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Chemical Plume Tracing by Discrete Fourier Analysis and Particle Swarm Optimization

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Abstract

A novel methodology for solving the chemical plume tracing problem that utilizes data from a network of stationary sensors has been developed in this study. During a toxic chemical release and dispersion incident, the imperative need of first responders is to determine the physical location of the source of chemical release in the shortest possible time. However, the chemical plume that develops from the source of release may evolve into a highly complex distribution over the entire contaminated region, making chemical plume tracing one of the most challenging problems known to date. In this study, the discrete Fourier series method was applied for re-construction of the contour map representing the concentration distribution of chemical over the contaminated region based on point measurements by sensors in a pre-installed network. Particle Swarm Optimization was then applied to the re-constructed contour map to locate the position of maximal concentration. Such a methodology was found to be highly successful in solving the chemical plume tracing problem via the sensor network approach and thus closes a long-standing gap in the literature. Furthermore, the nature of the methodology is such that a visual of the entire chemical dispersion process is made available during the solution process and this can be beneficial for warning purposes and evacuation planning. In the context of such chemical release scenarios, the algorithm developed in this study is believed to be able to play an instrumental role towards national defense for any country in the world that is subjected to such threats.

Keywords

Chemical plume tracing, sensor network, discrete Fourier series, particle swarm optimization, national defense

INTRODUCTION

The issue of terrorism has become a major concern for many nations throughout the world in recent years. Security measures have been stepped up in many countries and heavy investments have been made to develop countermeasures against the various possible types of terrorist threats – chemical, biological, radiological, explosive – that may arise. This paper focuses on the first type of threat that may arise through acts of terrorism, that of deliberate release of toxic chemicals into the environment with the intention to inflict human casualties through chemical poisoning. During a toxic chemical release and dispersion incident, the imperative need of first responders is to determine the physical location of the source of chemical release in the shortest possible time so that appropriate countermeasures can be carried out in a timely fashion so as to minimize the extent of human casualties. The first responders to such an incident may consist of ground troops from the defense forces or armed forces that are equipped with the necessary chemical suits and detectors. A massive search operation to locate the source of chemical release will be required before containment and subsequently, decontamination procedures can be carried out. Alternatively, to minimize human exposure to such potentially lethal chemicals, advanced technologies such as robots and sensors can be exploited to carry out the task of locating the position of the source. It is envisaged that such technologies when coupled with the necessary artificial intelligence afforded by appropriate numerical algorithms will be able to accomplish such tasks with minimal or even no human intervention. However, the requirement for an effective numerical algorithm to complement a sensor network or fleet of autonomous robots installed with chemical sensors for carrying out chemical plume tracing has received little attention to date. The development of such a capability would provide all nations throughout the world with a new technological edge to enable fast response to toxic chemical release scenarios.

In the published literature, research efforts have been directed towards development of olfactory-based mechanisms used by various biological entities to carry out search operations by autonomous vehicles. The latter may include both Unmanned Aerial Vehicles (UAVs) as well as Autonomous Underwater Vehicles (AUVs) for aerial and amphibious operations respectively. Farrell *et al.* (2003) presented a plume mapping approach based on hidden Markov methods (HMM) for odor source localization by a single autonomous vehicle moving in a high Reynolds number fluid. Li *et al.* (2006) developed a behaviour-based adaptive mission planner to trace a chemical plume to its source and reliably declare the source location. The strategy was inspired by the manoeuvring behaviours of moths flying upwind along a pheromone plume. Pang and Farrell (2006) derived a computationally efficient method based on stochastic process theory and Bayesian inference methods to yield algorithms for predicting likely source locations based on the measured flow and the detection or non-detection events that occur at the changing vehicle location of an AUV. Marques *et al.* (2006) presented a new algorithm for searching odor sources across large search spaces with groups of mobile robots. The odor search problem was formulated as a stochastic optimization problem in which the goal is to find the local

maxima in an average concentration map and the method of Particle Swarm Optimization (PSO) was applied. More recently, Jatmiko *et al.* (2007) also reported on a Modified PSO algorithm which combines chemotaxic and anemotaxic modelling for the odor tracing problem.

The localization of a source of chemical release by dynamic measurements of the plume it forms is a complex real-world problem because of the stochastic and dynamic nature of the physical environment. It contains a high degree of freedom and is a highly nonlinear problem for which no straightforward mathematical solution exists. Although there have been several attempts to address the problem of chemical plume tracing by the use of autonomous vehicles equipped with chemical sensors, the equally promising and alternative approach of utilizing a network of stationary sensors has also received increasing attention from research workers in recent years. Haupt (2005) first demonstrated the utility of an optimization approach for coupling a forward-looking Gaussian dispersion model with a backward-looking receptor model to identify a single source or combination of sources. This was extended to a method that simultaneously determines surface wind direction and source characteristics using a genetic algorithm (Allen *et al.*, 2007). More recently, this algorithm was combined with a gradient descent algorithm to allow back-calculation of seven variables that characterize the release (Long *et al.*, 2010). The approach was validated using the Gaussian puff as the dispersion model. Yee (2008) presented a Bayesian inference approach for multiple source reconstruction from concentration data obtained from an array of sensors. Bayesian probability theory was used to derive the posterior probability density function for the number of sources and parameters that characterize each source. Senocak *et al.* (2008) also developed a stochastic event reconstruction method based on the Bayesian inference approach with Markov chain Monte Carlo sampling. Gaussian plume dispersion models were adopted as the forward model within the Bayesian inference framework to achieve rapid-response event reconstructions. The authors commented that such a Gaussian plume model may not be suitable for release events at the neighbourhood scale where the impact of individual buildings on dispersion patterns is significant and advanced dispersion models should be considered in such cases. At Lawrence Livermore National Laboratory, a dispersion prediction modelling system based on urban parameterization was recently developed (Monache *et al.*, 2009). The parameterization was based on a conceptual model of the urban boundary layer consisting of four sublayers with specific vertical wind profiles, velocity variances and vertical eddy diffusivities to represent the urban roughness effects on atmospheric flow. The effect of near-source buildings on initial dispersion was represented by an initial Gaussian distribution. In the current study, a new approach for solving the chemical plume tracing problem is presented that does not require the use of a forward-looking dispersion model, assumptions about the characteristics of spread of the chemical plume or *a priori* knowledge of wind profiles, wind speeds or wind directions within the region of concern. The approach is tested with numerically generated concentration distributions that are non-Gaussian in nature to demonstrate the possibility of chemical plume tracing in an urban setting.

METHODOLOGY

The methodology proposed in this study for chemical plume tracing using a sensor network consists of two components that will hereafter be referred to as discrete Fourier series and Particle Swarm Optimization respectively. The mathematical bases of these methods will be discussed briefly in this section while their method of implementation will be presented along with the simulation results obtained in the following section.

Discrete Fourier Series

A periodic function f(x) with period L can be expressed as a Fourier series given by the expression:

$$f(x) = a_o + \sum_{n=1}^{\infty}\left[a_n \cos\left(\frac{n\pi x}{L}\right) + b_n \sin\left(\frac{n\pi x}{L}\right)\right] \quad (1)$$

where n = 1, 2, 3, … and the coefficients are given by the integrals:

$$a_o = \frac{1}{L}\int_0^L f(x)dx \quad (2)$$

$$a_n = \frac{2}{L}\int_0^L f(x)\cos\left(\frac{n\pi x}{L}\right)dx \quad (3)$$

$$b_n = \frac{2}{L}\int_0^L f(x)\sin\left(\frac{n\pi x}{L}\right)dx \quad (4)$$

For mathematical analysis, the Fourier series may also be expressed in exponential form with complex coefficients:

$$f(x) = \sum_{n=-\infty}^{\infty}\alpha_n e^{i\left(\frac{2\pi n x}{L}\right)} \quad (5)$$

where $\alpha_n = \frac{1}{2}(a_n - ib_n)$, n = 0, ± 1, ± 2, … and α_n is given by:

$$\alpha_n = \frac{1}{L}\int_{-L/2}^{L/2} f(x) e^{-i\left(\frac{2\pi n x}{L}\right)} dx \tag{6}$$

By the convolution theorem, it may be shown that the coefficients α_n of the Fourier series expansion of f(x) are equal to the values of the corresponding Fourier transform of f(x), denoted as F(f), evaluated at n/L. In other words, the Fourier transform of a periodic function is then an infinite set of sinusoids (i.e. an infinite sequence of equidistant impulses) with amplitudes F(n/L) (Brigham, 1974).

Consider a continuous function f(x) and its Fourier transform F(f) which are discretized by sampling and truncation so that only a finite number of points, say N, are considered. If it is assumed that the N samples of the original function f(x) are one period of a periodic waveform, the Fourier transform of this periodic function is given by the N samples as computed by the expression:

$$F\left(\frac{n}{N\ell}\right) = \sum_{k=0}^{N-1} f(k\ell) e^{-i\left(\frac{2\pi n k}{N}\right)} \tag{7}$$

where ℓ = L/N and n = 0, 1, …, N-1. This is the well-established discrete Fourier transform (Brigham, 1974).

The sampling theorem states that if the Fourier transform of a function f(x) is zero for all frequencies greater than a certain frequency f_c, then the continuous function f(x) can be uniquely determined from a knowledge of its sampled values. Consider a discrete function containing N data points for which the corresponding continuous function is to be determined. Without loss of generality, the smallest interval between any two adjacent data points may be used to define the highest frequency component of the Fourier transform of the corresponding continuous function. Further, the domain of the discrete function may be assumed to be one period of a periodic waveform of the corresponding continuous function. This allows Eq. (7) to be applied for calculating values of the discrete Fourier transform of the discrete function and by the convolution theorem mentioned earlier, these will be equal to the coefficients of the Fourier series expansion of the corresponding continuous function. By this argument, the following expression for the double Fourier sine series of a two-dimensional continuous function may be derived from its discrete counterpart:

$$f(x,y) = \sum_{m=1}^{M}\sum_{n=1}^{N} a_{mn} \sin\left(\frac{m\pi x}{L_x}\right)\sin\left(\frac{n\pi y}{L_y}\right) \tag{8}$$

$$a_{mn} = \frac{4}{MN}\sum_{h=1}^{M}\sum_{k=1}^{N} f\left(\frac{h}{M},\frac{k}{N}\right)\sin\left(\frac{m\pi h}{M}\right)\sin\left(\frac{n\pi k}{N}\right) \tag{9}$$

Particle Swarm Optimization

The most challenging global optimization problems are those that do not contain any known structure that can be exploited. However, stochastic methods which generally require few assumptions on the optimization problem are particularly suited for such problems. The Particle Swarm Optimization (PSO) algorithm is a population based search algorithm based on the simulation of the social behaviour of birds within a flock (Engelbrecht, 2002). The initial intent of the particle swarm concept was to graphically simulate the graceful and unpredictable choreography of a bird flock (Kennedy and Eberhart, 1995), with the aim of discovering patterns that govern the ability of birds to fly synchronously and to suddenly change direction with a regrouping in an optimal formation. In PSO, a swarm of individuals are referred to as particles, with each representing a potential solution. Each particle is flown through a hyperdimensional search space in such a manner that the behaviour of each particle is influenced by its own experience as well as those of its neighbours. The concept behind PSO is based on the social-psychological tendency of individuals to emulate the success of other individuals and therefore represents a kind of symbiotic cooperative algorithm. The position and velocity of each particle, P_i, in the swarm are updated at each time step according to the following equations:

$$x_i(t) = x_i(t-1) + v_i(t)\Delta t \tag{10}$$

$$v_i(t) = \varphi v_i(t-1) + \rho_1\{x_{pbest,i} - x_i(t-1)\} + \rho_2\{x_{gbest} - x_i(t-1)\} \tag{11}$$

where $x_i(t)$ and $v_i(t)$ are the position and velocity of particle P_i at time t respectively, Δt is the time step which is assigned an arbitrary value of 1.0, ϕ is an inertia weight, ρ_1 and ρ_2 are random variables, $x_{pbest,i}$ is the position giving the best performance of P_i up to time t and x_{gbest} is the position giving the globally best performance of the entire swarm up to the current time. In the current implementation, particles that attempt to travel out of the domain of the function to be optimized are constrained to remain stationary at the edge of the domain until they reverse their direction of motion.

The second and last terms above are commonly referred to as the cognitive and social components respectively. The further away a particle is from its own best solution and the global best solution, the larger the driving force provided by these components to move the particle towards the best solutions. The random variables ρ_1 and ρ_2 are defined as $\rho_1 = r_1c_1$ and $\rho_2 = r_2c_2$, with r_1 and r_2 randomly selected from a uniform distribution U(0,1) and c_1 and c_2 are positive acceleration constants. Kennedy (1998) has shown that $c_1 + c_2 \leq 4$ is a necessary condition in this formulation. Velocities and positions tend to diverge to infinity otherwise. The inertia weight ϕ provides improved performance of the algorithm by controlling the influence of previous velocities on the new velocity. Physically, larger inertia weights cause larger exploration of the search space and vice versa. However, studies have also shown that the PSO algorithm does not converge for all combinations of the inertia weight and the acceleration constants c_1 and c_2. To ensure convergence, the following relation must hold (Van den Bergh, 2002):

$$\varphi > \frac{1}{2}\left(c_1 + c_2\right) - 1 \tag{12}$$

with $\phi \leq 1$. The PSO algorithm tends to exhibit cyclic or divergent behaviour if the above relation is not satisfied. In the present study, values of the above parameters used were $c_1 = 1.0$, $c_2 = 1.0$ and $\phi = 0.5$.

RESULTS AND DISCUSSION

We first suppose a scenario whereby a region measuring 1 km by 1 km is contaminated with a toxic chemical or pollutant that is released from an unknown location within the region. The chemical forms a gaseous plume that is invisible and odorless. Due to turbulent atmospheric conditions, geographical landscapes, natural and man-made structures within the region, a complex distribution of the chemical results. Figure 1a shows a randomly generated two-dimensional function that is used to simulate such a scenario. The colour contours represent concentrations of the chemical with red and blue indicating high and low concentrations respectively. In comparison with Gaussian plume or puff types of dispersion patterns, such a concentration distribution is more likely to arise in a chemical release incident that occurs in an urban setting due to the complex boundary conditions imposed by the buildings and structures as well as other factors such as street canyon effects. Pockets of chemicals may form at various positions within the region as a result of the chemical being trapped in dead zones around buildings and structures. However, in an actual chemical release incident, such a contour map is almost certainly unavailable for analysis. If it were, the chemical plume tracing problem would be solved instantaneously simply by a visual search for the location of highest chemical concentration within the region. In principle, the entire contour map can be constructed by performing a very large number of measurements at different positions in the region but this is almost never practically possible in an emergency situation. Instead, we assume that a network of stationary sensors had been pre-installed within the region prior to the chemical release incident.

Each sensor, represented by a white dot in Figure 1a, is capable of making concentration measurements in real time at its own location and transmitting those measurements to a central computer system for analyses. With a network containing 10 × 10 sensors, this is equivalent to taking 100 point measurements of the continuous concentration distribution and we then ask whether it is possible to achieve an accurate re-construction of the entire contour map with these discrete data points. Treating this set of discrete values as a discrete function whose continuous equivalent was to be derived, the discrete Fourier series method was applied to this discrete function. Figure 1b shows the resulting contour map that was re-constructed from this set of discrete values. On comparison between the two panels, it may be seen that the major features of the original contour map in terms of approximate regions where high and low concentrations of chemical occur had been re-constructed although quantitative differences in the actual concentration distributions may be discerned. The re-constructed contour map may be adequate for chemical plume tracing if it allows a good approximate of the global maximal point of the original concentration distribution to be located. Otherwise, a larger number of discrete values of the concentration distribution may be required for a more accurate re-construction.

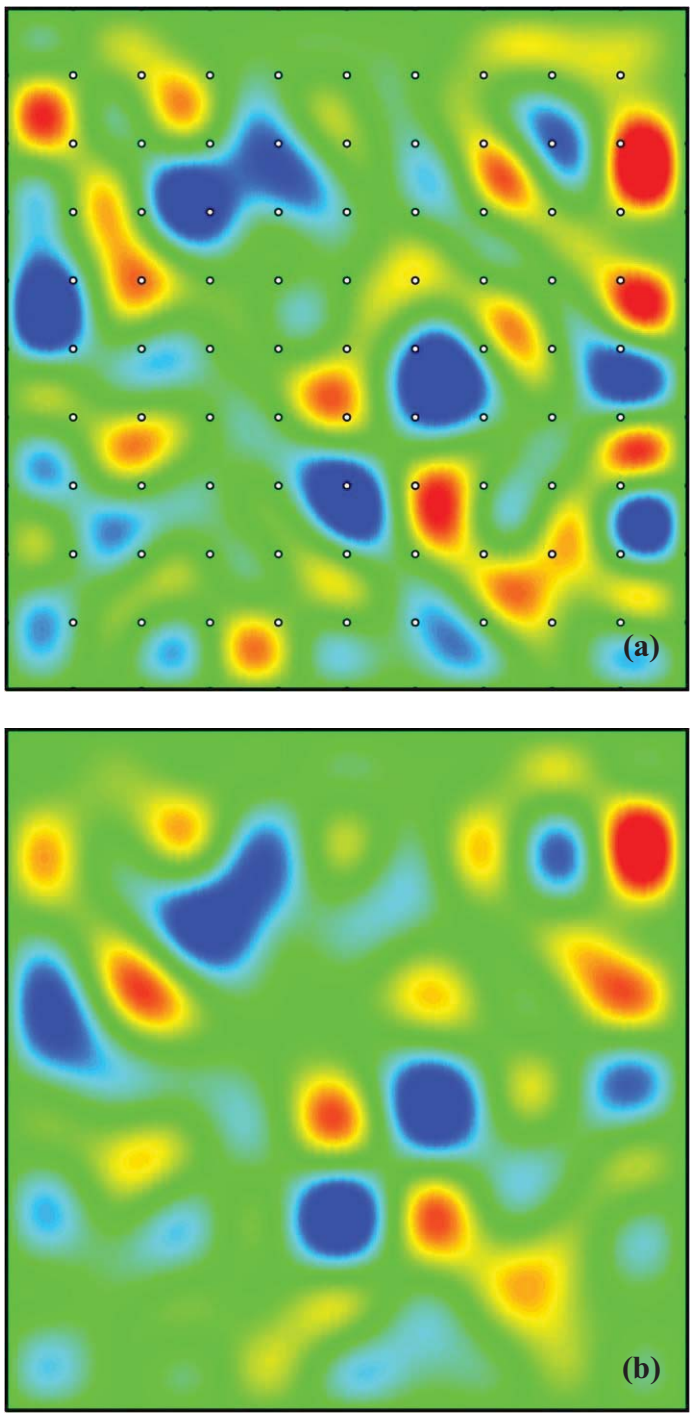

Figure 1. Concentration distribution of a chemical released from an unknown location within a 1 km by 1 km region. The colour contours represent concentrations of the chemical with red and blue indicating high and low concentrations respectively. (a) A network of 10 × 10 chemical sensors represented by white dots is assumed to have been pre-installed before the chemical release incident. Each sensor is capable of making concentration measurements in real time at its own location and transmitting those measurements to a central computer system for analyses. (b) Concentration distribution of the chemical that has been re-constructed from the sensor measurements using the discrete Fourier series method. Major features of the original contour map have been re-constructed although quantitative differences may also be discerned.

Figure 2a shows another arbitrarily generated concentration distribution which contains a larger number of high and low concentration regions. Correspondingly, as depicted by the white dots shown on the figure, it was assumed that a larger number (20 × 20) of sensors were present in the region for concentration measurements. On performing the re-construction process by applying the discrete Fourier series method to this set of discrete values, Figure 2b shows that a much more accurate representation of the original concentration distribution is obtained. In fact, the original and re-constructed contour maps are almost indistinguishable from each other. It may then be expected that a good

approximate of the global maximum of the original concentration distribution can be obtained by applying the PSO algorithm to the re-constructed contour map and this will be presented next. It may be noted at this point that the re-construction process applied here did not require any prior assumptions about the characteristics of spread of the chemical plume or *a priori* knowledge of wind profiles, wind speeds or wind directions within the region as mentioned earlier. The sensors were assumed to be capable of measuring concentration of the chemical or pollutant at their respective positions only and no other information was utilized.

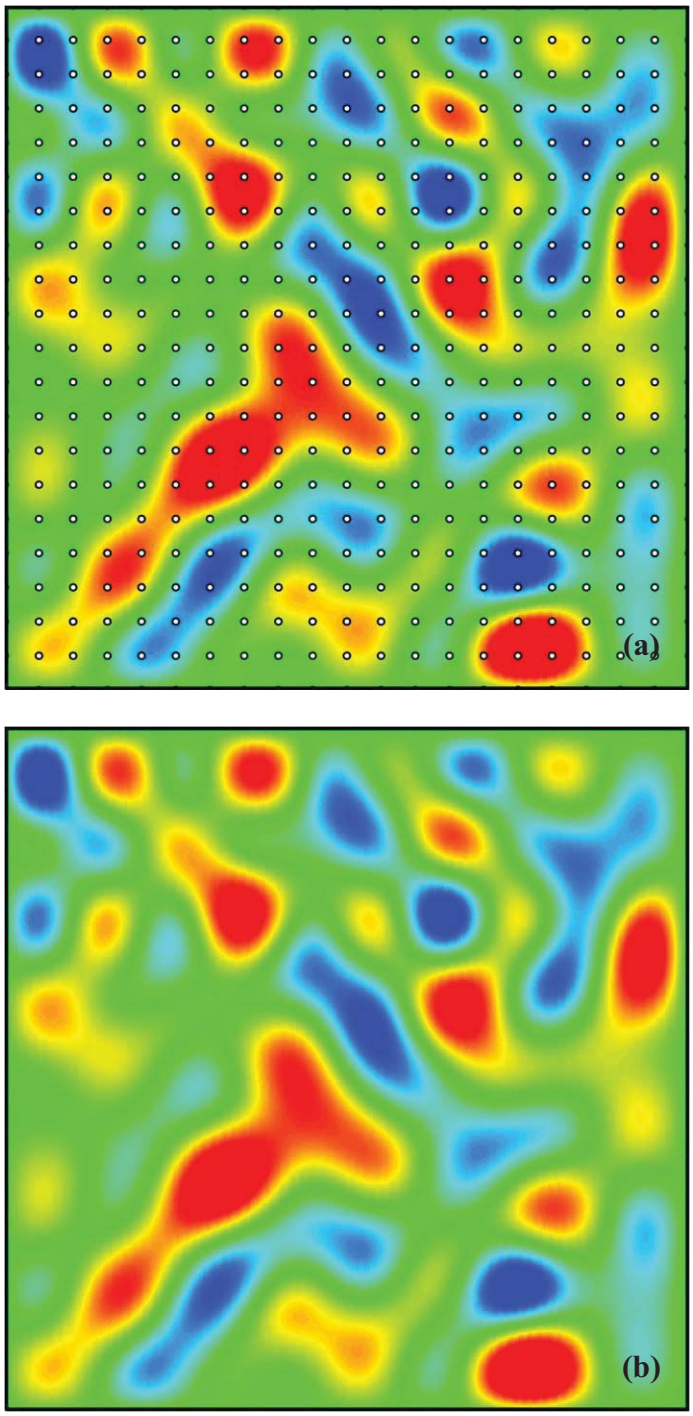

Figure 2. Concentration distribution for a more complex chemical release scenario. (a) Correspondingly, a larger number of sensors represented by white dots is assumed to have been pre-installed. As with the previous scenario, the sensors report point measurements of the continuous concentration distribution. (b) Treating the set of discrete values from the sensor network as a discrete function whose continuous equivalent is to be derived, the discrete Fourier series method is applied and a much more accurate representation of the original concentration distribution is obtained.

With an accurate re-construction of the chemical concentration distribution, the chemical plume tracing problem is essentially solved as what remains is simply determination of the location of highest concentration within the region.

This necessarily assumes that the source is continuing to emit the chemical or pollutant during the plume tracing process. The contrasting scenario whereby the source is empty and no longer emitting is considered to be outside the scope of the present study. The chemical plume tracing problem may then be treated as an optimization problem in which the objective function to be maximized is the discrete Fourier series representation of the concentration distribution given by Eq. (8) and (9). The PSO algorithm introduced earlier may then be applied to locate the global optimum of this objective function. Figure 3a shows positions of 10 PSO particles randomly distributed over the domain of the re-constructed contour map from Figure 2b at the start of the optimization process. The positions of these particles were updated iteratively via Eq. (10) and (11) and after 1000 iterations, Figure 3f shows that all particles converged to a common location on the contour map. It was verified manually that this final position of all particles was the global maximal point of both the original and re-constructed contour maps. This indicates that the PSO algorithm had been successful in achieving global optimization of these functions. More importantly, this also means that localization of the source of chemical release had been successfully achieved. To our knowledge, this is the first report of solving the chemical plume tracing problem by the approach of global optimization of a re-constructed concentration distribution of the chemical.

Several such chemical plume tracing simulations had been conducted in the course of this study and the methodology presented here comprising of the discrete Fourier series method and PSO was found to be successful in solving the chemical plume tracing problem in each case. The program codes for the algorithm were executed on a typical personal computer and computation times were always negligible in the sense that results were always generated almost instantaneously. It may also be noted at this point that the only assumption required for the methodology to be successful is that the position of the source of chemical release to be located is also the point of maximal chemical concentration within the entire region. This assumption is expected to hold as long as chemical is still being released from its source during the search process and this allows the chemical plume tracing problem to be transformed into an optimization problem as has been done here. The contrasting problem where the source is depleted before the search begins may be referred to as a chemical puff tracing problem. Although not shown here for the sake of brevity, direct application of the methodology to such a scenario would lead to particles in the PSO algorithm ‘chasing’ after the most concentrated puff rather than converging towards the position of the depleted source. For both chemical plume and puff scenarios where a highly lethal but invisible cloud may be sweeping across a country rapidly, the ability to have a visual image of the entire dispersion process can be very beneficial for warning purposes and evacuation planning. This is especially so for residents who are situated in the path of the toxic cloud. In the context of such chemical release scenarios, it is believed that the algorithm developed in this study will be able to play an instrumental role towards national defense for any country in the world that is subjected to such threats.

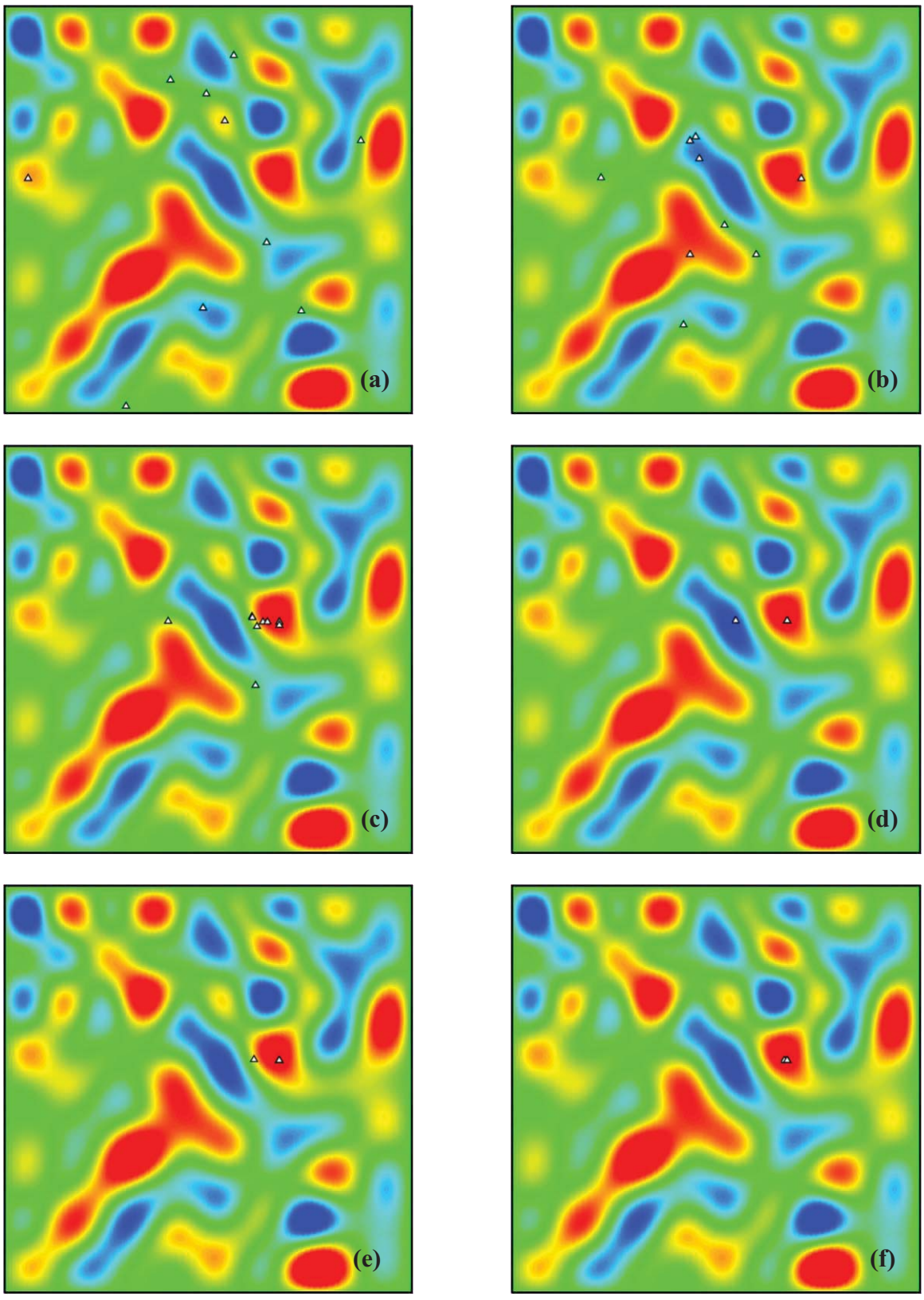

Figure 3. Chemical plume tracing by Particle Swarm Optimization (PSO) performed on the contour map that has been re-constructed by the discrete Fourier series method. (a) 10 PSO particles are initially randomly distributed over the domain of the re-constructed contour map. Snapshots of the search process show positions of the particles after (b) 200, (c) 400, (d) 600, (e) 800 and (f) 1000 iterations of the PSO algorithm. All particles converged to a common location on the contour map after 1000 iterations. This final position of all particles is the global maximal point of both the original and re-constructed contour maps. This indicates that the PSO algorithm has been successful in achieving global optimization of these functions and that localization of the source of chemical release has been successfully accomplished.

CONCLUSIONS

A novel methodology for solving the chemical plume tracing problem that utilizes data from a network of stationary sensors has been developed in this study. During a toxic chemical release and dispersion incident, the imperative need of first responders is to determine the physical location of the source of chemical release in the shortest possible time so that appropriate countermeasures can be carried out in a timely fashion so as to minimize the extent of human casualties. However, the chemical plume that develops from the source of release may evolve into a highly complex distribution over the entire contaminated region due to such factors as turbulent atmospheric conditions, geographical landscapes, presence of natural and man-made structures etc. In the face of such unpredictable conditions and mathematical complexities, the problem of chemical plume tracing by the use of a sensor network has not been resolved satisfactorily to date.

The methodology presented in this study for solving this problem comprises of contour re-construction and global optimization to locate the source of chemical release. The discrete Fourier series method was applied for re-construction of the contour map representing the concentration distribution of chemical over the contaminated region based on point measurements by sensors in a pre-installed network. PSO was then applied to the re-constructed contour map to locate the position of maximal concentration representing the position of the source of chemical release. This methodology was found to be highly successful in solving the chemical plume tracing problem via the sensor network approach. It does not require the use of a forward-looking dispersion model, assumptions about the characteristics of spread of the chemical plume or *a priori* knowledge of wind profiles, wind speeds or wind directions within the region of concern. The approach has been tested with randomly generated concentration distributions that are non-Gaussian in nature to demonstrate the possibility of chemical plume tracing in an urban setting. Furthermore, the nature of the methodology is such that a visual image of the entire chemical dispersion process is made available during the solution process and this can be beneficial for warning purposes and evacuation planning in scenarios where a highly lethal but invisible chemical cloud may be sweeping across a country rapidly. In the context of such chemical release scenarios, the algorithm developed in this study is believed to be able to play an instrumental role towards national defense for any country in the world that is subjected to such threats.

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