Main menu

H13-15b
METHOD FOR COMPARISON OF LARGE EDDY SIMULATION-GENERATED WIND FLUCTUATIONS WITH SHORT-RANGE OBSERVATIONS

Nathan Platt[1], Dennis DeRiggi[1], Steve Warner[1], Paul Bieringer[2], George Bieberbach[2], Andrzej Wyszogrodzki[2] and Jeffrey Weil[2]

[1]Institute for Defense Analyses, Alexandria, Virginia, USA
[2]National Center for Atmospheric Research, Boulder, Colorado, USA

Abstract: The often prohibitive costs of comprehensive field trials coupled with relatively cheap and abundant computational power leads to a strong desire to use modelling tools to supplement field testing of system components. These modelling tools must be capable of reproducing key environmental variables present during field testing and require rigorous validation. The Virtual THreat Response Emulation and Analysis Testbed (VTHREAT) modelling system is composed of a suite of models designed to provide a virtual Chemical, Biological, Radiological and Nuclear (CBRN) release environment. Two key variables that VTHREAT is designed to realistically simulate are agent concentration and wind velocity. Typical validation studies compare mean predicted and observed quantities of interest such as mean concentration and mean wind speed and direction. This paper attempts to develop techniques to evaluate fluctuations – in particular, two-dimensional wind vector fluctuations.

Key words: *virtual environment, transport and dispersion, concentration fluctuations, wind fluctuations, validation methodology, p-values*

BACKGROUND

As computational power becomes more available and relatively cheap there is desire to use computer modelling tools to supplement field testing of system components. The use of such tools holds the promise of increasing the efficiency of the field tests that are conducted, aiding the evaluation of results obtained from such tests, and reducing costs. To support virtual testing, computer modelling systems must be capable of reproducing key environmental variables. Therefore, the modelling system requires rigorous analysis to support confident validation efforts.

The National Center for Atmospheric Research (NCAR) Virtual THreat Response Emulation and Analysis Testbed (VTHREAT) modelling system (Bieberbach, G., et al. 2010) is composed of a suite of models designed to provide a virtual Chemical, Biological, Radiological and Nuclear (CBRN) release environment. This tool has the potential to support a wide range of analyses including: (1) development, test, and evaluation of chemical-biological defence and meteorological sensors, algorithms, and architectures, (2) acquisition studies (e.g., analyses of alternatives, trade-off studies), (3) planning of field trials, to include aiding in the evaluation of field trial results, and (4) formulation and investigation of concepts of operation. VTHREAT components include virtual chemical, biological, and meteorological sensors as well as background models (e.g., particulates). Ultimately, all of these components require analyses in support of validation.

A key feature of VTHREAT is the potential to produce realistic, representative, meteorological fields and threat clouds that include fluctuating and meandering components. Validation of this key feature should enhance acceptance for many potential uses and should include detailed comparisons of physical models with specific sets of observations as well as statistical comparisons of predicted distributions to observations. Two key variables that VTHREAT is designed to realistically simulate at multiple locations are: 1) scalar agent concentration, and 2) wind velocity vectors. Typical validation studies compare mean predicted and observed quantities of interest (i.e., mean concentration and mean wind speed and direction) and in some cases might involve analysis of variances. In contrast, we decided to concentrate our effort on developing techniques to evaluate fluctuations ─ in particular, two-dimensional wind vector fluctuations.

METHODOLOGY

For scalar variables, such as concentration, a validation methodology to compare predicted scalar fluctuations at multiple locations with a limited set of experimental data was presented by Hill, et al., 2002 using p-values or “tail probabilities”. This method requires that a set of model realizations of an experimental observation can be created. This allows a probability distribution function of the scalar of interest at a large number of receptors (both space and time) to be computed. Next, an observed scalar and predicted distribution of fluctuations are used to calculate the percentile in the predicted distribution that exceeds the observed value (p-value or “tail probability”). If the p-values are uniformly distributed, then the predicted distribution is consistent with the observations.

An extension of the p-values methodology described above to two-dimensions was proposed in Fries, 2001 and Comfort, et al., 2002. It involves either parametric or non-parametric constructions of equal probability contours in two dimensions. The scalar p-value is then calculated by integrating the probability outside of the equal probability contour where the particular observation resides. By testing whether or not the distribution of resulting p-values (from nominally independent observations) are uniformly distributed, one can determine if the predicted distribution is consistent with observations. We note that some caution should be exercised when using this approach. To demonstrate, assume that the two-dimensional modelled distribution is a bivariate Normal distribution centred at the origin with $\sigma_x = \sigma_y = 1$. We write this as $(X,Y) = (N(0,1),N(0,1))$ where $N(0,1)$ stands for normal distribution with $\mu = 0$ and $\sigma = 1$ with X and Y independent. For any observation (x,y) the scalar p-value is given by $e^{-(x^2+y^2)/2}$. If observations come from the same two-dimensional distribution (X,Y) then the calculated p-values are uniformly distributed as demonstrated in Figure 1. Now, consider that the observations are coming from the scalar distribution defined by $Z = \sqrt{X^2+Y^2}$. We note that Z is a Rayleigh distribution with parameter σ = 1. Please recall that standard deviation of this distribution is $\sigma\sqrt{2-\frac{\pi}{2}}$.Then calculated p-values are still uniformly distributed as shown in Figure 2.

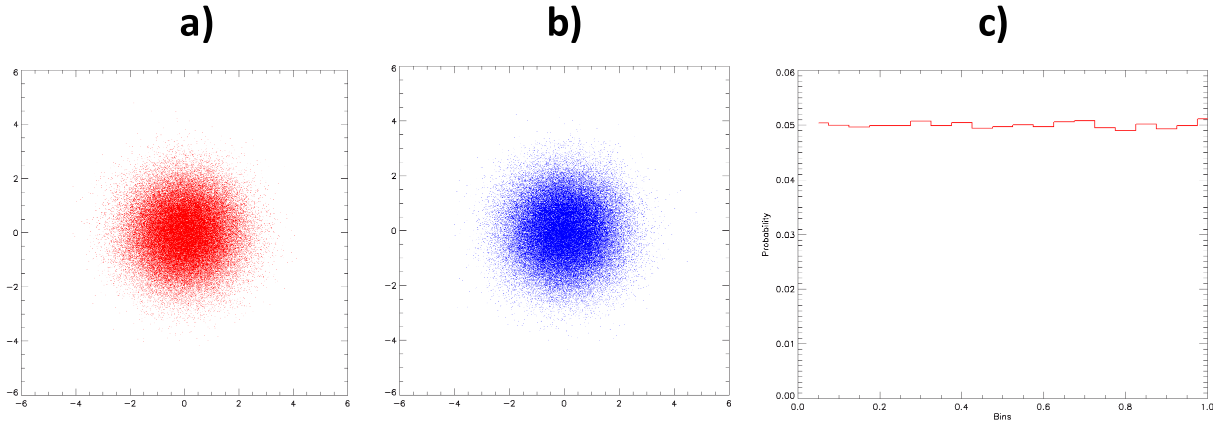

Figure 1. Demonstration of distribution of scalar p-values when modelled and observed distributions are bivariate normal: a) depicts modelled distribution, b) depicts observations, and c) shows distribution of scalar p-values which is close to theoretical uniform distribution.

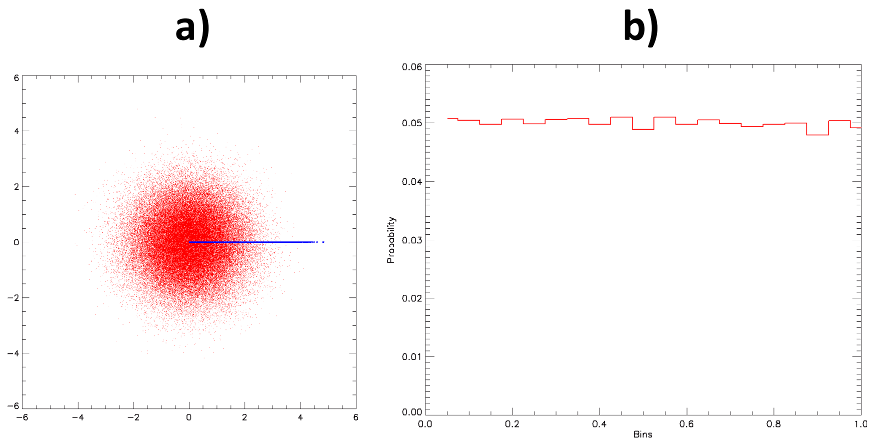

Figure 2. Demonstration of distribution of scalar p-values when modelled distribution is bivariate normal and observed distribution is Rayleigh: a) depicts predictions (in red) and observations (in blue), and b) shows distribution of scalar p-values which is close to theoretical uniform distribution.

To better understand the example described above, we note that individual scalar p-values based on contouring the two-dimensional probability density function do not vary along equal probability contour lines. This allowed us to construct a one-dimensional illustration by specifically selecting observations along a ray emanating from the origin with a probability density function defined by angular projection of circular contours of normal bivariate distribution onto the radial ray. These examples need not be one-dimensional – one could easily construct two-dimensional observations by allowing some variation in angle along circular contours that would still yield a uniform distribution of p-values.

Intuitively, one needs to extend the definition of scalar p-values to two-dimensional p-values to be able to capture the full dynamics of potential two-dimensional distribution functions. We’re still working out some general details describing classes of two-dimensional distribution functions that are amendable to this and will present a simplified case here. Assume that we have two continuous independent random variables X and Y. Then the joint distribution function is defined by $f_{X,Y}(x,y) = f_X(x)\,f_Y(y)$ for all (x,y). For any observation (x,y) we could calculate two separate p-values called p_x and p_y which are based on individual independent random variables X and Y. It can be shown, that if two-dimensional p-values (p_x,p_y) are uniformly distributed in the unit square $[0,1]\times[0,1]$ then the underlying observations are consistent with the joint probability defined by independent random variable X and Y. Furthermore, if there is a linear and invertible transformation that takes random variables X' and Y' into X and Y, and if calculated two dimensional p-values (p_x,p_y) are uniformly distributed in the unit square, then the underlying observations are consistent with the joint probability function defined by random variables X' and Y'.

Figures 3 and 4 demonstrate the application of two-dimensional p-values to the examples discussed earlier and shown in Figures 1 and 2, respectively. As expected, the two-dimensional p-values shown in Figure 3 are uniformly distributed in $[0,1]\times[0,1]$, while the two-dimensional p-values shown in Figure 4 reduce to non-uniformly, one-dimensionally distributed p_x values and constant p_y values.

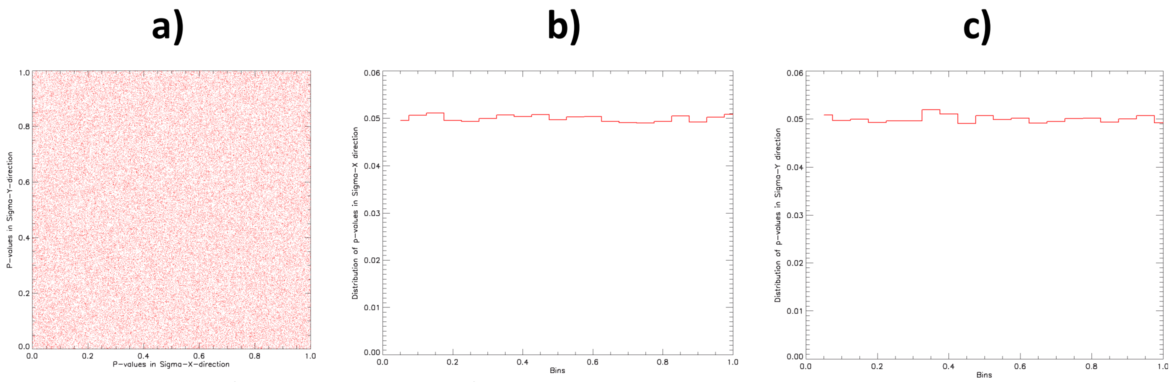

Figure 3. Demonstration of two-dimensional p-values for the case when predictions and observations are drawn from a bivariate normal distribution: a) shows calculated two-dimensional p-values that *look* uniformly distributed in the unit square, b) and c) show individual distribution of p_x and p_y values, respectively, which appear uniform in one-dimension. Please note that no formal test was applied to check for uniformity of the two-dimensional p-values and uniformity of individual p_x and p_y values *does not* necessary imply uniformity of the two-dimensional p-values.

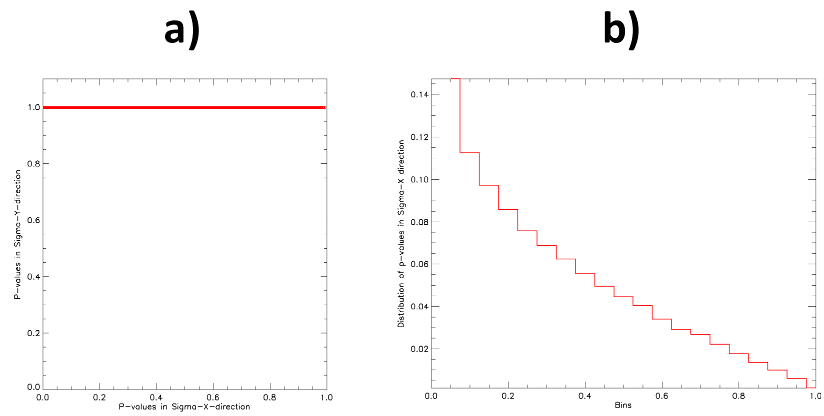

Figure 4. Demonstration of two-dimensional p-values for the case when predictions are drawn from a bivariate normal distribution and observations are drawn from Rayleigh distribution: a) shows calculated two-dimensional p-values that are constant in y-direction, b) shows individual distribution of p_x values which is clearly different from a uniform distribution.

Given a large finite set of VTHREAT predicted wind vector fluctuations $\{\underline{w}_i = (u_i, v_i) \mid i = 1..N\}$ that could be used to define a continuous probability density function for two random variables (*U*,*V*) and another set of observed wind vector fluctuations (e.g., samples) $\{\underline{\mathbf{s}}_j = (u_j^{(s)}, v_j^{(s)}) \mid j = 1..M\}$, we propose the following procedure to ascertain whether or not samples $\underline{s}_j$ are consistent with being drawn from random variables (*U*,*V*):

1. Find a rotation matrix **R** that decorrelates predictions $\underline{w}_i$. Apply this rotation matrix **R** to both predictions $\underline{w}_i$ and samples $\underline{s}_j$. For simplicity, assume that the new decorrelated sets use the same name.
2. Test transformed $\underline{w}_i=(u_i,v_i)$ to see if u_i and v_i are independent. If u_i and v_i are not independent then the procedure to calculate two-dimensional p-values described earlier might not be applicable.
3. Calculate two-dimensional p-values (p_x^i, p_y^i) using transformed samples $\underline{s}_j$.
4. Test to see if two-dimensional p-values (p_x^i, p_y^i) are uniformly distributed in [0,1]×[0,1]

We're still working out details about particular statistical tests to be applied in steps 2 and 4. We note that failure in step 2 involving testing for independence of the transformed predictions might result in unpredictable conclusions based on this procedure.

APPLICATION TO VTHREAT WIND VECTOR FLUCTUATION PREDICTIONS

VTHREAT was used to simulate trial 54 from the Fusing Sensor Information from Observing Networks (FUSION) Field Trial 2007 (FFT 07) (Storwold, 2007). This highly instrumented test was conducted at the U.S. Army's Dugway Proving Ground (DPG) and was designed to collect data to support the further development of prototype source term estimation algorithms. As part of the meteorological instrumentation of the test site, 40 Portable Weather Information Display Systems (PWIDS) were arranged on a regular rectangular grid to collect wind speed and direction, temperature, relative humidity and pressure at 2 meters above ground at 10 second time intervals. Trial 54 involved the continuous release of propylene gas for 10 minutes from a single source. Propylene concentrations were continuously sampled at 50Hz at 100 digiPID (digital photoionization detector) and 20 UVIC (ultraviolet ion collector) sensors densely arranged at the test site. Out of the 40 deployed PWIDS, only 39 collected useable data.

VTHREAT predictions, including wind speed and direction at PWIDS locations, were started ten minutes prior to tracer release and continued for 1800 seconds. VTHREAT output resolution was set to 1 sec. Twenty VTHREAT realizations of trial 54 were performed. To match the frequency of observations, VTHREAT output wind measurements were bin averaged to 10 seconds. VTHREAT was allowed to settle for 600 seconds to spin up its turbulence before wind comparisons with observations were performed. Thus, there were a total of ([1800-600]/10+1)×39 = 4719 observed wind speed and direction measurements available for the comparison (i.e., number of p-values that could be calculated). Before any analysis and averaging, both VTHREAT predictions and PWIDS observation of wind speed and direction were transformed into (*u*,*v*) space. To calculate wind fluctuations in (*u*,*v*), a 60-second running window average was constructed for each individual PWIDS data stream (VTHREAT or observations) and fluctuations were calculated with respect to this average. The resulting predicted and observed fluctuations were plotted at each available time at 10 second increments and visually compared. Figure 5 shows a few example plots for VTHREAT predicted (20 realizations in red) and observed (in black) wind fluctuations.

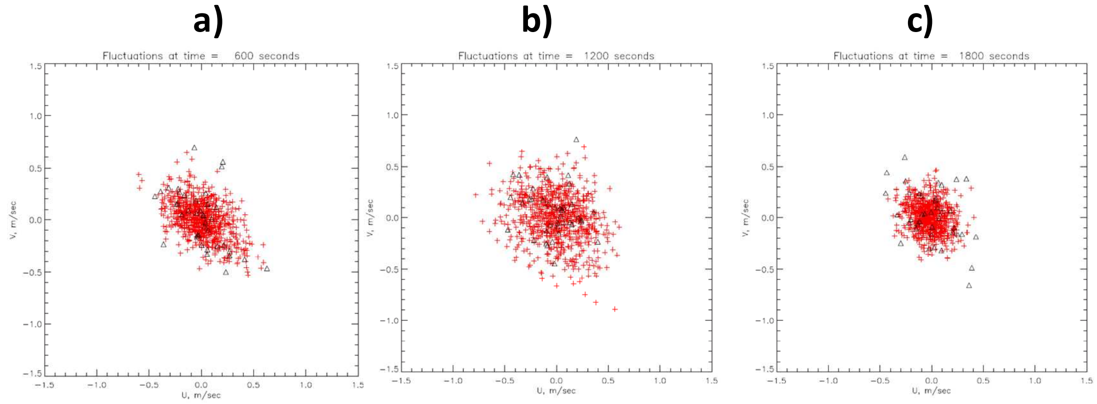

Figure 5. Examples of VTHREAT predicted (20 realizations in red) and observed (in black) wind fluctuations for a) 600 sec, b) 1200 sec, and c) 1800 sec after the start of the simulation.

To simplify the calculation of scalar and two-dimensional p-values, for this demonstration of the methodology and based on visual inspection of Figure 5, we assume that the VTHREAT-based fluctuations are drawn from an elliptical-normal distribution. Additionally, we note that potentially there is a significant spatial and temporal correlation between individual observations (i.e., nearby PWIDS observations and VTHREAT predictions are correlated in space and time) that we will ignore for now. We note that the elliptical-normal distribution assumption and rotation of the ellipse based on computed correlation between individual components of this distribution to align the axis of the ellipse with coordinate axis results in de-correlated normal distributions along the axis which are independent. Figure 6 depicts p-values calculated as follows: a) depicts scalar p-values based on the *distance*, b) depicts two-dimensional (p_x,p_y) values, c) depict distribution of individual p_x values, and d) depicts distribution of individual p_y values.

While Figure 6b seems to indicate uniformly distributed two dimensional p_x and p_y values, Figure 6c and 6d along with Figure 6a indicate a slight peak in the distribution near the origin. We note that while uniformly distributed individual p_x and p_y does not necessarily imply uniform distribution of two-dimensional (p_x,p_y) values, non-uniformity of either individual p_x or p_y values does imply non-uniformity in the two-dimensional (p_x,p_y) values. We further investigate two-dimensional (p_x,p_y) values by constructing a frequency table in 0.05 increments in Table 1. The values that are highlighted in light/dark red cells are the top 20 frequencies and frequencies whose counts exceeded 30. Looking at this table, we infer that indeed the two-dimensional p-values have a primary peak near the origin and secondary peaks along the axes where the value of either p_x or p_y is near 0.

DISCUSSIONS AND FUTURE WORK

In this paper we demonstrated a potential extension of a scalar p-value methodology to statistically compare predicted distributions with a limited set of observations to two-dimensional (p_x,p_y) p-values. An initial application of these techniques to help validate wind fluctuations predicted by VTHREAT was shown as well. The distribution of VTHREAT predicted wind fluctuations visually appears close to the observed fluctuations (i.e., it appears that the observations could have been randomly drawn from the predicted distributions. Nevertheless, two-dimensional (p_x,p_y) p-values indicate a slight diversion from a uniform distribution in the unit square [0,1]×[0,1] around the edges and the origin. There are a number of potential reasons for this. First, to simplify the calculation of p-values, an elliptical-normal distribution of VTHREAT predictions was assumed. Additionally, there is potential for a significant spatial and temporal correlation between neighbouring PWIDS that could affect the resulting p-value estimates. Future work with VTHREAT-simulated results will replace the elliptical-normal distribution assumption with a non-parametric estimation of the cumulative probability function that will be used to estimate p-values. Additionally, we'll consider several data reduction techniques to attempt to remove spatio-temporal correlations that might be inherent in neighbouring PWIDS observations and simulations. In addition, relevant statistical tests both for independence of the rotated two-dimensional VTHREAT wind fluctuations and uniformity of the two-dimensional p-values will be developed and applied.

Table 1. Two-dimensional (p_x,p_y) p-values tables. Each entry correspond to number if (p_x,p_y) values that fall into appropriate bin that are selected in 0.05 increments. Boundary cells shaded in gray are bin values, cells shaded in light/dark read are top 20 values and cells shaded in dark read are frequencies whose count exceeds 30.

	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50	0.55	0.60	0.65	0.70	0.75	0.80	0.85	0.90	0.95	1.00
0.05	**52**	**36**	26	**39**	**33**	25	16	22	22	25	16	18	24	14	14	24	23	26	21	20
0.10	22	19	8	13	11	16	10	14	11	12	12	9	18	20	13	16	11	11	14	13
0.15	20	12	16	14	17	13	8	15	12	12	11	10	16	8	19	10	13	17	13	14
0.20	15	14	14	12	12	14	13	11	16	16	12	6	11	13	7	9	13	12	6	16
0.25	15	17	9	13	12	13	15	11	12	12	13	17	11	14	9	10	10	6	5	12
0.30	16	17	7	14	16	14	16	12	5	8	7	16	7	11	9	3	20	16	15	10
0.35	18	16	7	13	10	11	10	15	14	10	8	16	9	8	13	13	13	7	16	9
0.40	20	9	11	11	14	10	14	18	10	8	14	9	7	11	13	14	13	14	15	10
0.45	11	7	9	6	12	11	12	7	13	5	9	10	7	17	18	10	9	8	11	14
0.50	19	14	14	15	13	11	11	10	3	11	9	11	11	11	8	7	16	7	6	7
0.55	20	10	9	15	12	11	12	5	8	4	11	9	8	8	17	11	10	12	13	7
0.60	22	6	14	22	9	8	15	10	11	11	11	8	8	9	10	14	10	9	15	12
0.65	15	13	11	8	10	15	10	8	12	15	7	22	9	11	7	9	6	9	9	12
0.70	17	10	3	5	12	9	8	9	15	13	10	12	18	7	4	8	11	9	12	14
0.75	6	6	13	7	8	8	11	11	5	11	9	14	9	6	12	5	11	6	6	10
0.80	14	13	14	8	11	8	10	8	16	10	13	13	10	16	9	9	10	8	14	9
0.85	15	14	13	12	14	10	8	15	18	18	7	5	11	8	7	10	7	10	7	13
0.90	15	7	5	9	9	10	9	8	12	10	8	4	13	7	15	8	12	9	8	7
0.95	14	6	8	10	7	14	4	5	6	11	12	18	12	11	7	14	13	8	8	6
1.00	16	7	8	8	3	8	10	10	9	8	4	7	18	14	10	9	9	11	14	11

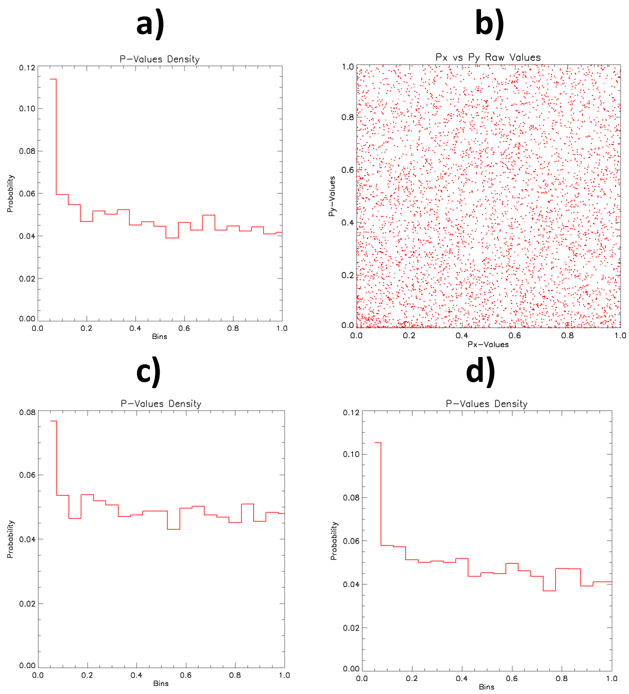

Figure 6. Calculated p-values: a) scalar p-values based on the distance, b) two-dimensional (p_x,p_y) values, c) distribution of individual p_x values and d) distribution of individual p_y values.

Acknowledgements
This effort was supported by the Defense Threat Reduction Agency with Dr. John Hannan as the project monitor and Institute for Defense Analyses professional development program. The views expressed in this paper are solely those of the authors.

REFERENCES

Bieberbach, G., Bieringer, P.E., Wyszogrodzki, A., Weil, J., Cabell, R., Hurst, J., and J. Hannan, 2010: *Virtual chemical and biological (CB) agent data set generation to support the evaluation of CB contamination avoidance systems*, The Fift Symposium on Computational Wind Engineering (CWE 2010), Chapel Hill, North Carolina.

Comfort, G.C., Rivolo, A.R, and A. Fries, 2002: *Validation of Missile Fly-Out Simulations*, Institute for Defense Analyses, paper P-3697.

Hill, R., Lowles, I., Auld, V., and T. Parker, 2001: *Probabilistic Evaluation of Models for the Atmospheric Dispersion of Effluents Released From a Complex Site*, Proceedings of the 8th Int. Conf. on Harmonization within Atmospheric Dispersion Modelling for Regulatory Purposes, Sofia, Bulgaria.

Fries, A., 2000: *Another "New" Approach For "Validating" Simulation Models*, American Statistical Association 2000 Proceedings of the Section on Physical and Engineering Sciences, Indianapolis, IN, August 13-17, pp. 61-66.

Storwold, D.P, 2007: *Detailed test plan for the Fusing Sensor Information from Observing Networks (FUSION) field trial 2007 (FFT 07*. West Desert Test Center, U.S. Army Dugway Proving Ground, WDTC Document No. WDTC-TP-07-078.