CHEMICAL ENGINEERING TRANSACTIONS
VOL. 31, 2013
Guest Editors: Eddy De Rademaeker, Bruno Fabiano, Simberto Senni Buratti
ISBN 978-88-95608-22-8; ISSN 1974-9791
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at: www.aidic.it/cet
DOI: 10.3303/CET1331021

Sensitivity Analysis of Dispersion Models for Jet Releases of Dense-Phase Carbon Dioxide

Simon E. Gant*[a], Adrian Kelsey[a], Kevin McNally[a], Henk Witlox[b], Mike Bilio[c]

[a] Health and Safety Laboratory, Harpur Hill, Buxton, SK17 9JN, UK
[b] DNV Software, Palace House, 3 Cathedral Street, London SE1 9DE, UK
[c] Health and Safety Executive, Redgrave Court, Merton Road, Bootle, L20 7HS, UK
simon.gant@hsl.gov.uk

A global sensitivity analysis is performed on Phast's dispersion model for simulating jet releases of dense-phase carbon dioxide (CO_2). The releases studied consist of above-ground, unconfined, horizontal, steady-state orifice discharges, with orifices ranging in diameter from ½ to 2 inch (12.8 to 50.4 mm), and the liquid CO_2 reservoir maintained at between 100 and 150 bar and close to ambient temperatures. These scenarios are relevant in scale to leaks from large diameter above-ground pipes or vessels.
The sensitivity analysis is performed using a Gaussian emulator that is constructed from 100 Phast simulations. The parameters varied include the reservoir temperature and pressure, orifice size, wind speed, humidity, surface roughness and height of the release. The emulator is used to identify the input parameters that have a dominant effect on the dispersion distance of the CO_2 cloud. The whole analysis (including the Phast simulations) runs on a laptop computer in less than 30 minutes.
The study demonstrates that Bayesian analysis of model sensitivity can be conducted rapidly and easily on consequence models such as Phast. There is the potential for this to become a routine part of hazard assessment.
A more limited set of results is also presented using the Computational Fluid Dynamics (CFD) software, ANSYS-CFX13, which is used to examine the effect of the solid CO_2 particle size, which cannot be examined using Phast. The results show that the CO_2 particle size has a relatively minor effect on the dispersion distance in the scenarios considered here.

1. Introduction

The next decade is likely to see the rapid growth of Carbon Capture and Storage (CCS) infrastructure both in the UK and internationally. As a consequence, significant efforts are currently being directed towards understanding the hazards posed by atmospheric discharges of high-pressure CO_2. In many of the planned UK CCS infrastructure projects, the CO_2 will be transported or stored in a dense-phase state, i.e. as a liquid or supercritical fluid (the critical temperature of CO_2 is 31 ºC). In a planned or accidental release from a CO_2 pipeline or compressor station, the CO_2 will rapidly expand from the operating conditions and change state into a mixture of gaseous and solid CO_2 at atmospheric pressure. This complex release behaviour presents novel challenges for consequence modelling and risk assessment, and there remain a number of uncertainties associated with the depressurisation behaviour of pipelines, the CO_2 particle size and the deposition of solid CO_2.
Over the last five years, there have been a number of publications examining the release and dispersion of CO_2. The study by Dixon et al. (2012) is particularly relevant to the present work as it involved a comparison of three different dispersion models: the integral model in Shell FRED and two different CFD codes, OpenFOAM and ANSYS-CFX. Both the FRED and the OpenFOAM models assumed that the two-phase flow was in homogeneous equilibrium, i.e. the CO_2 particles and surrounding vapour shared the same temperature and velocity, whilst the ANSYS-CFX model used a particle-tracking approach. Predictions from the three models were in generally good agreement with the measurement data. The ANSYS-CFX model used in that study is the same as that used in the present paper.

Please cite this article as: Gant S., Kelsey A., McNally K., Witlox H. and Bilio M., 2013, Sensitivity analysis of dispersion models for jet releases of dense-phase carbon dioxide, Chemical Engineering Transactions, 31, 121-126 DOI: 10.3303/CET1331021

DNV Software has produced three key papers on CO_2 release and dispersion modelling. In the first of these, Witlox et al. (2009) described an extension to PHAST version 6.53.1 to account for the effects of solid CO_2. The modifications consisted principally of changing the way in which equilibrium conditions were calculated in the expansion of CO_2 to atmospheric pressure, to ensure that below the triple point the fluid conditions followed the sublimation curve in the phase diagram. In the second paper, Witlox et al. (2011) reported the results of a sensitivity analysis for both liquid and supercritical CO_2 releases from vessels and pipes with the revised PHAST version 6.6 model. The sensitivity analysis was performed using a local "one-at-a-time" approach to model input variation, where each parameter was varied in turn whilst holding all other parameters fixed. In contrast, in the global sensitivity analysis presented here, all of the parameters are varied simultaneously to calculate the effect of each parameter over the full range of other input parameters. In the third paper by Witlox et al. (2012), the results of the model validation study using measurements from a series of field-scale tests originally commissioned by BP and Shell were published.

In addition to these CO_2 dispersion studies, a comprehensive model sensitivity analysis of Phast for three different atmospheric releases of toxic substance was reported recently by Pandya et al. (2012). This involved running Monte-Carlo (MC) experiments on Phast directly, with sample sizes of 20,000 simulations and computing times of around 24 h, using several computers in parallel.

The principal contribution of the present paper is a global sensitivity analysis of the Phast model for simulating atmospheric dispersion of CO_2. No comparisons of model predictions to experiments are presented but instead the focus of the analysis is on understanding which model input parameters (or combinations of input parameters) have a significant influence on the resulting CO_2 plume size, within a given range of conditions.

The type of sensitivity analysis undertaken is novel and it involves building a Bayesian statistical model from the results of a number of Phast simulations. The sensitivity analysis is then performed on the Bayesian model, not on Phast directly. It is demonstrated that this approach is sufficiently accurate and can yield results within a very short time-frame. Although the sensitivity analysis is demonstrated for application to dense-phase CO_2 releases, the approach can equally be adopted for other hazard analyses. It is anticipated that this will become routine practice in the coming years, since it provides model users with an improved understanding of the important physical processes controlling sometimes very complex flows, and it can assist greatly in directing further modelling efforts or measurements.

2. Calculation Methods

The CO_2 releases simulated in the present work consist of above-ground, unconfined, horizontal, steady-state orifice discharges from vessels in atmospheric conditions of neutral (D-class) stability. The range of conditions modelled using Phast is given in Table 1.

Table 1: Parameters varied in Phast global sensitivity analysis

Number	Parameter	Minimum	Maximum
1	Reservoir temperature	5 °C	30 °C
2	Reservoir pressure	100 bar	150 bar
3	Orifice diameter	½ inch (12.6 mm)	2 inch (50.8 mm)
4	Wind speed	0.5 m/s	50 m/s
5	Humidity	0 % RH	100 % RH
6	Ground surface roughness	0.0001 m	1.0 m
7	Release height above ground	0.5 m	3 m

The model output parameter that has been considered to be of primary importance is the distance from the orifice to a predicted concentration of 6.9 mol% of CO_2 (termed "dispersion distance" here). For a steady exposure duration of 30 min, this concentration corresponds to a Dangerous Toxic Load (DTL) of 1.5×10^{40} ppm.min^N (with N=8), which is the Specified Level of Toxicity (SLOT) for CO_2 used by the UK Health and Safety Executive (HSE, 2012).

In steady-state releases, the resulting plume concentrations are not constant over time but instead naturally vary about the mean concentration due to turbulence. Any such variations are important in the case of CO_2 since the DTL increases rapidly with concentration (to the power eight in HSE's model). It was highlighted by Gant and Kelsey (2012) that predictions of the hazard range would be non-conservative if turbulent concentration fluctuations were neglected. Care should therefore be exercised in interpreting the output quantity used here as the distance to SLOT.

2.1 Phast

The discharge and dispersion models of the consequence modelling software Phast (Version 6.7) have been used in the present study, details of which can be found in the papers of Witlox et al. (2009, 2011, 2012). The guidance provided in the Phast 6.6 release notes on the correct model configuration for CO_2 releases has been followed. Expansion from the reservoir conditions to atmospheric pressure has been calculated by assuming conservation of mass, momentum and energy (labelled “conservation of energy” in Phast) and the fluid at the orifice has been assumed to be in a meta-stable liquid state.

2.2 Gaussian Emulation Machine (GEM)

The global sensitivity analysis has been conducted using the Gaussian Emulation Machine (GEM) software, produced by Marc Kennedy and colleagues at Sheffield University (Kennedy, 2005). A useful introduction for non-specialists to the techniques employed by GEM is given in the paper by O’Hagan (2006) with further details provided by Oakley and O’Hagan (2004).

In essence, the Gaussian emulator is a sophisticated curve-fit to a number of “training” data points. In the present work, these data points are the results output from a number of Phast simulations. The emulator’s principal underlying assumption is that the output is a homogeneously smooth, continuous function of the input parameters. Rather than return just a single output value for a given set of input conditions, the emulator returns a probability distribution. This is used to provide the user with both a mean output value and some indication of the statistical spread about the mean, i.e. the uncertainty in the emulator. This uncertainty varies according to the location on the (multi-dimensional) curve of output values. At the points that were used to construct the emulator, the emulator gives an output value equal to the true value with minimal uncertainty. As one moves away from these points, the uncertainty gradually increases in response to interpolation and/or extrapolation errors. The uncertainty can be reduced by increasing the number of training data points, but typically just a few hundred training points may be required to produce results with an acceptable level of accuracy. To obtain a similar level of accuracy using a standard “brute-force” MC method applied directly to Phast (without the emulator) would usually require many thousands of Phast runs, with much longer computing times.

There were several steps to performing the sensitivity analysis of Phast using GEM. Firstly, the input parameters for a set of 100 Phast model runs were defined, using the maximin Latin hypercube algorithm in GEM, which selects input values to obtain good coverage of the sample space. In practice, this step simply requires the specification of minimum and maximum values for each of the seven input variables, given in Table 1 in the GEM Graphical User Interface (GUI). A short MATLAB script (Mathworks, 2011) was then used to take the file produced by GEM and modify a template Phast text-input (*.PSU) file to create 100 separate Phast input files. The Phast simulations were then run in batch mode, typically taking a few seconds each. The text output (*.OUT) files from Phast were then post-processed using another MATLAB script to extract the desired output (in this case, the dispersion distance) and this data was written to an output file. Finally, the input and output files were read into GEM, which constructed the Gaussian emulator and ran the sensitivity analysis in typically around 30 s.

The results produced by GEM showed in some cases that there were some interactions between model input parameters. To assess the magnitude of these interactions, it was relatively simple to select those parameters to examine for joint effects using the GEM GUI, and then re-run the analysis.

“Cross-validation” tests (Bastos and O’Hagan, 2008) were performed to assess the uncertainties in the Gaussian emulator and check that a sufficient number of training points had been used to construct the emulator. This involved using the full set of 100 Phast results to first estimate the parameters for the Gaussian emulator, but then using just 99 of the 100 Phast results for the interpolation step to predict the output at the conditions of the hundredth Phast run. This process was repeated over all hundred runs (leaving out each one in turn) to obtain an overall picture of the emulator accuracy across the whole sample space. Again, this process was made easy using the GEM GUI.

The whole sensitivity analysis (including the Phast runs) was performed in less than 30 min of computing time on a standard laptop computer. The most time-consuming aspect of the study, which required a few days effort, was to write the MATLAB scripts to process the data and interface GEM and Phast. However, these scripts needed to be written only once.

2.3 ANSYS-CFX

There is some uncertainty in the size of solid CO_2 particles produced by large jet releases and it is unlikely that experiments will be able to determine this directly. In order to assess the impact of this uncertainty on the resulting plume extent, a limited number of CO_2 dispersion simulations were performed using a model developed in the ANSYS-CFX CFD version 13 (ANSYS Inc, 2010). This uses a Lagrangian particle-tracking model for the solid CO_2 particles that accounts for the exchange of mass, momentum and energy

between the solid and gas phases. Unlike Phast, the CO_2 particles therefore do not necessarily have the same velocity or temperature as the surrounding vapour.
The inlet conditions for the ANSYS-CFX model were prescribed from the Phast model results at the point where the jet had expanded to atmospheric pressure. In the sensitivity tests, the solid CO_2 particles at this position were all assigned a uniform initial diameter of either 5 μm, 50 μm or 100 μm. The smallest of these corresponds roughly to the size predicted by the particle model of Hulsbosch-Dam et al. (2012a,b) for CO_2 releases at a pressure of 100 bar and superheat of around 80 ºC. In total, nine separate simulations were performed using the CFD model, using three different orifice sizes of ½, 1 and 2 inch diameter. In all of these cases, atmospheric conditions were neutral, the ambient temperature and humidity was 10 °C and 60 % RH, the wind speed at a reference height was 5 m/s and the ground surface was smooth. The inlet conditions from the Phast calculations used a reservoir pressure and temperature of 150 barg and 10 °C. Further details of the ANSYS-CFX model can be found in the paper by Dixon et al. (2012).

3. Results

The results from the variance-based global sensitivity analysis are shown in Figure 1 in the form of a "Lowry plot". The vertical bars show the main and total effect for each parameter, ranked in order of importance, whilst the lower and upper bounds of the curve show the cumulative sum of the main and total effects, respectively. More than 70 % of the variance in the Phast results is due to the orifice diameter (Parameter 3 in Table 1). The second highest contribution comes from the release height above the ground (Parameter 7). The remaining factors (or combinations of factors) account for less than 12 % of the total variance.

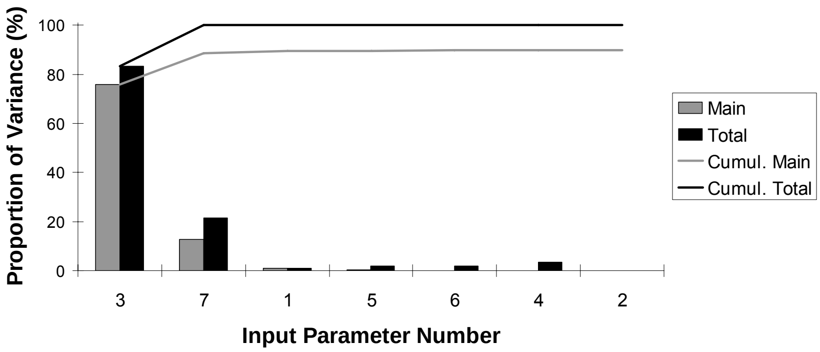

Figure 1: "Lowry" plot showing main and total effects for Phast model input parameters given in Table 1

Figure 2 depicts the predicted dispersion distance as a function of the orifice diameter and release height. The dispersion distance increases with the orifice diameter, roughly proportional to the mass release rate (i.e. orifice diameter squared). The dispersion distance increases with decreasing release height, due to the reduced air entrainment when the jet is closer to the ground.

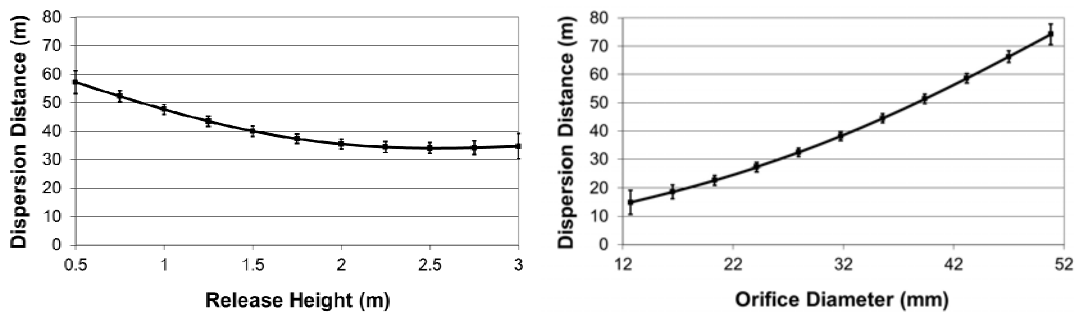

Figure 2: Main effects (including overall mean) from the Gaussian emulator, showing how the dispersion distance varies as a function of orifice diameter and release height.

The size of the total effect relative to the main effect in Figure 1 provides an indication of the degree of interaction between different model input parameters. The results indicate that there is some interaction between the orifice diameter and release height. These interactions are shown graphically in Figure 3, which plots the three-dimensional surface of the dispersion distance as a function of these two input parameters.

It is important to check that a sufficient number of model realizations have been performed in order to construct a reliable emulator. The results of cross-validation tests are presented in Figure 4, which shows the emulator's prediction of the dispersion distance against that predicted by Phast. As noted previously, the emulator provides results in terms of a statistical distribution about the mean. The results presented in Figure 4 shows the emulator mean (square symbol) and the emulator standard deviation (the error bar) for all 100 cross-validation tests. In total, 93 % of the emulator's mean predictions of the dispersion distance were within 4 m of that predicted by Phast. Since the purpose of the emulator is primarily to predict the trends in the Phast output and identify important parameters, this was considered to be an acceptable degree of accuracy. Additional tests using 400 Phast runs to construct the emulator gave similar results to those presented here.

A comparison of the shape of the CO_2 jet produced by Phast and ANSYS-CFX is given in Figure 5. The plume is more wedge-shaped in the CFD model results and hence the maximum distance to a concentration of 6.9 mol% is greater. However, at a height of 1 m above ground level, the distance to a concentration of 6.9 mol% is roughly comparable in the two models. Similar levels of agreement were obtained for all three orifice diameters tested. The effect of varying the CO_2 particle size from 5 μm to 100 μm in the CFD model led to a minor difference of around 2 % in the predicted dispersion distances.

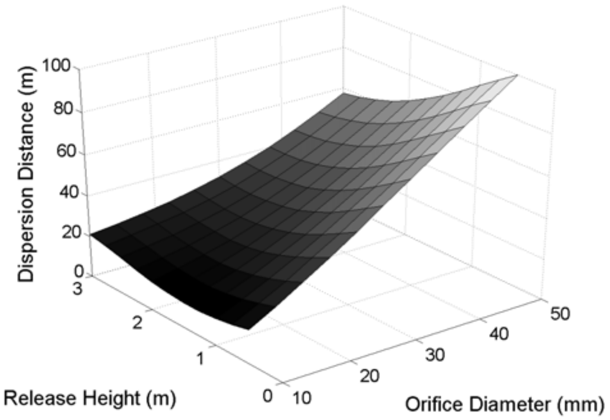

Figure 3: Joint effects resulting from varying the orifice diameter and release height simultaneously

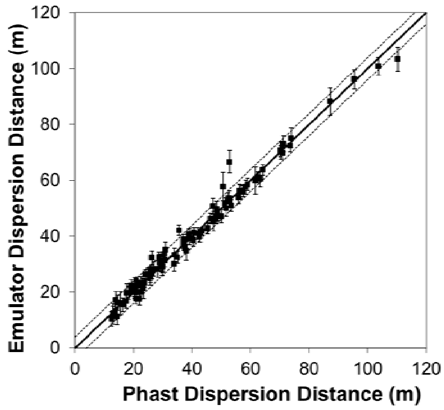

Figure 4: Results from cross-validation of the emulator

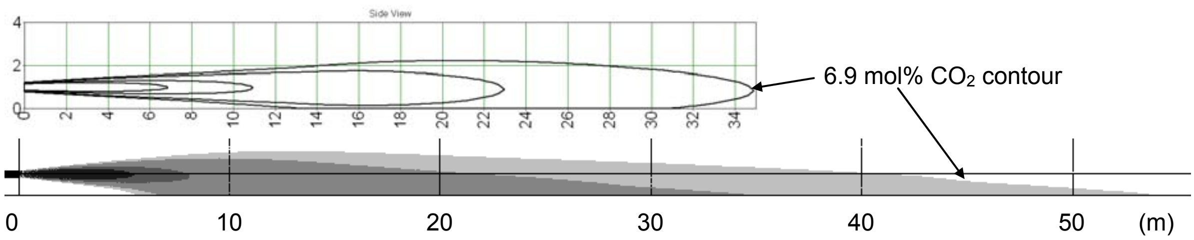

Figure 5: Vertical cross-sections of the Phast (top) and CFD (bottom) CO_2 plumes for a 1-inch (25.4 mm) diameter orifice. Contours of concentration are shown in each case for 6.9, 10, 20 and 30 mol% CO_2

4. Conclusions

A variance-based global sensitivity analysis has been performed on Phast to identify the important factors affecting the dispersion distance. The parameters varied include the CO_2 reservoir temperature and pressure, orifice size, wind speed, humidity, surface roughness and height of the release. The results show that for the range of conditions tested here, the orifice diameter has a far greater impact than any of the other parameters varied. The second-largest effect was from the release height, with a lower release height producing a plume that extends further, due to the reduction in air entrainment. Separate tests using

a CFD model showed that the dispersion distance was little affected by the size of solid CO_2 particles in the two-phase jet.
The global sensitivity analysis of Phast required less than 30 minutes of computing time on a standard laptop computer. This study has demonstrated that Bayesian analysis of model sensitivity can be conducted rapidly and easily, using tools such as the GEM software tested here. There are significant benefits to be gained from running such analyses in terms of identifying the important physical processes in complex flows, and in narrowing the scope of further simulations or experimental measurements.
In the present work, uniform probability distributions were applied for each of the input variables. For example, any wind speed was considered equally likely, within the range of conditions modelled. In future work, techniques for uncertainty analysis will be tested which apply realistic probabilities for wind speed, atmospheric stability etc. based on meteorological data. Further extensions to this work may also consider model calibration, using experimental datasets.

5. Disclaimer

The contributions made to this paper by Simon Gant, Adrian Kelsey, Kevin McNally and Mike Bilio were funded by the Health and Safety Executive (HSE). The contents, including any opinions and/or conclusions expressed, are those of the authors alone and do not necessarily reflect HSE policy.

References

ANSYS Inc., 2010, ANSYS-CFX Release 13.0, <www.ansys.com>, Accessed 20.08.2012.

Bastos L.S., O'Hagan A., 2008, Diagnostics for Gaussian process emulators, Technometrics, 51, 425-438.

Dixon C., Gant S.E., Obiorah C., Bilio M., 2012, Validation of dispersion models for high-pressure carbon dioxide releases, Proc. IChemE Hazards XXIII Conference, 153-163, Southport, UK, 12-15 November 2012.

Gant S.E., Kelsey A., 2012, Accounting for the effect of concentration fluctuations on toxic load for gaseous releases of carbon dioxide, Journal of Loss Prevention in the Process Industries, 25, 52-59.

Kennedy M.C., 2005, GEM-SA, Version 1.1. Software: Gaussian Emulation Machine for Sensitivity Analysis. Available from <www.tonyohagan.co.uk/academic/GEM/index.html>, Accessed 20.08.2012.

Hulsbosch-Dam C.E.C., Spruijt M.P.N., Necci A., Cozzani V., 2012a, An approach to carbon dioxide particle distribution in accidental releases, Chemical Engineering Transactions, 26, 543-548 DOI: 10.3303/CET1226091.

Hulsbosch-Dam C.E.C., Spruijt M.P.N., Necci A., Cozzani V., 2012b, Assessment of particle size distribution in CO_2 accidental releases, Journal of Loss Prevention in the Process Industries, 25, 254-262.

HSE (Health and Safety Executive), 2012, Toxicity Levels of Chemicals, <www.hse.gov.uk/chemicals/haztox.htm>, Accessed 20.08.2012.

Mathworks, 2011, MATLAB version 2011b. MathWorks Inc., Natick, Massachusetts, USA, <www.mathworks.co.uk>, Accessed 20.08.2012.

Oakley J.E., O'Hagan A., 2004, Probabilistic sensitivity analysis of complex models, Journal of the Royal Statistical Society B, 66, 751–769.

Pandya N., Gabas N., Marsden E., 2012, Sensitivity analysis of Phast's atmospheric dispersion model for three toxic materials (nitric oxide, ammonia, chlorine), Journal of Loss Prevention in the Process Industries, 25, 20-32.

O'Hagan T., 2006, Bayesian analysis of computer code outputs: A tutorial, Reliability Engineering & System Safety, 91, 1290-1300.

Witlox H.W.M., Harper M., Oke A., 2009, Modelling of discharge and atmospheric dispersion for carbon dioxide releases, Journal of Loss Prevention in the Process Industries, 22, 795-802.

Witlox H.W.M., Stene J., Harper M., Nilsen S.H., 2011, Modelling of discharge and atmospheric dispersion for carbon dioxide releases including sensitivity analysis for wide range of scenarios, Energy Procedia, 4, 2253-2260.

Witlox H.W.M., Harper M., Oke A., Stene J., 2012, Phast validation of discharge and atmospheric validation for carbon dioxide releases, Proc. 15th Annual Symposium, Mary Kay O'Connor Process Safety Centre, 306-326, Texas A&M University, College Station, Texas, USA, 23-25 October 2012.