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ASSESSING OPERATIONAL URBAN AND INDOOR CONTAMINANT DISPERSION MODELING CAPABILITIES WITH A GPU-LES SYNTHETIC DISPERSION ENVIRONMENT SYSTEM

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Abstract: Conducting casualty assessments associated with human exposure is a critical function of emergency response modelling tools. This calculation is based on a combination of models that represent the material release fate and transport, and human response to the exposure. The calculation becomes even more complex for urban areas where the presence of buildings and other structures affects wind fields and the corresponding outdoor contaminant transport, and high population densities and distributions which complicate the accurate assessment of consequences. In this paper we illustrate the relative inaccuracies associated with calculating human casualty and injury estimates from the ensemble averaged AT&D simulations available in the current generation of emergency response tools for open terrain, urban, and indoor environments. Results will be shown for a variety of idealized scenarios that illustrate the impact of making the casualty estimates from an ensemble of human toxic load calculations vs. making a single human-effects estimate from an ensemble of AT&D solutions.

Key words: *Urban and Indoor Dispersion Modeling, Large Eddy Simulation (LES), Graphics Processing Unit (GPU) Computing, Indoor-Outdoor Contaminant Transport and Dispersion, Exposure and Human Health Assessments*

INTRODUCTION

Modelling approaches used to assess human injury and casualty estimates are a critical component of the emergency response tools used to assess the risks associated with exposures to airborne hazardous materials. These tools link a combination of physical processes which include the release of the material into the atmosphere, the fate and transport of the material, and the inhalation/exposure and associated human response of people who are in the path of the material. Each element of this chain of models is frequently complex and there is often considerable uncertainty in the information used as input to each of the models. Furthermore, the modelling technologies used to represent three main elements (e.g. release, fate/transport, and human response) are largely developed separately and then combined by an integrator with a limited understanding of the nuances of the science in each element. Collectively these issues make estimating human casualties associated with the exposure to hazardous airborne materials in an operationally relevant time-frame very difficult. Little, if any, data exists to validate this system of models.

In spite of these challenges, modelling systems exist for making these types of casualty estimates. Examples include the Human Exposure Model (HEM) (EPA, 2019), the Hazardous Pollutant Exposure Model (HAPEM) (EPA, 2015), and the Hazard Prediction and Analysis Capability (HPAC) system developed by the Defence Threat Reduction Agency (DTRA) (DTRA, 2008). HEM is typically used to calculate near range (e.g. within 50 km of the source) chemical inhalation exposure risks downwind of industrial facilities. HAPEM is designed to estimate long term inhalation exposure for selected population groups at scales ranging from urban to continental. HPAC is a fast-running modeling capability used to assist in the emergency response to the release of hazardous industrial and chemical, biological, radiological, and nuclear (CBRN) materials. HPAC includes capabilities for assessing hazard areas and human collateral effects and can provide solutions within minutes in open terrain, urban, and indoor environments. While different in many respects, these models all share a common approach that calculates human risk and/or casualty estimates from an ensemble averaged atmospheric transport and dispersion (AT&D) solution.

In this paper we use high fidelity dispersion simulations from a Large Eddy Simulation (LES) model to illustrate the relative inaccuracies associated with calculating human casualty and injury estimates from the ensemble averaged AT&D simulations available in the current generation of emergency response tools like HPAC. Examples demonstrating the impact of making the human effects estimate from an ensemble of human toxic load calculations are contrasted with making a single human casualty estimate from an ensemble of AT&D solutions. Results are presented using models currently available within the HPAC system for outdoor open terrain, urban locations, and indoor environments.

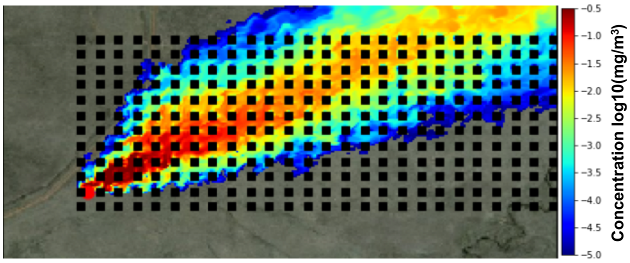

Figure 1. A GPU-LES dispersion solution for an urban stable PBL.

STUDY DESIGN AND ANALYSIS SCENARIOS

Airborne Material Fate and Transport Simulations

LES models, when combined with an AT&D model, either an inline Eulerian model that solves for the advection diffusion of the airborne material at each model grid point Bieringer et al. (2017), or with a Lagrangian Particle Dispersion Model (LPDM) (Weil et al. 2012), have been shown to produce accurate simulations of airborne material dispersion. When configured to resolve the spatial and temporal scales of the physical processes that dominate airborne material dispersion, LES has been shown to be an effective means to create ensembles of short time-averaged “single-realization” dispersion solutions that can be used to assess air sampling network designs, pollutant measurement systems performance, and characterizing the impact of hazardous airborne materials on human health (Bieringer et al. 2014). For this study we used a modeling system called the Joint Outdoor-indoor Urban LES (JOULES). JOULES couples a building-aware LES atmospheric model, with an integrated outdoor airborne material transport and dispersion model, and models that simulate the transport of contaminants across the building envelope. A key enabling technology is an LES model that has been implemented on a Graphics Processing Unit (GPU) computing platform that is over 150 times faster than conventional LES models implemented on a Central Processing Unit (CPU) system (Bieringer et al. 2017). This GPU-LES enables us to create the ensembles of high-resolution microscale atmospheric and dispersion solutions used in this study.

JOULES was able to produce simulations for both open terrain and a simple urban environment with an array of equally spaced small buildings. The model was configured to simulate daytime convectively unstable and night-time moderately stable planetary atmospheric boundary layer (PBL) with a meandering surface wind. A nested model grid design was used. The outer nest was configured so that the entire depth of the PBL was represented in the model and cyclic boundary conditions could be used to spin up the turbulent eddies. The inner nest used a one-way lateral boundary conditions to downscale the eddies and turbulence from the large nest to a finer scale. The inner nest used a 3-meter horizontal and vertical grid spacing. This spatial grid increment was necessary to resolve both the small buildings and the stable PBL scenarios. Figure 1 illustrates an example of a dispersion solution for the stable PBL in the urban location. All of the simulations use a 4-minute continuous release of a unit, passive (non-reactive) tracer. An ensemble of 30 dispersion simulations were developed and used for all of the analyses.

This study also utilized models from HPAC to represent the types of models used in operational emergency response tools. To ensure that the meteorological conditions were consistent between the LES and operational tools, the relevant meteorological variables from the LES simulation were averaged over a 30 minute period and then written to HPAC formatted weather files for use in driving the operational dispersion simulations. The Second-order Closure Integrated PUFF (SCIPUFF) model (Sykes et al. 2008) was used for the open terrain simulations and the Micro-Swift-Spray (MSS) model (Tinarelli et al. 2007) was used for the urban simulations. The buildings were represented by simple rectangular objects with dimensions of (x=12m, y=15m, z=10m) and were spaced 25 meters apart. As shown in Figure 1, the LES resolved the flow deformations associated with these building obstacles and the contaminant dispersion around them. The indoor spaces were represented by a simplified, single-zone (often referred to as a “box” or “reduced-geometry”) building model developed by scientists at Lawrence Berkeley National Laboratory (LBNL). This type of model is frequently used in operational emergency response tools for scenarios involving modeling many buildings at urban scale, or when the details of a particular building are unknown and must be covered probabilistically. In such cases, the lack of detailed information about building interiors, and the computational burden of a general-purpose model, may make simple models more appropriate than a running a full multizone model. For this study the indoor concentration were calculated with the box model for air change rates (ACR) of 0.5, 2 and 10 air changes per hour. Concentrations from a location at the center of the upwind face of each building were used as the entry point of the contaminant to the building.

Human Toxic Load and Casualty Calculations

Human casualty and injury estimates for many materials are represented by a combination of time-integrated exposures and a representation of the toxicity of the material. This method is commonly referred to as toxic load. Toxic load was originally assumed to be a linear function of the total quantity of material inhaled. Experimental studies conducted by ten Berge et al. 1986 and Sommerville et al (2009) suggested that for many materials, the health effects are dependent upon how the contaminant is inhaled. The results from these experiments led to the subsequent development and use of a modified toxic exposure model that defines a material specific exponent to the material concentration in the toxic load equations as shown in Equation 1. The value of the exponent is related to the toxicity of the material and makes the toxic load calculation sensitive to fluctuations in the concentration (Bieringer et al. 2014 and Urban et al. 2014).

$$TL(x,t) = \int_0^t C^n(x,t')dt' \tag{1}$$

Probit analysis is one of the most common methods for translating toxic load exposures of individuals to the human health response to that exposure (Montoya and Planas, 2009). In emergency response systems like HPAC, this approach is used to estimate injuries and casualties associated the hazardous material release. Here, the probit analysis approach is used to integrate the impact of the material release across the entire area impacted to produce a single estimate of impact of the hazardous material release as a function of time since the release. For the purpose of illustrating the effects of averaging on casualty estimates, we use the toxicity characteristics and corresponding human response associated with exposures to chlorine. The toxic load exponent (n) for chlorine is 2.75 and the probit model developed by Sommerville et al. (2010) for military and general populations are given in equation 2 below.

$$Y_{n\,(military)} = -31.25 + 2.91 log(C^nT) \qquad Y_{n\,(civilian)} = -22.698 + 2.18 log(C^nT) \tag{2}$$

How the impacted population is distributed also impacts the assessment. To illustrate this property we explore scenarios ranging from (simple and less realistic) where the population is uniformly distributed to more realistic scenarios where the population is distributed clusters of varying sizes. This approach is used for both the outdoor and indoor casualty estimates. The uniformly distributed population is presented in this paper.

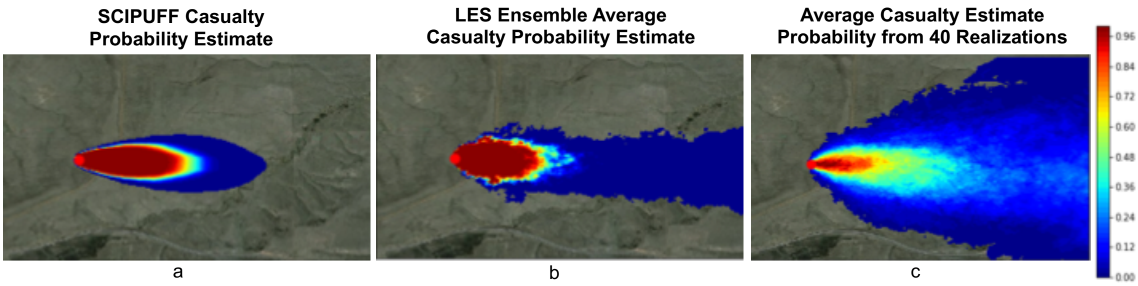

Figure 2. Two-dimensional casualty probability for a chlorine release in an unstable boundary layer. Figure a. is the estimate for SCIPUFF, figure b. is the estimate when averaging 40 realizations before the toxic load calculation, and figure c. is the casualty probability estimate from averaging the 40 realizations after the toxic load calculation.

RESULTS

Open Terrain Outdoor Casualty Assessment

Simulations from the both LES and SCIPUFF models for an open terrain unstable and stable PBL scenario served as the input for the analysis results presented here. Concentration values from each were used to calculate toxic load and casualties using the toxicity characteristics of chlorine described above. Figure 2 illustrates a mapping of the casualty calculations from the unstable PBL simulations for the uniformly distributed population scenario. The left image shows the casualty probability calculated from the SCIPUFF model, the center image represents the casualty probability from the LES simulations when the average is calculated before the casualty probability calculation, and the right image is the casualty probability when an average of the 'single realization' toxic load estimates is computed. Figure 3 shows a timeseries of the total casualty estimates corresponding with the three panels in Figure 2. The plots display the casualty estimate for figures 2b (orange line) and 2c (blue lines), and each estimate is normalized by the SCIPUFF solution, 2a. The individual realizations are denoted by the blue, dotted lines. A normalized value of one implies that the casualty estimate is identical to the SCIPUFF solution. Both figures highlight that the use of an ensemble averaged dispersion model can provide both over and under estimates of casualties in this scenario. It suggests that overestimates occur near the release location and a general underestimation occurs further downwind in scenarios where turbulent induced variability is high. Figure 3b displays a stable case where turbulent variability is low. For this case the plume remains compact, and larger scale turbulent variations cause slight meandering of the plume allowing it to behave similar to a near-field release for a much longer downwind distance For this case, the ensemble average provides a higher casualty estimate than the mean of the 'single realization' estimates.

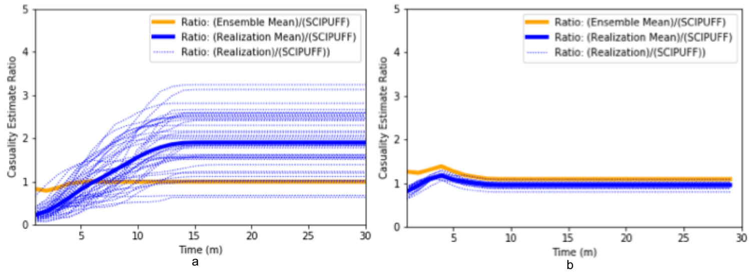

Figure 3. Outdoor casualty estimates for a chlorine release. Figure a. depicts results convective PBL and figure b. depicts releases within a stable PBL.

Urban and Indoor Casualty Assessment

LES and MSS model simulations for unstable and stable PBL urban scenarios serve as the input for the analysis results presented here. Figure 4 is similar to Figure 2 but for indoor casualty estimates for a uniformly distributed building array. The top image shows the casualty probability calculated from the MSS model, the center image represents the casualty probability from the LES simulations when the average is computed before the casualty probability calculation, and the bottom image is the casualty probability when the ensemble average is computed after the box model and toxic load calculations. Similar to the outdoor open terrain results, the operational model produces an overestimate of the casualties closer to the release location and an underestimate further downwind. Indoor casualty calculations were also calculated for the scenarios described above. Figure 5 depicts a timeseries of the total casualty estimates indoors that were derived from outdoor concentrations from both the ensemble averaged MSS and the ensemble of the single realization LES calculations for the unstable and stable PBL scenarios. Figure 5a shows the timeseries of outdoor casualty ratios for an unstable PBL scenario and Figure 5b shows the same results for stable scenario. Unlike the outdoor scenario, there isn't a large difference in total casualty estimates between the average of the 'single realization' and operational approaches. However, from figure 4, the area where casualties can occur is different where operational model over-estimates the casualty calculation close to the source location and under-estimates the casualty calculation farther downwind.

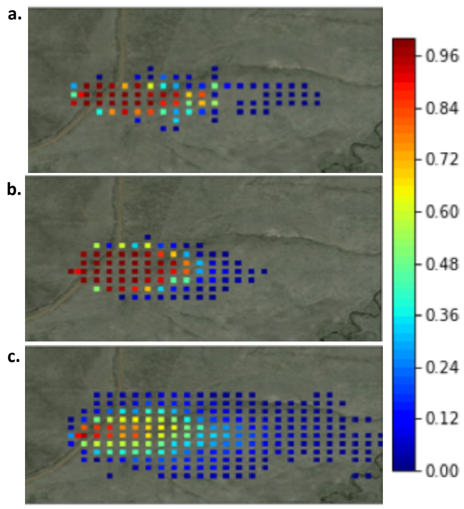

Figure 4. Indoor casualty probability estimates. Same as figure 2.

CONCLUSIONS

In this paper we have illustrated that significant inaccuracies in human casualty and injury estimates can be associated with how these estimates are calculated. As expected, the non-linear operator in the toxic load calculation will not commute with the average, and therefore results in different casualty estimates when computed from an ensemble of "single-realization" solutions vs. an ensemble averaged solution. Results were presented illustrating this effect when using a simple assumption that population is uniformly distributed. In this situation, this effect results in both overestimates of casualties near the release location and underestimates of casualties further from the release location. The magnitude of the over and underestimates is dependent on the magnitude of turbulent variability. Due to the localized areas of higher concentrations the effects of averaging have a larger influence on casualty estimates in rural areas than in urban environments. The impact that spatial averaging has on the over and underestimates in the casualty estimates indoors is significantly diminished relative to the outdoor results. While not fully explored in this study, preliminary results also suggest that this effect is also present with the population is not uniformly distributed and the impact of averaging on casualty estimates is even more pronounced. Finally, this study illustrates the utility of using the JOULES system to assess the accuracy of the operational emergency response tools and as a tool for improving them.

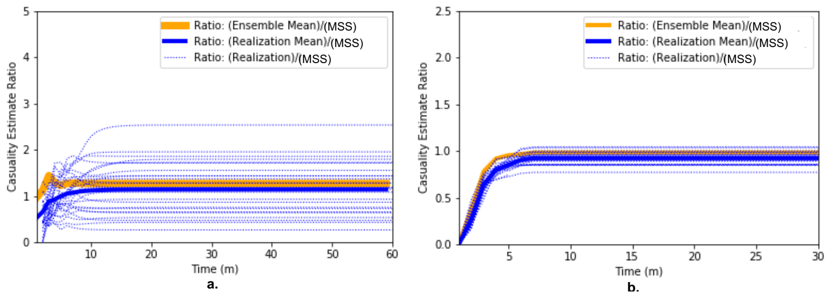

Figure 5. Indoor casualty estimates for a chlorine release. Figure a. depicts results unstable PBL and Figure b. depicts results for releases within a stable PBL.

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