center, Aberdeen Proving Ground, MD.

APPENDIX B.
GRAPHICAL COMPARISONS OF PREDICTED AND OBSERVED DIPOLE PRIDE 26 DOSAGES

The plots in this appendix compare the predicted and observed dosages for the Dipole Pride 26 (DSWA II) trials. For each trial, the results are shown from left to right for Samplers 100-130 (the northernmost sampling line), Samplers 200-230 (the center sampling line), and Samplers 300-330 (the southernmost sampling line).

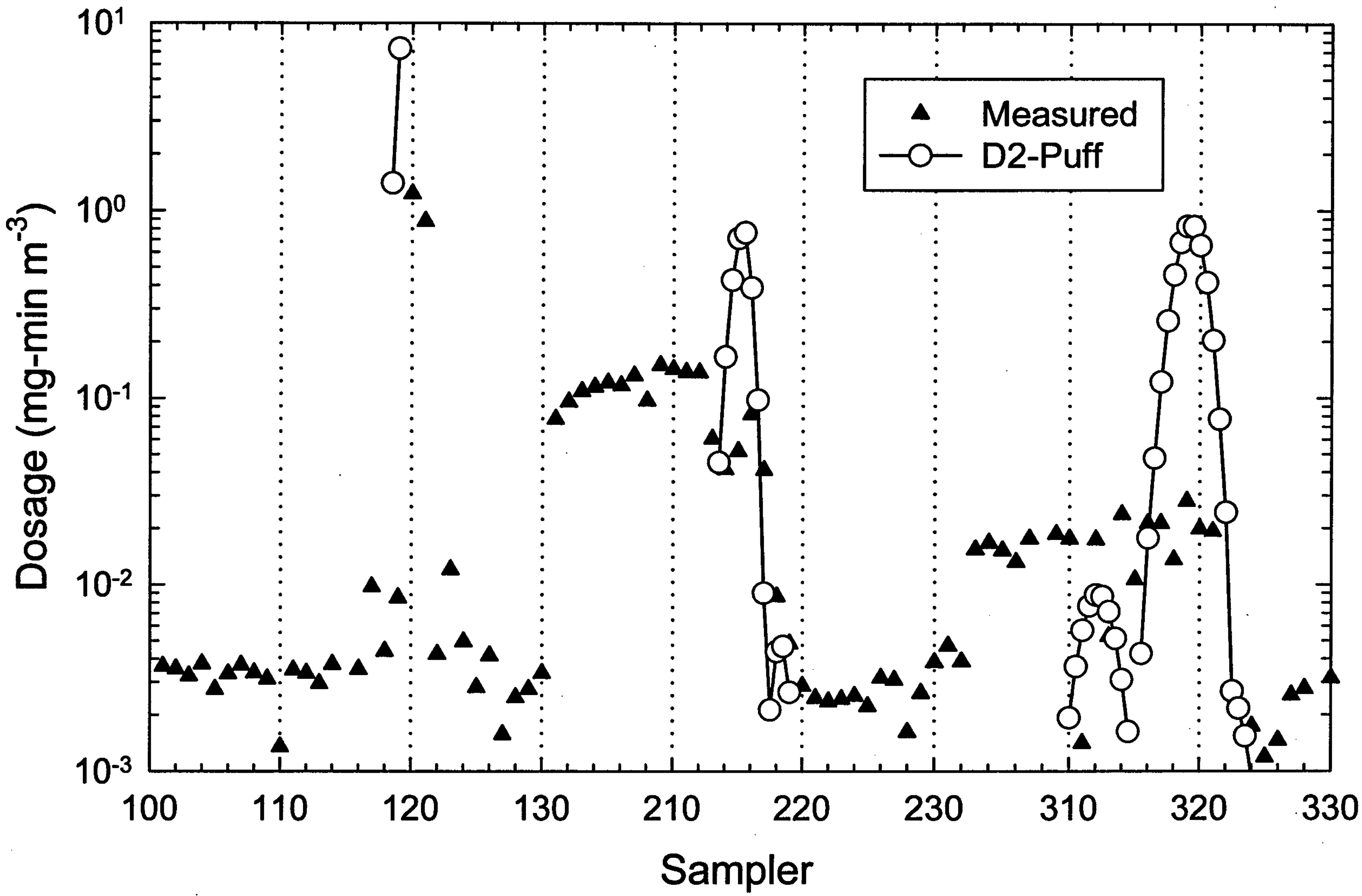

Figure B-1. Plot of measured versus D2-Puff calculated total SF_6 dosages at all three Dipole Pride 26 sampling lines for Trial 3. D2-Puff data points include an additional pseudo sampler between the field samplers to improve the plot definition.

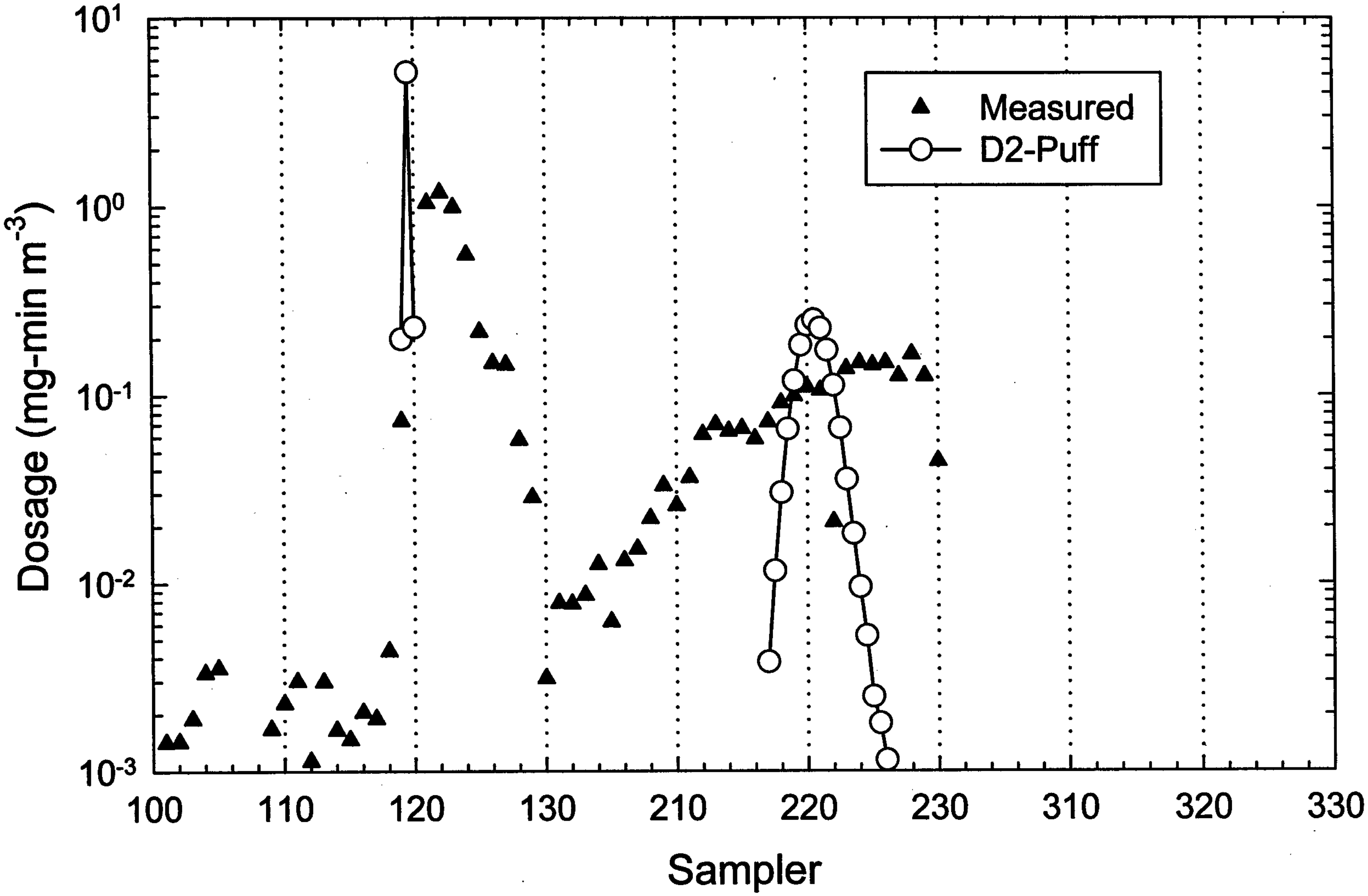

Figure B-2. Plot of measured versus D2-Puff calculated total SF_6 dosages at all three Dipole Pride 26 sampling lines for Trial 4A. D2-Puff data points include an additional pseudo sampler between the field samplers to improve the plot definition.

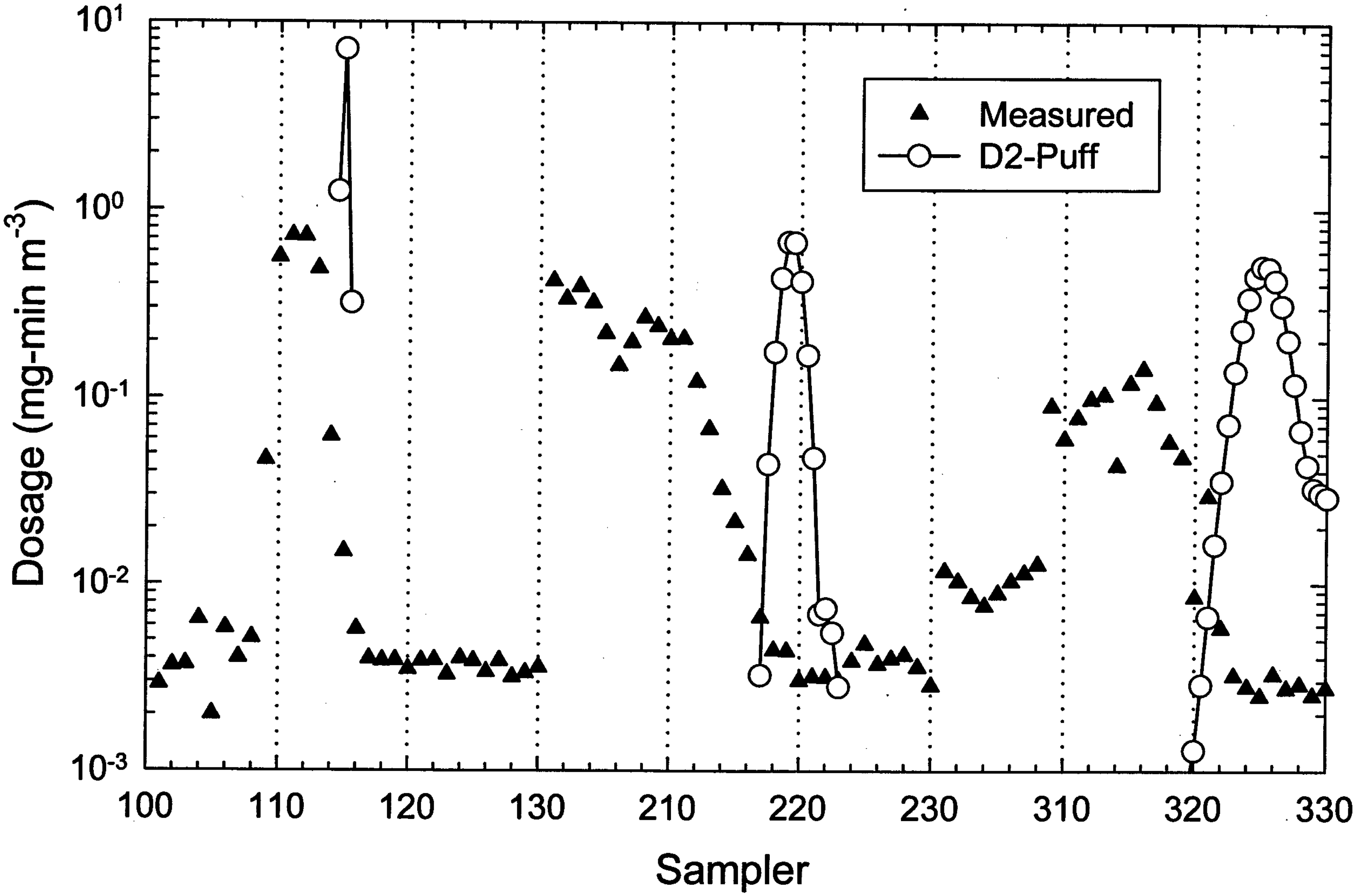

Figure B-3. Plot of measured versus D2-Puff calculated total SF_6 dosages at all three Dipole Pride 26 sampling lines for Trial 5. D2-Puff data points include an additional pseudo sampler between the field samplers to improve the plot definition.

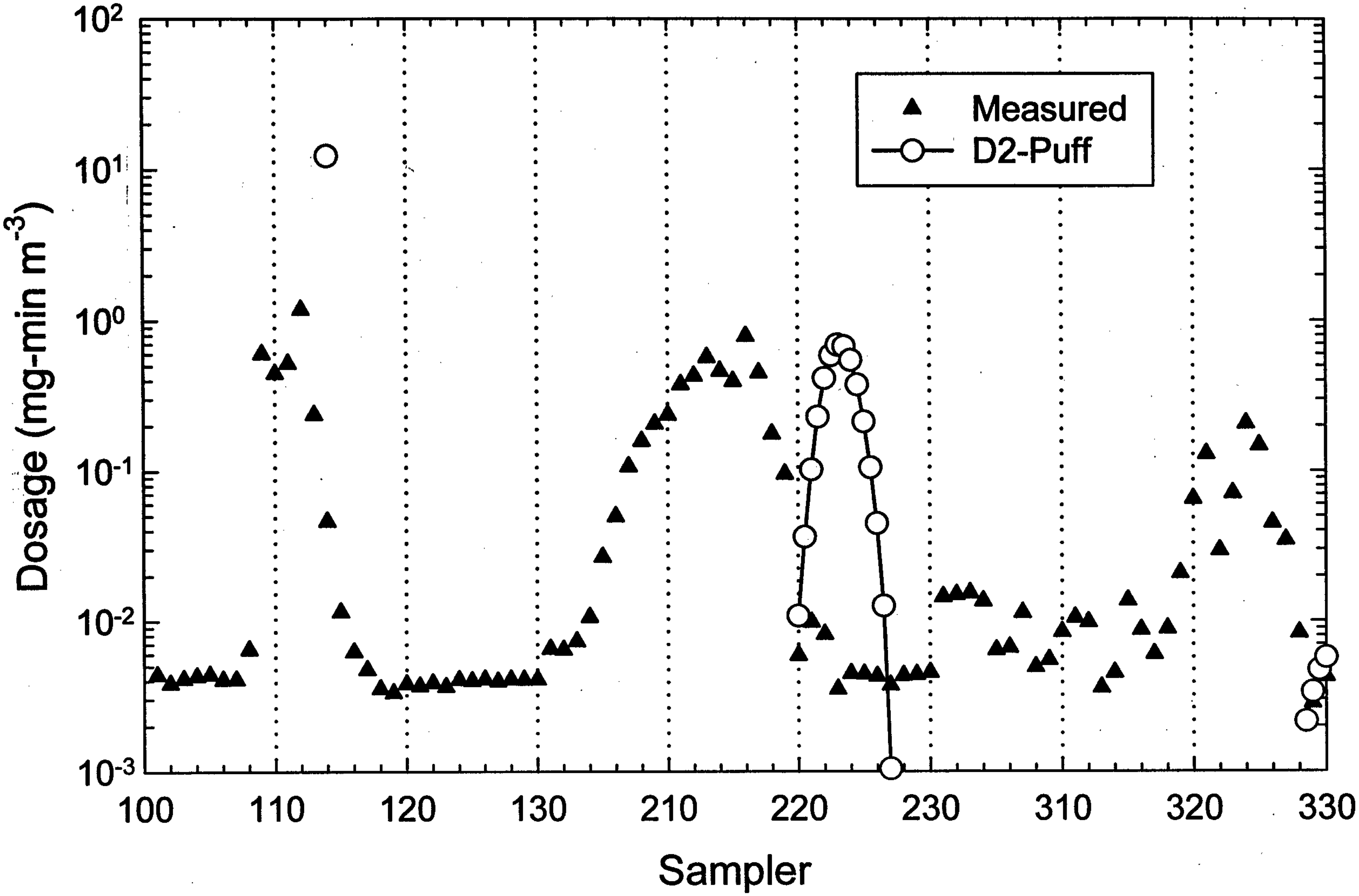

Figure B-4. Plot of measured versus D2-Puff calculated total SF_6 dosages at all three Dipole Pride 26 sampling lines for Trial 6. D2-Puff data points include an additional pseudo sampler between the field samplers to improve the plot definition.

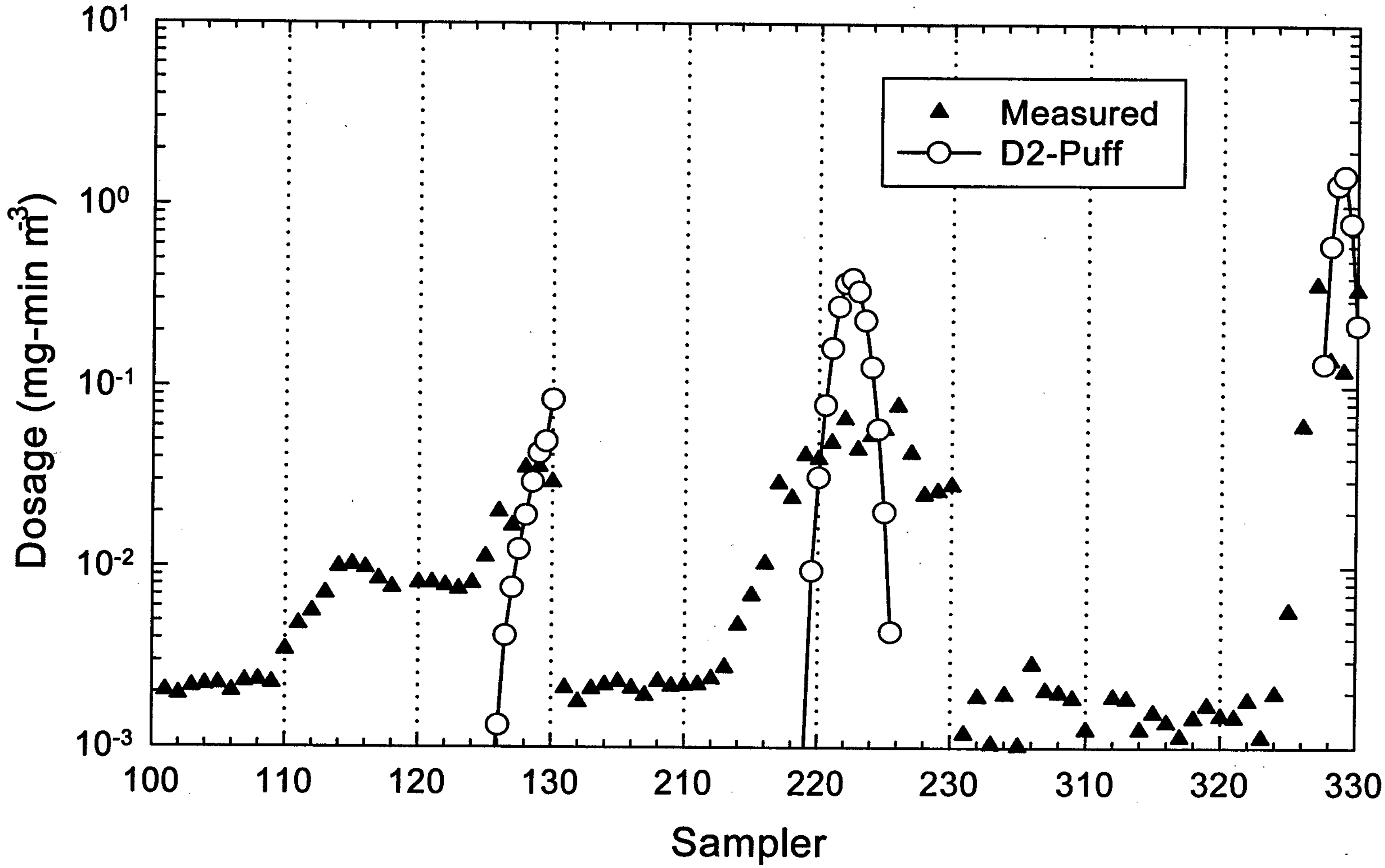

Figure B-5. Plot of measured versus D2-Puff calculated total SF_6 dosages at all three Dipole Pride 26 sampling lines for Trial 7. D2-Puff data points include an additional pseudo sampler between the field samplers to improve the plot definition.

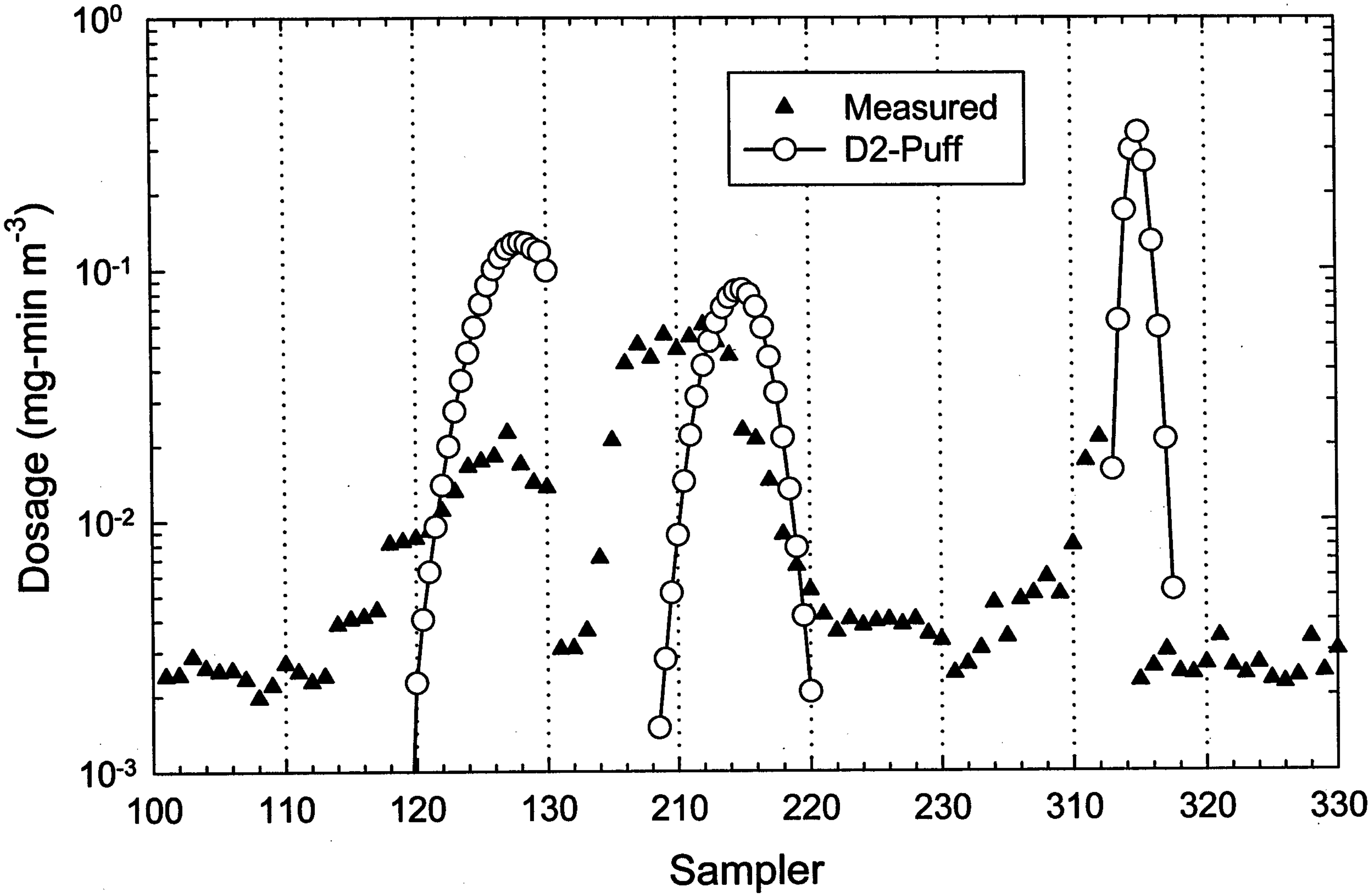

Figure B-6. Plot of measured versus D2-Puff calculated total SF_6 dosages at all three Dipole Pride 26 sampling lines for Trial 9. D2-Puff data points include an additional pseudo sampler between the field samplers to improve the plot definition.

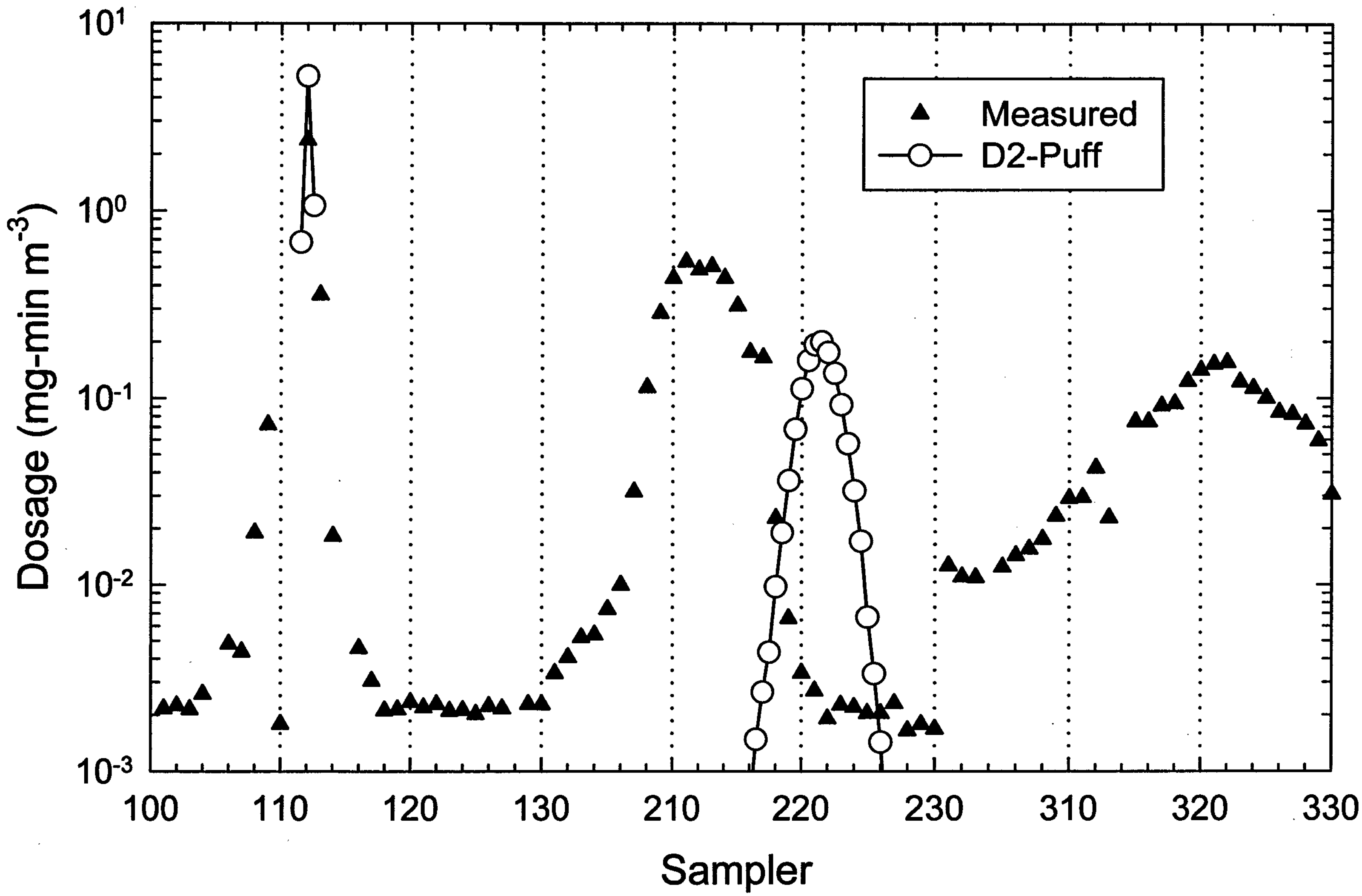

Figure B-7. Plot of measured versus D2-Puff calculated total SF_6 dosages at all three Dipole Pride 26 sampling lines for Trial 11B. D2-Puff data points include an additional pseudo sampler between the field samplers to improve the plot definition.

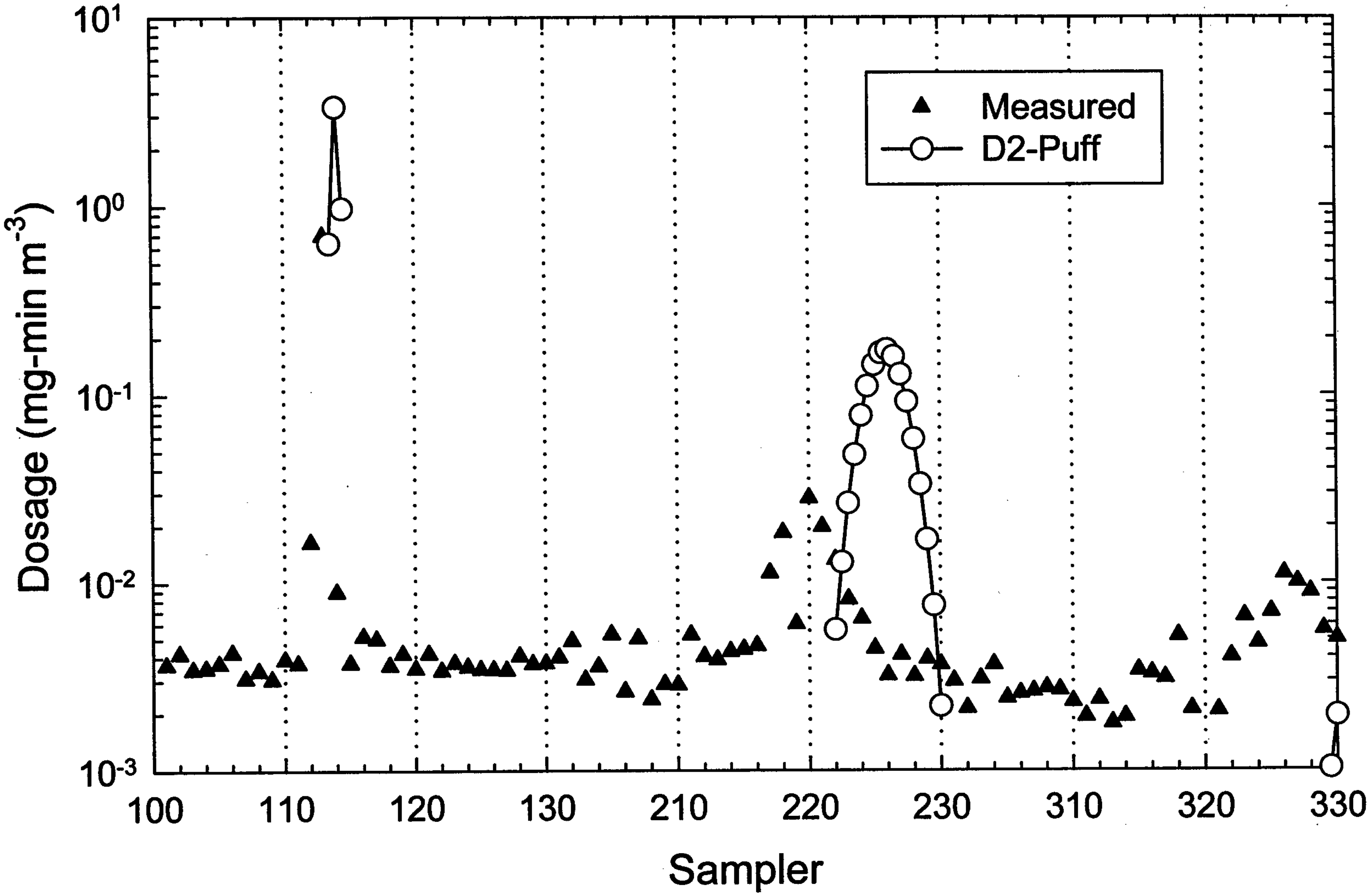

Figure B-8. Plot of measured versus D2-Puff calculated total SF_6 dosages at all three Dipole Pride 26 sampling lines for Trial 13. D2-Puff data points include an additional pseudo sampler between the field samplers to improve the plot definition.

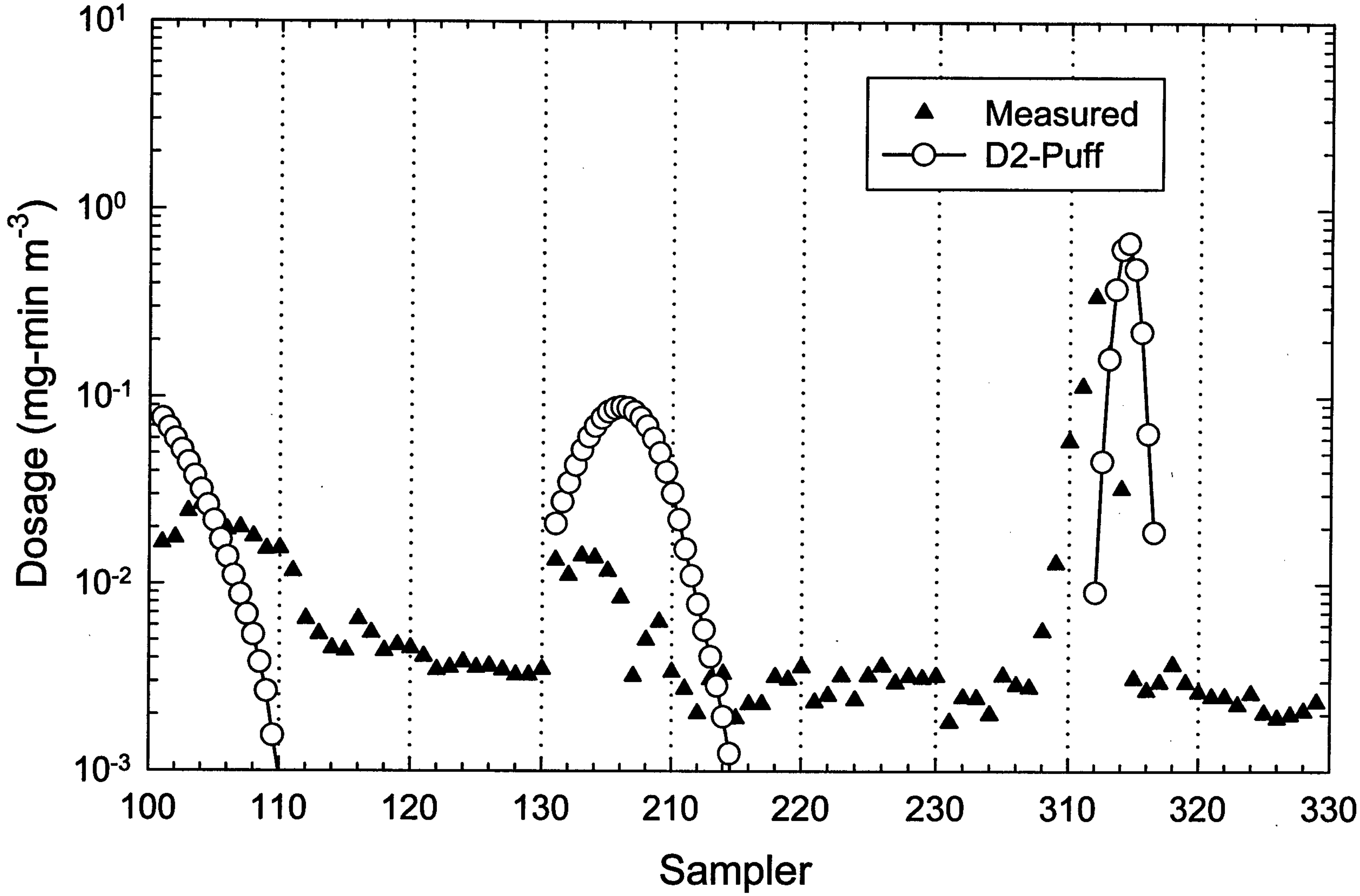

Figure B-9. Plot of measured versus D2-Puff calculated total SF_6 dosages at all three Dipole Pride 26 sampling lines for Trial 14. D2-Puff data points include an additional pseudo sampler between the field samplers to improve the plot definition.

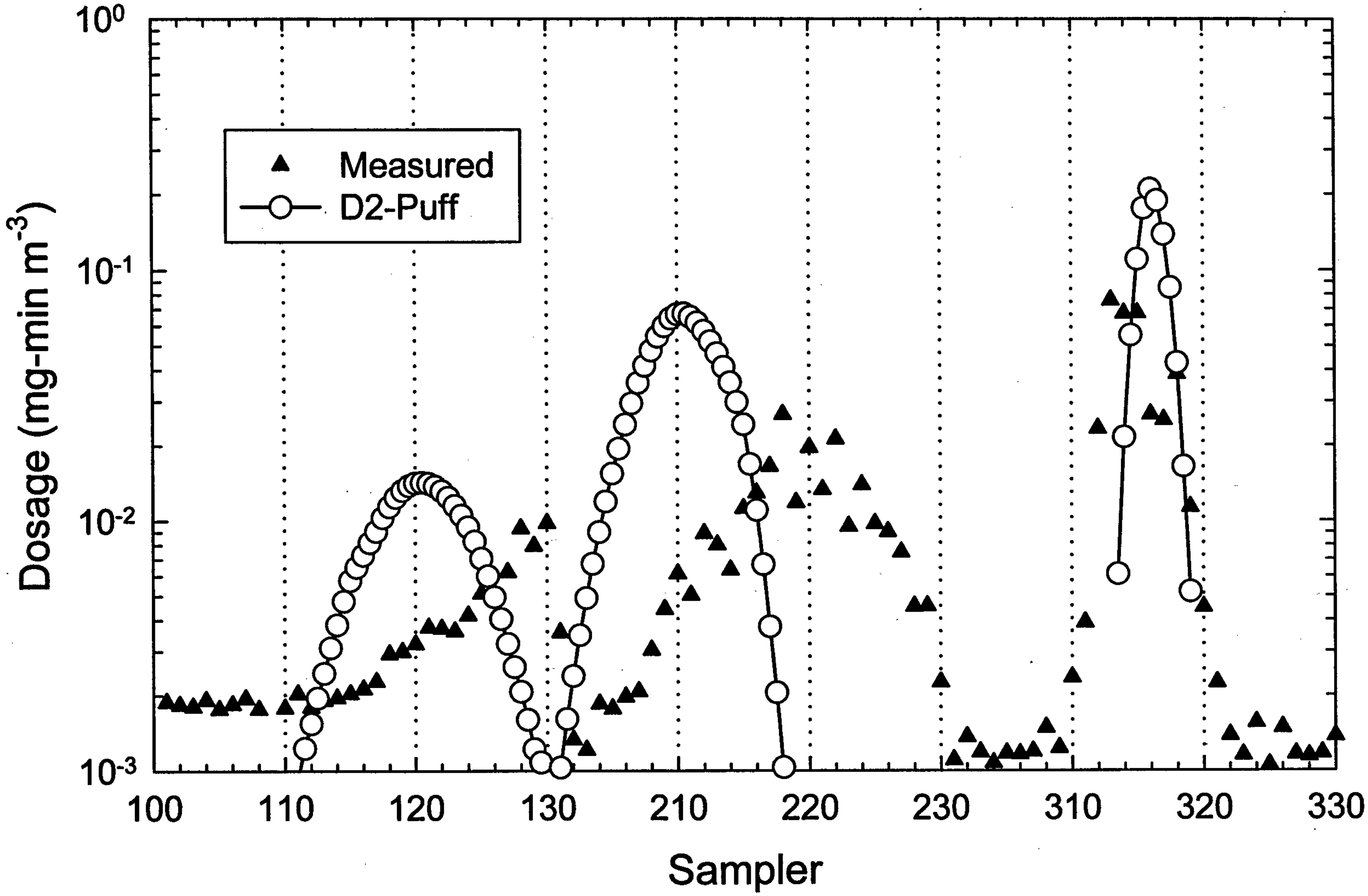

Figure B-10. Plot of measured versus D2-Puff calculated total SF_6 dosages at all three Dipole Pride 26 sampling lines for Trial 15A. D2-Puff data points include an additional pseudo sampler between the samplers to improve the plot definition.

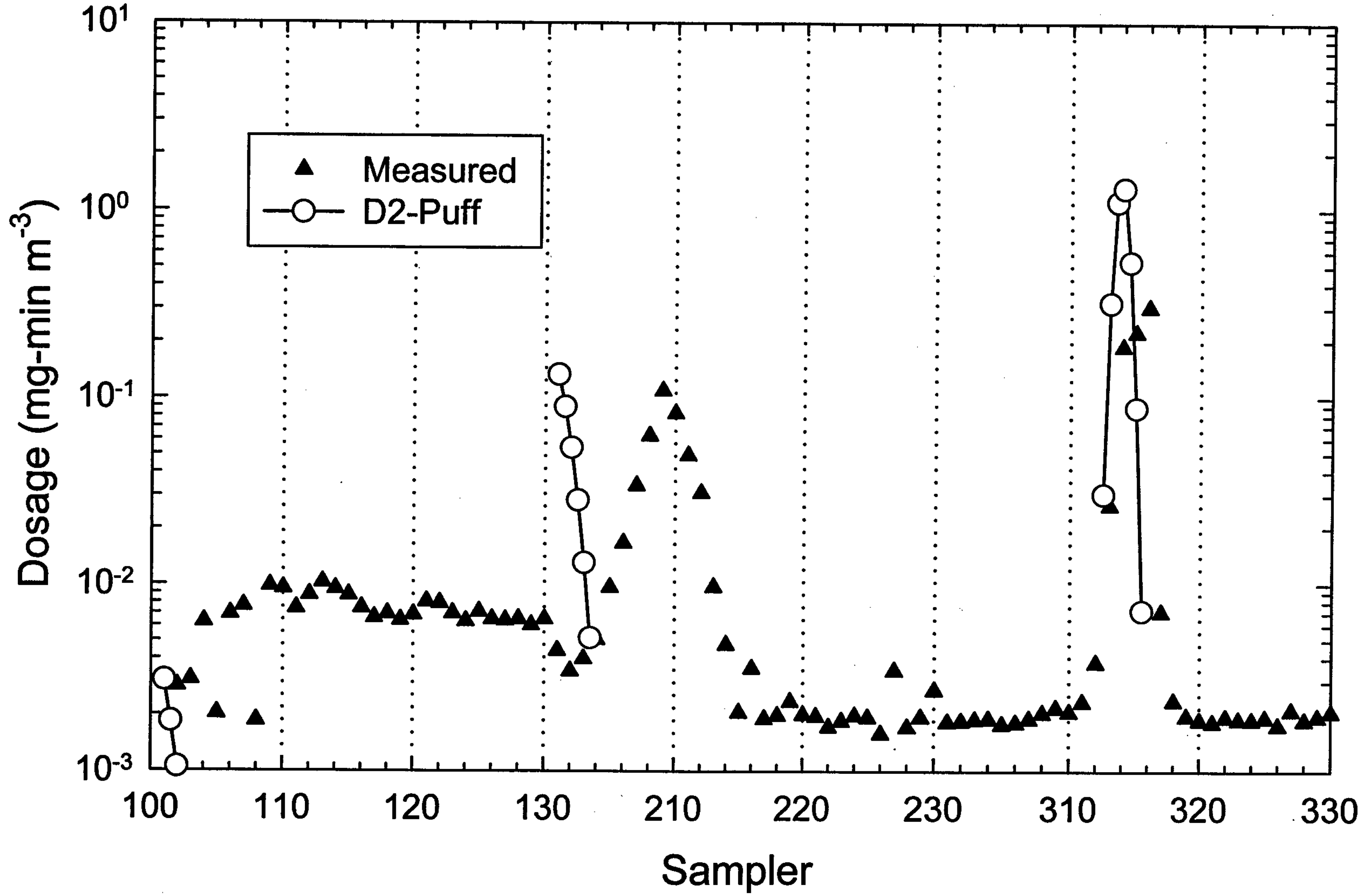

Figure B-11. Plot of measured versus D2-Puff calculated total SF_6 dosages at all three Dipole Pride 26 sampling lines for Trial 16B. D2-Puff data points include an additional pseudo sampler between the samplers to improve the plot definition.

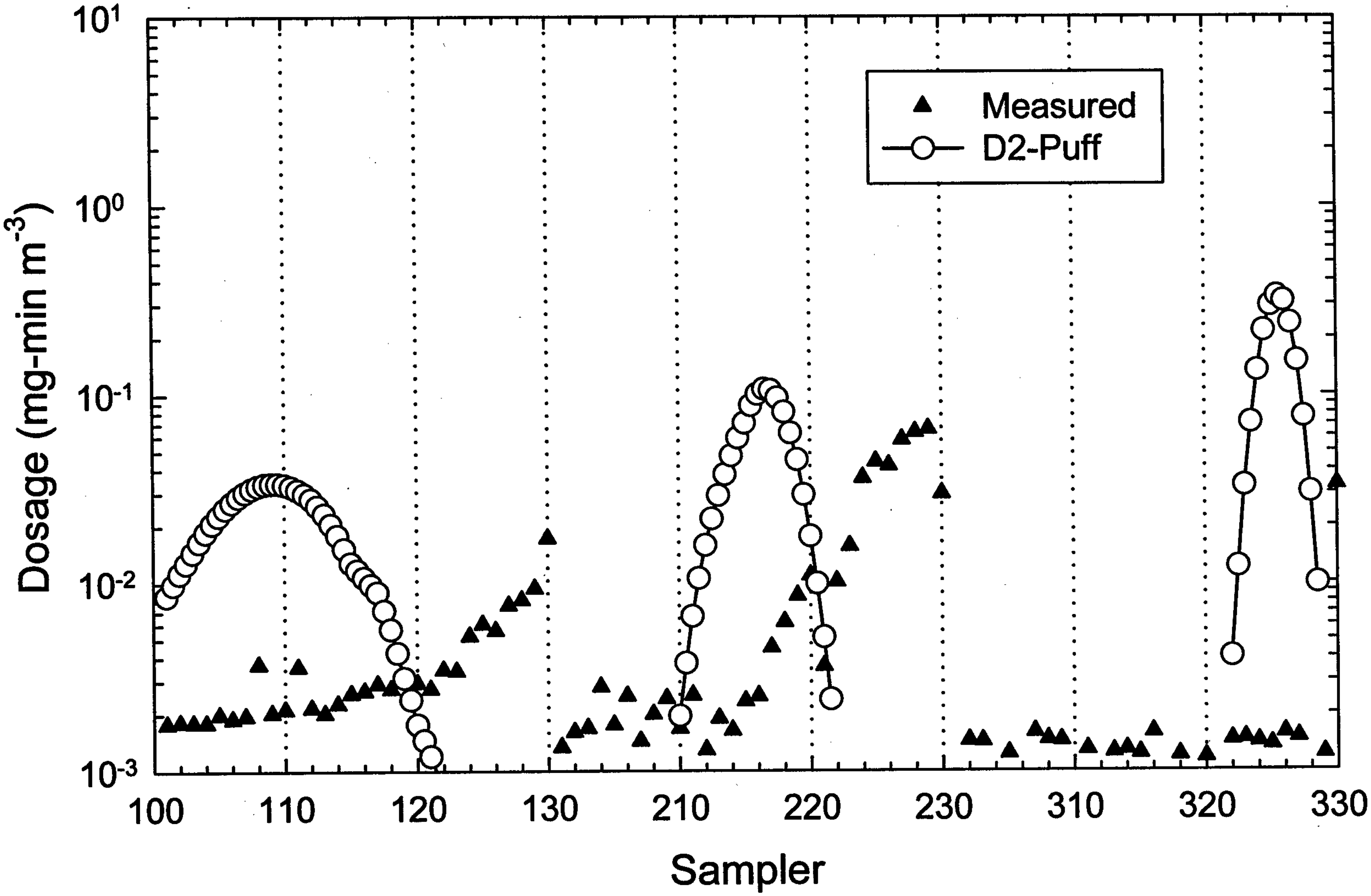

Figure B-12. Plot of measured versus D2-Puff calculated total SF_6 dosages at all three Dipole Pride 26 sampling lines for Trial 17A. D2-Puff data points include an additional pseudo sampler between the samplers to improve the plot definition.

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APPENDIX C. REFERENCES

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