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Modeling dense gaseous contaminant pathways over complex terrain using a geographic information system

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Abstract

An impedance surface approach within a geographic information system (GIS) is used to model dispersion pathways for dense, gaseous, hazardous contaminants across complex terrain. The impedance surface methodology is tested using the Nogales Arizona–Sonora region of the US–Mexico border for simulation under varying wind conditions. This approach provides a realistic approximation of potential dispersion patterns in complex terrain where most existing dispersion models are inappropriate.

1. Introduction

Most attempts at modeling the dispersion of denser-than-air contaminant clouds focus on the fluid mechanics and atmospheric dynamics of the advection–dispersion problem with minimal attention given to the effects of complex terrain on gas movement. This is acceptable for many regions of the earth and for many airborne contaminant typologies. Indeed, many of the currently available models have been validated with data from releases of liquefied natural gas (LNG), liquefied petroleum gases (LPG), and ammonia over water or flat, dry lake beds [1–4]. These are all cases where the terrain complexity can reasonably be assumed unimportant. In areas with very complex terrain, however, the character of the terrain may dominate flow and models built for flat terrain would not provide adequate results. This research focuses explicitly on the characteristics of the terrain to delineate pathways for dense gas dispersion. A model is developed which integrates terrain factors that impede or enhance the flow across the surface. The form of the model is based upon impedance surfaces, and the development of impedance surface models is only possible with

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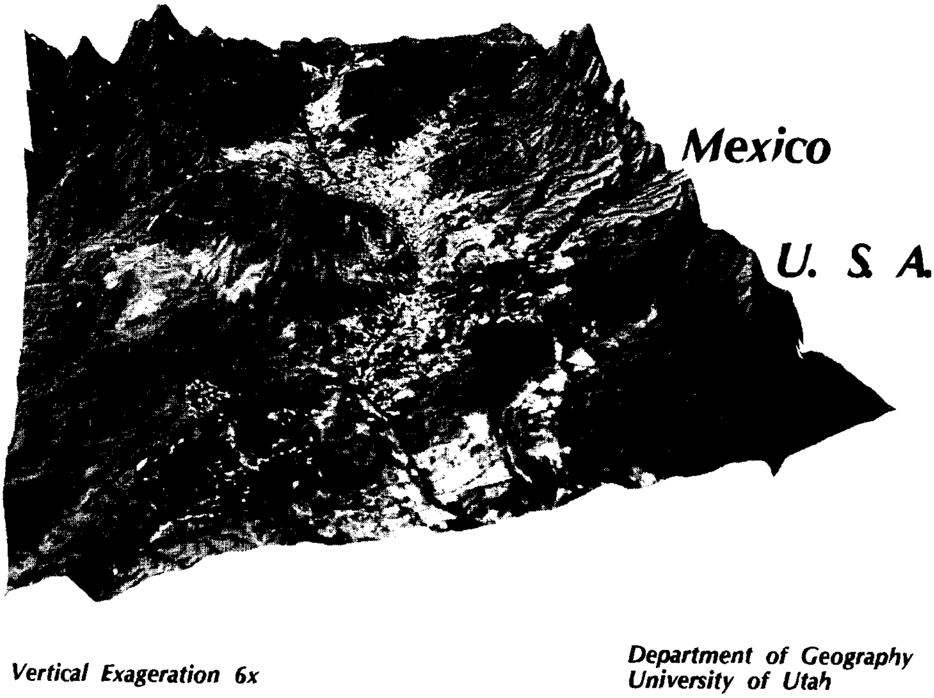


Fig. 1. Panchromatic Landsat composite image draped over a digital terrain model of Nogales Arizona–Sonora. The urbanized area (shown by lighter values in the image) is contained by a generally north–south trending valley. Note: elevations are exaggerated 6 ×.

advancements in raster geographic information systems (GIS) technology. The region of Nogales, Arizona–Sonora is used as the research site due to its complex terrain and channeling, valley topography (Fig. 1). Also, numerous trans-national industrial facilities, known as maquiladoras, are located in Nogales, Sonora and are located primarily upslope from densely settled residential and commercial areas straddling the United States–Mexico border. This research develops realistic simulations of the pathways a dense, gaseous contaminant would take in complex terrain.

2. Existing dispersion models

Interest for modeling dense gas dispersion has been primarily motivated by the consequences of flammable or toxic chemical releases [5–7]. In the dense gas dispersion literature the term "model" can mean a physical model or a numerical model of the area and release. The fluid mechanics inherent in physical models are only understood in a limited way, and are impossible to fully incorporate in a numerical model [8]. The high cost of constructing and operating a physical model can often be prohibitive, however, and numerical models are used as a more cost effective, flexible, and often more expeditious alternative.

In order to address the complexities of the physical problem, numerical models must make assumptions about the fluid dynamics and chemistry occurring in the dense gas cloud. One of the first and often most unrealistic assumptions made by most existing numerical models is that of flat terrain. As Britter and Snyder [6] state,

> "... the eventual user of this knowledge (attempting, for example, a risk assessment study) must consider the far more complicated problems of incorporating real terrain and local obstacles, and, as a result, has sought more effort in these areas. Common sense suggests that topography, in the form of ground slope, isolated hills or more complex terrain, will alter or divert the cloud or plume. The topography may enhance plume dilution and divert the plume away from regions of elevated terrain. Alternatively, the dense gas plume may be channeled into valleys or low-lying areas and be protected there from the diluting influence of the ambient flow".

Nevertheless, most existing dense gas numerical models do not consider the effects of terrain and focus exclusively on the fluid mechanics for the flat terrain problem.

All of the existing numerical models use the fundamental physical laws of conservation of mass, energy, and momentum to model the dense gas dispersion and can be assigned to one of three general categories [9, 10]. Box models treat the cloud as a uniformly mixed volume and use a lumped parameter model. Intermediate models break the cloud into smaller pieces and use mean variables in the conservation equations to model dispersion. Several box and intermediate models are compared in [11]. In this study each model is given the same input parameters and the model outputs are compared to each other in a "code comparison" (i.e. no comparison to empirical data). Full, time variant, 3-D finite element models are the only existing models to integrate topography. These models solve the conservation equations in their full forms within a 3-D finite element mesh [9].

Several of the public domain and proprietary numerical dispersion models available for the flat terrain dispersion scenario are listed in Table 1. The HEGADAS/HEGABOX models combine a box model of the initial release and gravity slumping (HEGABOX) with an intermediate model (HEGADAS) of the subsequent gravity spreading of the phase of the dispersion process. As with most box models, HEGABOX assumes a uniform concentration cylinder of gas as the source and models gravity slumping with top and edge entrainment of air into the slumping cylinder [12]. DEGADIS models dense gas dispersion in three distinct phases: near field, intermediate field, and far field dispersion [10, 13]. Near field dispersion is a box model of the gravity slumping much as in the HEGABOX model. As atmospheric flow becomes more important DEGADIS uses an intermediate field model which disperses the cloud in x, y, and z dimensions until the cloud is neutrally buoyant. At this point, a far field model is used to model the dense gas as a trace gas in the atmosphere. SLAB and FEM3 are closely related models [14]. SLAB solves the cross-wind averaged equations which results in a "quasi" 3-D-model, and FEM3 is a fully time dependent, 3-D finite element model. FEM3 is the only model reviewed which can account for variable ground topography [9, 14]. The principal advantage

Table 1
Common dense gas dispersion models [12]

Model name	Institution
AFTOX	US Air Force
ALOHA	NOAA
AVACTA	Aerovironment, Inc.
DEGADIS	US Coast Guard and Gas Research Institute
HEGADAS	Shell Development Co.
OME	Ontario Ministry of the Environment
SLAB	Lawrence Livermore National Laboratory
AIRTOX	ENSR Corp.
CHARM	Radian Corp.
CHEMS-PLUS	Arthur D. Little
EAHAP	Energy Analysts, Inc.
MESOCHEM	Impell Corp.
SAFEMODE	Technology and Management Systems, Inc.
TRACE	E.I. DuPont DeNemours and Co.

of all other models over FEM3 is the relatively low computational effort required for a simulation.

All of these existing models focus on developing concentration profile estimates for flash point and toxicologic calculations in a flat terrain release. In contrast, the objective of this research is to estimate the pathway which a dense, gaseous contaminant would take in complex terrain. The complex terrain pathway estimates do not include chemical concentration profile information at this time; however, the pathway information itself is important information to people working in chemical emergency preparedness and community planning.

3. Impedance surface models in a GIS

A geographic information system, or GIS, is the integration of database management, analytic and cartographic display capabilities specifically focused on organizing, analyzing, and visualizing geographic and spatial data. Geographic data are characteristics about a phenomenon for which the absolute and relative positions (i.e. spatial context) are important. GIS's are much more than electronic maps, however. The database structure inherent in a GIS facilitates analysis and modeling of spatial processes (e.g. dispersion) [15–18]. GIS's are also very useful as integrators of geographic data from diverse sources, such as, digital elevation models (DEM), digital line graphs (DLG), census demographic data, and satellite imagery.

A raster GIS represents geographic space as a regular, 2-dimensional tessellation of the earth's surface. The tessellation typically divides an area into many small, contiguous squares. Conceptually, each small square, or cell, contains a value for a single

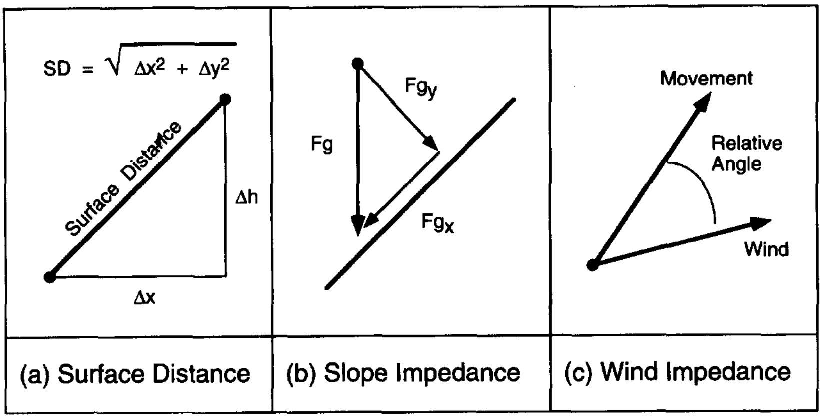


Fig. 2. Three factors for developing an impedance surface dispersion model–surface distance, slope impedance, and wind impedance. The product of these factors forms the basis for the dense gas dispersion model.

phenomenon (e.g. elevation) which is representative of the level of the phenomenon at the center point of the cell. Implicit in the raster data structure is a network which connects the center point of each cell with its four adjacent and four diagonal neighbors. The network structure creates eight (8) neighbors for each cell, and results in a queen's case neighborhood. This implicit network in a raster GIS is used as the foundation for impedance surface modeling. Impedance surfaces are raster data sets in which the value in each cell represents the difficulty of movement over that cell. Using a distance weighted average between cells a unique impedance can be calculated for each link between adjacent center points in the network. Summing impedances between adjacent cells calculates the overall impedance between any two cells. Identifying the significant factors contributing to the impedance and developing the functional dependence between those factors and the impedance variable are the major tasks in impedance surface modeling. In addition to the impedance surface data layer, dispersion modeling requires a second GIS data layer which identifies the location of the contaminant source. The dispersion model assigns to each cell in an *accumulated* impedance layer the total *accumulated* impedance for the path between that cell and the nearest (in impedance measure) contaminant source cell. In dispersion terms, this makes the cell locations with higher impedance more difficult to reach by the source of a dense gas contaminant.

Three major factors have been incorporated into the dispersion model. They include surface distance, slope impedance, and wind impedance [19, 20] . Surface distance is simply the distance between adjacent nodes taking into account variable slopes in the terrain (Fig. 2(a)). Using the raster representation of space the surface distance is approximated using the known distance between cells (Δx), a DEM (Δh), and the Pythagorean theorem. Because a negatively buoyant gas is being modeled, a slope impedance factor is also required. This factor accelerates the dense gas flow down steeper slopes more rapidly than shallow slopes. Therefore, as the downhill angle increases the gas velocity increases, or conversely the impedance between cells decreases. The functional dependence between slope angle and impedance is derived by vector decomposition of the gravitational force vector into components parallel and perpendicular to the surface slope (Fig. 2(b)). The slope impedance is then inversely proportional to the gravitational component parallel to the surface slope. Winds are accounted for in a similar manner. The relative angle between the movement direction and the wind direction is used to determine the amount which the wind either assists flow or retards flow (Fig. 2(c)). The wind impedance factor changes the overall impedance of cell-to-cell links based on this angle, resulting in downwind travel which is easier (i.e. lower impedance) than upwind travel.

The three factors, surface distance, slope impedance, and wind impedance, multiplied together functionally define the overall impedance (Eq. (1)).

$$I_T = (D_s \times I_s \times I_w), \tag{1}$$

where I_T is the total impedance; D_s is the surface distance; I_s is the slope impedance; and I_w is the wind impedance. Surface distance and slope impedance are required inputs to the model. If meteorologic data are unavailable then the wind impedance is set equal to one, and does not affect the impedance surface calculations (see Fig. 4 for an example). The product of the three factors is used to compute the accumulated impedance surface. The impedance surface modeling for this research used the spatial and algebraic operators provided in the GRID spatial modeling module of ARC/INFO geographic information system software.

The impedance model requires assumptions about the environmental and physiochemical characteristics of the contaminant release. Terrain and wind flow are assumed to be the sole environmental determinants which define contaminant dispersion pathways. It is recognized that other factors, such as top entrainment, edge entrainment, and thermal mixing, are present in the dispersion process; however, at this time these factors cannot be integrated into the impedance surface model, and are beyond the scope of this paper. Industries in Nogales, Sonora are typically single level, low stack height facilities. Therefore, the model assumes the release to be near-ground-level. The model also assumes a sustained release, as opposed to instantaneous, finite duration, or time variant release, with no significant momentum or jetting. The chemical being released is assumed to be denser-than-air, non-reactive, and non-depositing.

4. Study area

The population in Nogales Arizona–Sonora has grown rapidly over the past 25 years. Nogales, Arizona currently has a population of approximately 20,000, while Nogales, Sonora has a population over 200,000 people [21]. Fig. 1 is a panchromatic satellite image of Nogales Arizona–Sonora draped over a digital terrain model. In this image, urbanized areas are shown by lighter values, and heavily developed areas (e.g. industrial locations) are nearly white. The urbanized area of both cities concentrates along the narrow, north–south trending valley surrounded by very steep and complex terrain.

Multinational firms relocate to the border region due to lower labor costs, tariff considerations, and limited enforcement of environmental regulations. At the same time, geographic proximity of firms to the US market is maintained. Approximately 80 maquiladora plants, including electronics manufacturing, plastics fabrication, and automotive part manufacturing sites, are located in Nogales, Sonora. Most of the maquiladoras, as well as several domestic firms, have located in industrial zones at the southern end of the Nogales, Sonora urbanized area. In addition to chemicals found in any urbanized area (e.g. LNG and gasoline), these manufacturing sites bring a variety of chemical species into the Nogales region, such as mono and polyhalogenated solvents and refrigerants (e.g. carbon tetrachloride, perchloroethylene, and freon), and various aromatic compounds (e.g. alkylated benzene's, halogenated benzene's, and phenols) [22]. Many of the chemicals listed above have been identified as human health hazards and pose a potential health risk to the community [23, 24].

Unique topography and present land use patterns make the environmental risk of contamination by liquid and airborne hazardous materials released from one of these industrial firms an issue of great concern to local residents on both sides of the border. The primary surface and sub-surface flows are from the higher elevation south toward the north and the Santa Cruz River. The major industrial zones in Nogales, Sonora are located at approximately 1300 m in elevation, whereas the primary business and residential areas of both Nogales' are located between 1150 and 1200 m in elevation [25]. Most hazardous contaminants released into the air or water will follow pathways from the higher elevation industrial areas to the lower elevation commercial and residential areas. The steep-sided valley configuration will hold airborne contaminants within the populated area, thereby, increasing the potential risk to human health. The valley topography also creates a diurnal wind cycle in this region [26]. Depending on the time of the day, the diurnal cycle can either hold airborne contaminants within the valley or flush the contaminants out of the valley. This nexus of human settlement and activities with an unusual set of environmental conditions makes this region an ideal simulation test area.

5. Impedance model results

A base map (Fig. 3) is provided for geographic reference to Nogales, Arizona–Sonora and shows important topographic, population, and industrial features of the region. Features to note are the major north-south trending valley and the large hill (point A) just south of the international border. As indicated by the density of roads, a majority of the population lives west and north of point A. Diamonds indicate the location of maquiladoras, and a circle indicates the location of the simulated release. The simulated release is at the center of the southern-most cluster of maquiladoras, and represents the location of one of the largest (by employment) industrial sites in Nogales, Sonora. This site was chosen because the results of the

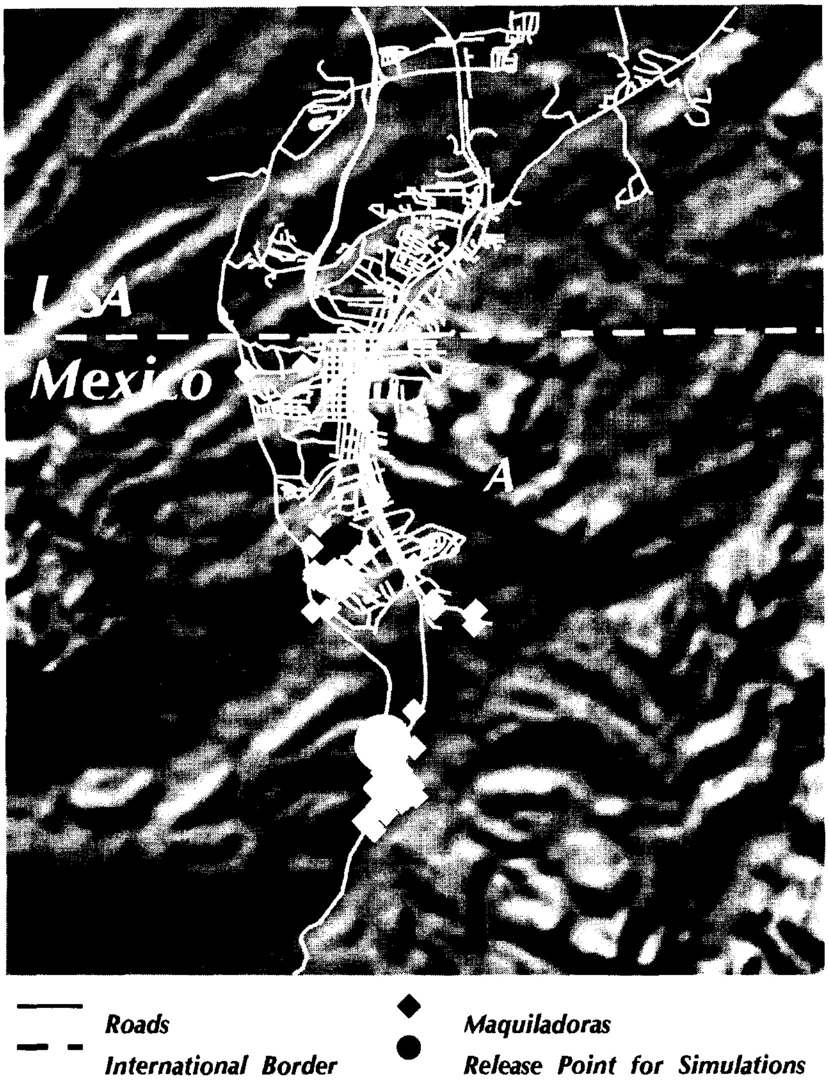
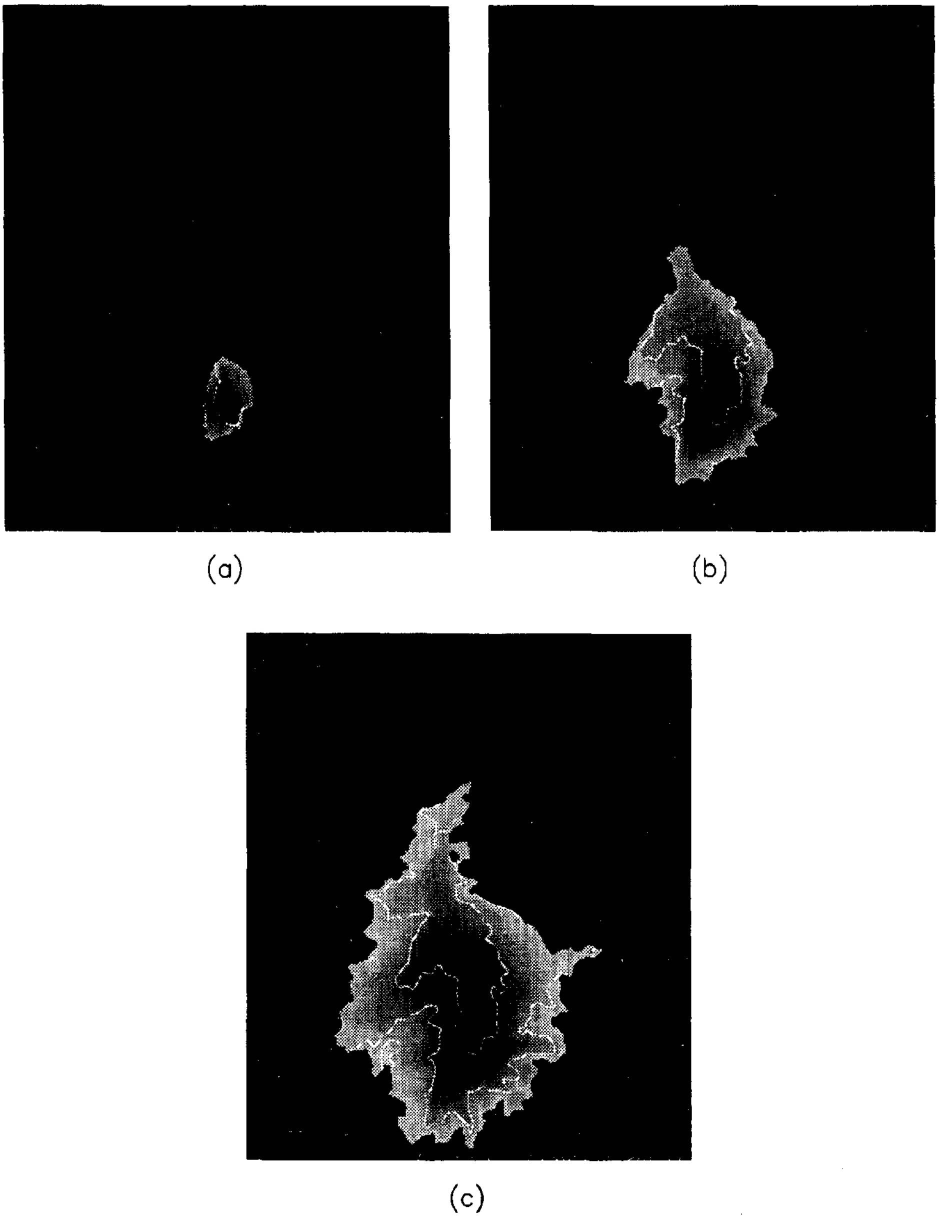


Fig. 3. Shaded relief, major roads, and industrial activity in Nogales Arizona–Sonora. Density of the roads is indicative of population density. Maquiladoras are represented by diamonds and the simulated release site is represented by a circle.

simulations would be representative of the chemical dispersion pathway created by a release from any of the maquiladoras in the area.

Results from the impedance surface model are presented in Figs. 4 and 5. The DEM used in the model has 25 m × 25 m cells and was generated by spatially interpolating digitized hypsography of the area. Fig. 4 shows model results when there is no wind in the valley and gravity flow is the major driving force for contaminant movement.

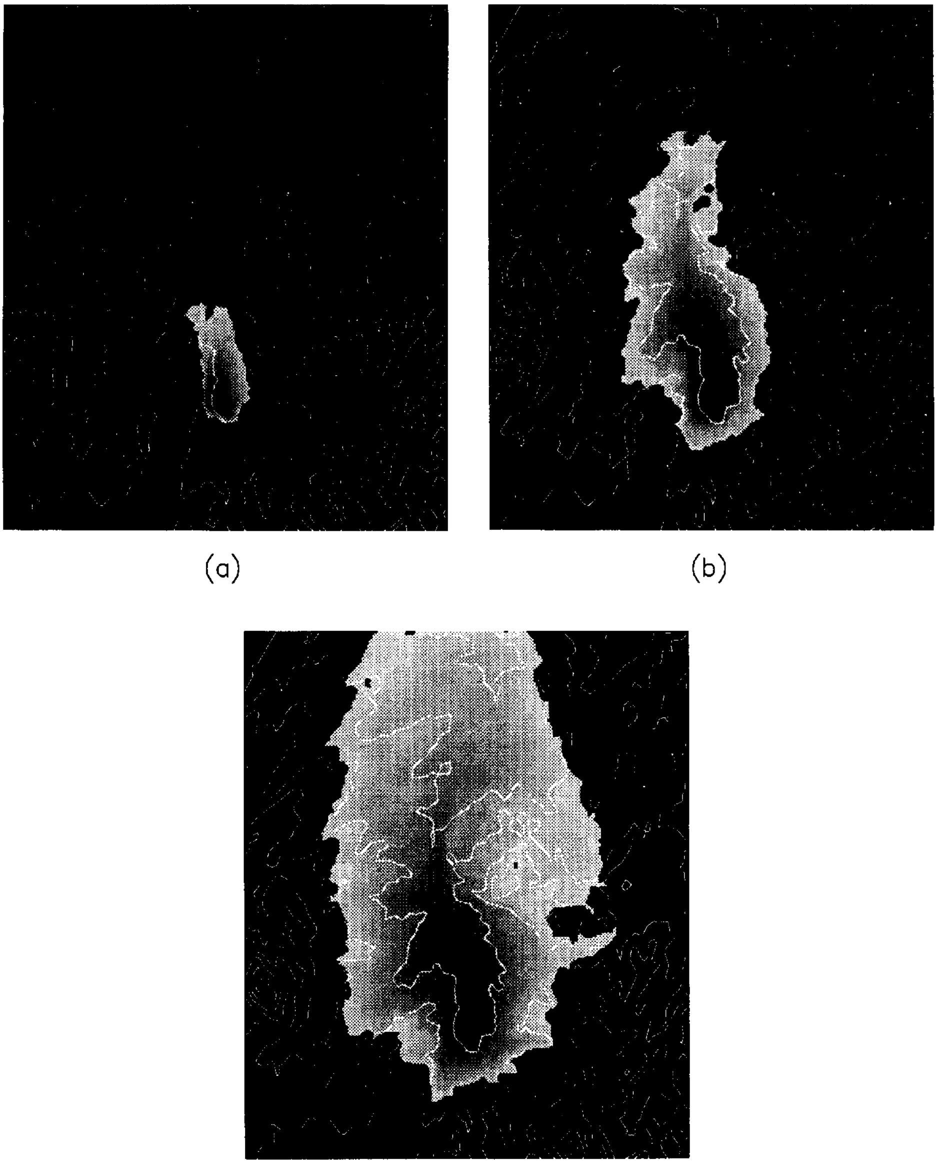

(a)

(b)

(c)

Fig. 4. Impedance surface model results with no wind.

Fig. 5 presents model results when the effects of gravity are combined with a southerly wind. A southerly wind is defined as a wind which is uniformly from the south at a constant velocity over the entire study area. More complex wind vector maps may



(a)

(b)

(c)

Fig. 5. Impedance surface model results with a southerly wind.

be used in the impedance surface model, however no such maps are yet available for the Nogales area. Both figures are a series of level slices from the accumulated impedance surface for each wind scenario. The gray scale range within the level slice is indicative of the accumulated impedance at each cell, with darker grays connoting low accumulated impedance and lighter grays connoting higher impedance. The black background and white, 50 m contour lines are provided as a georeference. Because level slices for each wind scenario are equivalent, they can be compared directly to track the progress of the contaminant and qualitatively evaluate the model.

Initial contaminant spread in the no-wind scenario (Fig. 4(a)) flows toward the valley channel to the north and east of the initial release point. Down-channel spread in Fig. 4(b) is higher due to the steeper downhill gradient, and this forces the contaminant cloud around the aforementioned hill (point A) rather than over it. In Fig. 4(c) the cloud has worked its way around the hill and into a low lying valley to the south and east of the hill. The movement of the gas is entirely determined by the accumulated impedance surface for each senario. The lesser impedance path determines whether the gas engulfs or goes around the hill. With the notable exception of FEM3, none of the existing dense gas dispersion models consider the effects of the valley channeling topography. Indeed, it would be inappropriate to use these other models in the Nogales area, or any other area with similar terrain. Fig. 5 demonstrates the simultaneous effects of a southerly wind and terrain on dense gas dispersion. In this series of level slices there is much less lateral dispersion compared to the same level slice in the no-wind scenario. The wind forces the cloud down the valley more quickly while terrain still contains flow to the valley bottom and around the hill. Comparison of Figs. 4(c) and 5(c) demonstrates the acceleration of the cloud to the north by the southerly wind, causing the cloud to engulf the hill (point A) which was previously unaffected.

6. Impedance model evaluation

The impedance model presented in this paper produces georeferenced simulations of pathways taken by a dense gas dispersing over complex terrain. The impedance model dispersion patterns channel and conform to the confining valley topography. Two wind scenarios, no wind and southerly wind, are presented for comparison. Each simulation produced results which are consistent with the general understanding of how dense gases would disperse in complex terrain, and simulate the channeling characteristics described by Britter and Snyder [6]. Unfortunately, empirical validation of the model is not possible at this time. Controlled, monitored, dense gas release data in complex terrain is not available for any location. The output of the impedance model simulations are expected pathways which are georeferenced and ready for analysis with other geographic datasets, such as population density and school locations. The impedance model approach creates the pathway information quickly and in a less complex, and more integrated computing environment than complex finite element models.

Potential refinements to this approach would use gas density and wind velocity data to estimate chemical concentration profiles. These enhancements would add value to the model by providing chemical emergency response units with geographically referenced, near real-time chemical concentration profiles, as well as pathway estimates. This advancement is currently being investigated. To refine the model, surface wind data will be required. This task is being accomplished by Berman et al. [26]. In addition, the functional relationship between the rate of dense gas descent, slope steepness, and gas density needs to be understood. With this understanding the impedance surface could be modified to create estimates of concentration profiles for specific gases over time and geographic space.

Estimating and mapping the dispersion pathways in complex terrain, with or without concentration profiles, is an important achievement. Knowledge of these pathways serves as valuable input into chemical emergency preparedness and community development plans. The impedance model provides these inputs, and is able to give planners near-real-time estimates of dispersion path(s) for release(s) anywhere in the area. Incorporating this capability in a GIS, where georeferenced population density, age structure, land use, transportation, and overall human vulnerability information are readily integrated, is a major advancement in the use of dense gas dispersion models for realistic risk assessment and emergency response in regions with high topographic relief.

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