Enabling Large-scale Fine-grained Simulation of IED Vapor Concentration in Open-air Environments

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***Abstract*—Ammonium nitrate and nitromethane are two of the most prevalent ingredients in improvised explosive devices (IED). Developing a detection system for IEDs in open public events where no specific check points are available requires many large scale, fine-grained simulations to estimate the explosive vapors. However, such large scale molecular simulations at the required granularity is very time consuming and in most cases not feasible. In this paper, we propose region-specific meshing to alleviate the computational cost. The proposed simulation methodology provides accurate results as compared with a baseline simulation of fine grained mesh (in a small area) while providing significant reduction in simulation time. Thus, large scale simulations at feasible computational burden can be achieved.**

***Index Terms*—IED, Ammonium, Nitromethane, Concentration**

I. Introduction

Improvised explosive devices (IEDs) typically contain four components: an initiator, a switch, a main charge, a power source, and a container [1]–[4]. Detection of these devices in an open-space uncontrolled area (soft target) without disrupting daily life remains very difficult and requires sensitive, specific, yet low-cost systems. Ion spectrometer and high-power laser beams are frequently used to detect explosives in airports and checkpoints [5]–[8]. However, with moving crowds in an open environment without any specific checkpoints, such as open-air concerts, sporting events, and public festivals, the above-mentioned techniques are not feasible.

Recently, significant research has focused on designing sensors to detect very low concentrations of explosive vapor that are released from IEDs. As an example, in [7], the authors propose to use CMOS capacitive sensor arrays that mimic a dog's nose. The active region (dielectric) of capacitors are coated with receptors which are sensitive to the $-NO_2$, $-ONO_2$ and $-NHNO_2$ groups. These capacitive sensors are able to detect the vapors released by the IED in the level of several parts per billion (ppb) [7]. In [8], the authors design and demonstrate sensors based on silicon nanotube transistors coated with similar receptors with sensitivity the parts per quadrillion range. The aforementioned examples show that it is possible to detect very small concentration of vapors. However, a complete detection system, needs to include sensor design, estimation of concentration profiles, and a detection and alert algorithm that takes into account sensor inaccuracies, drift, and offset. In order to design such a system, one needs to estimate the concentration profiles of the compounds over a large area and over a long duration. Multi-physics simulators, such as COMSOL [9], can be used to determine the necessary distribution and sensitivity of sensors to detect IEDs. However, fine-grained COMSOL simulations over a large area with many obstacles and wind conditions is not feasible due to computational complexity. Reducing the granularity of simulations is also not useful since vapor concentrations fall drastically with distance and the range for detection is typically small but changes dramatically with obstacles and wind conditions. Thus, we need a simulation framework that can merge the detailed information from fine-grained simulations with that of a coarse-grained simulations.

In this paper, we propose a hybrid simulation framework that adaptively selects areas of interest, *important grids*, from coarse-grain simulations to adjust the mesh size and location for fine-grained simulations. Our simulator then merges the two sources information via interpolation to obtain detailed simulation of concentration profiles over a large, open area with feasible computational burden. We show that this approach yields accurate results when compared to a baseline (fine-grained simulation of both compounds in a small area) but scales at lower computational cost to make large-scale simulations feasible.

II. Proposed Adapive Mesh Simulation Framework

Among the various types of IEDs, a combination of Ammonium Nitrate (AN) and Nitromethane (NM), (ANNM), which is a 60:40 mix of AN and NM (60% ammonium nitrate, 40% nitromethane by mass) is one of the most prevalent choices. To determine the diffusion profiles of explosive vapors, we start with the molecular diffusion model where ammonium nitrate (or nitromethane) is located in a simple cylindrical container (see Figure 1) (e.g. in the shape of a pipe bomb), with no wind and any other obstructions, such as buildings.

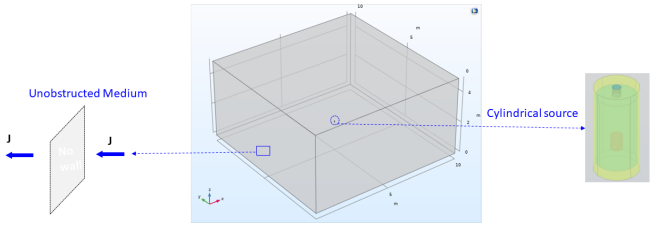

Fig. 1. Simulation set-up. Ammonium in IED in unobstructed medium.

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TABLE I
TABLE 1. SIMULATION SET UP PARAMETERS

Medium	Open environment
Contamination Material	NH_3
Temperature	293.15 K
Dimensions	x=10m, y=10m, z=4m

Here, our aim is to decide the possible detection distance range for sensors where the concentration level reaches the reported sensitivity levels of low-cost sensors (20-100ppb). Rectangular geometry with (x=10, y=10 and z=4 meters; see the Table1) dimensions is selected as the environment. The ammonium nitrate as a source inside the container (represents the IED) with a cylindrical shape(h=10 cm, r=5cm) is placed at the center (x=5m, y=5m). The container wall prevents permeation of vapor molecules, so vapor molecules can only diffuse from a 1 cm hole atop the container. The transient behavior of gas diffusion profile based on Fick's law was simulated using the transport of diluted species interface tool [10]. Figure 2 shows the 2D slices and 3D diffusion concentration profile considering a source at the center. The 2D slices represent the concentration of ammonia at a height of 1.5 m. Results show concentrations diffusing uniformly in all directions.

A. Region specific meshing

Simple geometry in a small map with uniform fine meshing (0.1 m resolution) is employed to run the previous simulation. However, a realistic large-scale open environment scenario also includes wind, obstacles, such as buildings, and walls, which adds complexity to the system, and increases the simulation time considerably. One way of overcoming this issue is reducing the mesh resolution, however, these results lack accuracy. As an example, Figures 3 shows the simulation results, concentration profile of ammonium nitrate in 2D slices at a height of 1.5 m at different time lapses when extremely fine mesh with 0.1 m grid size is used. Figure 4 shows the same profile with a coarse mesh with 1 m grid size. While a uniform concentration pattern is observed in Figure 3, it is clear that distortions on concentration pattern near the source are observed in Figure 4. Thus, using such coarse meshing where concentrations change significantly does not provide accurate results.

To alleviate this problem, we propose a hybrid simulation framework that adjust the mesh locations and sizes according to simulation results. The overall flow of the proposed algorithm is shown in Figure 5.

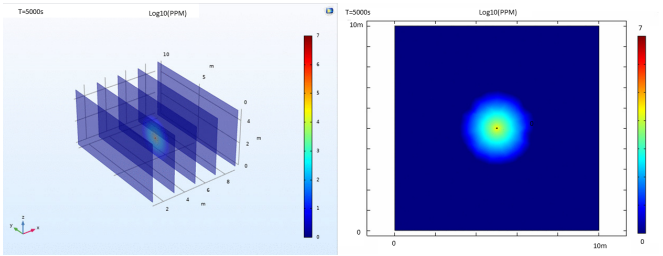

Fig. 2. Ammonium nitrate concentration over time in non-obstructed medium.

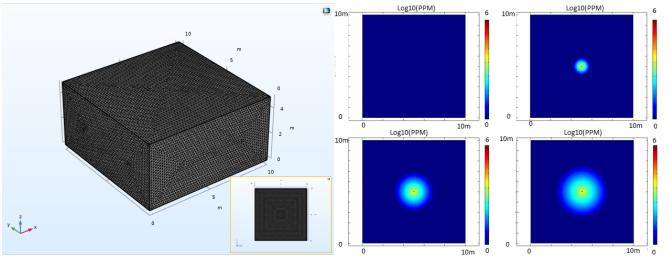

Fig. 3. Right: Simulated environment with extremely fine meshes. Left:Concentration profile of Ammonium at z=1.5m at time intervals: 0, 1000s, 5000s and 1000s

First, we introduce a new box around the source where the vapors can diffuse freely without any obstruction. Since we already know that concentration profiles near the source will be highest, this box will act as a *seed region* for fine-grained simulations. Then, we perform coarse-grained simulations in the given area outside the box to obtain an initial estimate of concentration profiles. We then determine *important grids*, which are the grids with concentrations above the detection threshold (C_{thresh}), or grids in the immediate neighborhood of this level of concentration. This detection threshold can be set based on the sensor sensitivity (e.g. 20ppb is used in this work). The coarse grids that are deemed important are further divided into fine meshes and these areas are simulated again. The concentration profiles in the remaining coarse grids are interpolated to match the grid sizes and the data are merged. We then increase the new simulation duration and repeat this process.

Figure 6 shows the mesh distribution and simulation results for the same simulations as in Figures 3 and 4, but using our proposed adaptive meshing algorithm. The source box (1 m x 1 m) is also shown in the concentration map as a black rectangle. The course-grained simulations are obtained with 1 m grid size, and the fine-grained simulations are obtained with 0.1 m grid size. Since there is no obstruction and/or wind, the important grids are determined at around the source (outside of the source box), as expected. It is also clear from the concentration map that no distortions in concentration profile and no discontinuity in concentration pattern are present.

B. Computational cost comparison

The primary goal of the hybrid simulation framework is to reduce the overall simulation time. Reducing the mesh grid

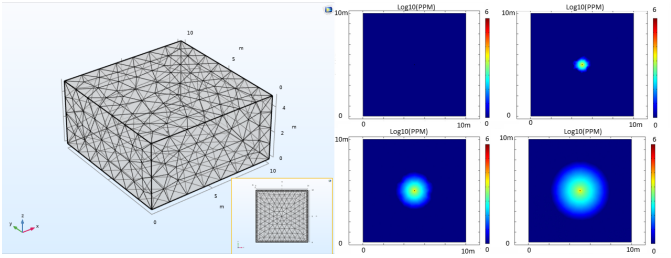

Fig. 4. Right: Simulated environment with coarse meshes. Left:Concentration profile of Ammonium at z=1.5m at time intervals: 0, 1000s, 5000s and 1000s.

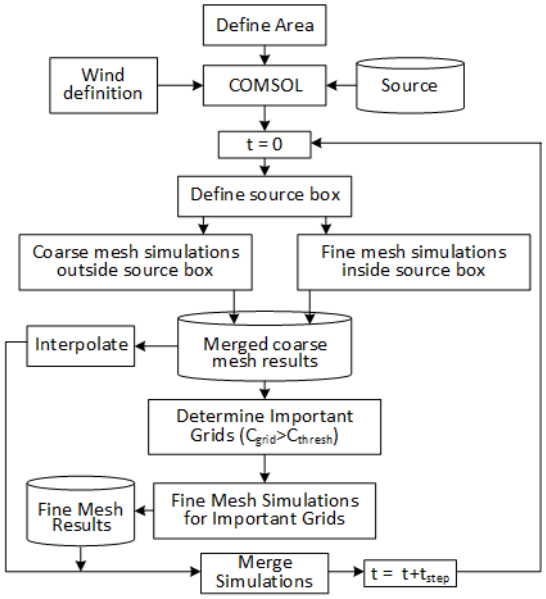

Fig. 5. The proposed adaptive mesh simulation algorithm

size increases the number of elements as well as increase memory requirements of the simulation, resulting in significant increase in simulation time as the simulation area gets larger. Table II compares the simulation time necessary for fine-grained and coarse-grained simulations as the simulation area is increased. We observe that speed ratio between fine-grained and coarse-grained simulations increase as the simulation area increases. Thus, for large-area simulations, fine-grained simulations will not be feasible.

TABLE II
COMPUTATION TIME COMPARISON BETWEEN MESH SIZES OVER INCREASING SIMULATION AREA

Area	Coarse	Fine	Ratio
5m x 5m	17s	468s	27
10m x 10m	31s	903s	29
20m x 20m	108s	4249	40

To evaluate the impact of hybrid meshing on computation time, we also add wind to the simulation for the 20m x 20m simulation area. In this specific experiment, wind in the direction of the x-axis is imposed, increasing the number of *important grids*. Figure 7 shows the selected important grids (at 500s time point). The area outside of this box is simulated in coarse mesh size, whereas the area inside this box is simulated with fine mesh size at this point. Table III shows the effect of hybrid simulations on computation time for the 20m x 20m area that is simulated in both fine-grained and coarse-grained mesh grid sizes. We can see that he hybrid simulation requires much less time compared to the fine-grained simulation, although it requires significantly more time than coarse grained simulations.

TABLE III
SIMULATION TIME SAVINGS USING THE HYBRID SIMULATION APPROACH AND THE NUMBER OF BOUNDARY ELEMENTS SIMULATED IN EACH CASE

	Coarse	Hybrid	Fine
# Elements	14478	62460	749878
Time (s)	108	629	4249

C. Accuracy comparison

The proposed hybrid mesh provides accurate results in comparison to uniform fine-grained mesh while providing the aforementioned computation time savings. As an example, Figure 8 shows the concentration profiles from the edge of the simulation boundary to the edge of the source in the horizontal dimension (y=10m). Note that in this simulation, wind with the speed of 2.8m/s is introduced. The two simulation results track well in terms of concentration along the line shown. Slight differences can be attributed to the interpolation that is used to align the simulation locations in both simulations due to different grid sizes.

III. SIMULATION OF REALISTIC MEDIUM

The simulations are extended to realistic scenario where several blocks and sidewalks are included.The Figure 9(a) shows the 412 m x 312m parts of University of Delaware stadium where the black blocks represent obstructions that vapors cannot permeate and white spacing represent the place where spectators can stand or move freely. Here, in addition to ammonium nitrate, nitromethane is also present in IED as shown in Figure 9 (c), where the blue and red sources inside the IED represent the ammonium nitrate and nitromethane respectively. The small opening on top of the bomb represent the hole where the vapors diffuse. The complex geometry requires region specific meshing to alleviate the computation

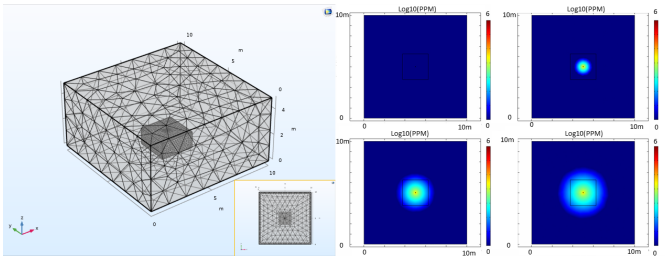

Fig. 6. Right: Simulated environment with hybrid meshes. Left:Concentration profile of Ammonium at z=1.5m at time intervals: 0, 1000s, 5000s and 1000s.

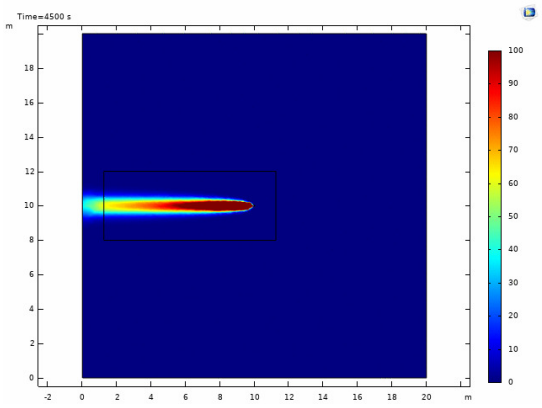

Fig. 7. Hybrid mesh simulation at 500s time point. The box indicates the location of identified important grids.

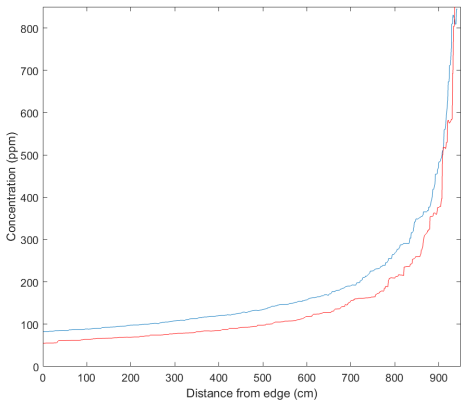

Fig. 8. Comparison of simulation results with fine-grained mesh (blue line) and the proposed hybrid mesh (red line) at a random time point (1800s).

cost, therefore we introduced a new box (shown in Figure 3) with dimensions of 20 m x 20 m around the source, where the vapors can permeate the walls of box without any obstruction. Then we used the proposed adaptive meshing algorithm as described in Figure 5 Wind with following speeds: v_1=2.82 m/s in X direction and time dependent v_2= 2.82 m/s in Y directions are introduced to the model to make realistic scenario. Simulation duration is set to 1000 second with 10 second intervals.

Figure 4 plots the 2D concentration of ammonium nitrate and nitormethane in terms of LSB (20 ppb = 1 LSB) at a randomly selected point in time (410s). The left side maps represent concentration of ammonium nitrate, while right side represents nitromethane concentration. These results demonstrate that concentration levels are strongly wind velocity dependent, and concentration accumulations take place around obstacles. Thus, the proposed adaptive meshing is necessary to enable accurate simulation of concentration profiles. Table IV shows the simulation time of coarse mesh and the proposed hybrid mesh, and compares this with the simulation time of fine mesh, as projected from the number of necessary finite elements. It should be noted that the fine mesh simulations are not feasible to complete even with given time as the server does not have the required memory. Thus, we verify that using the proposed hybrid mesh enables this scale of simulation without losing critical information.

TABLE IV
SIMULATION TIME AND THE NUMBER OF BOUNDARY ELEMENTS FOR COARSE AND HYBRID SIMULATIONS AND PROJECTED SIMULATION TIME FOR FINE MESH SIMULATIONS

	Coarse	Hybrid	Fine
# Elements	577,278	2,278,507	35,067,145
Time	1.5hr	3 days	50 days (projected)

IV. Conclusion

We investigated the concentration distribution of vapors released from IEDs, namely, ammonium nitrate and nitromethane. The region specific meshing is employed to simulate the very large scale geometry. Results shows that 20 ppb

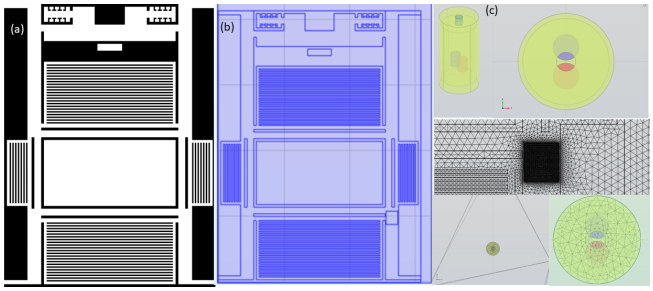

Fig. 9. (a) and (b) University of Delaware stadium map. (c) Sources in IED. Regions specific meshing.

of vapors released from IED can be detected at 1 m from an IED source. Furthermore, the 2D concentration map of ammonium nitrate and nitromethane show that both vapors are present at various locations depending on obsruction and wind conditions. This simulation framework is intended to help to build a cyber physical system that uses distributed gas sensors to protect the crowd in open environments.

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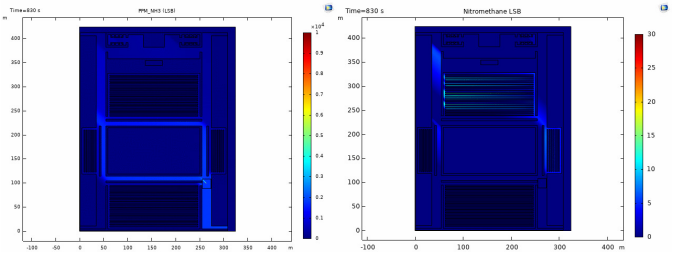

Fig. 10. Simulated University of Delaware stadium to determine the concentration profile of targeted molecules.