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Control of Chemical Spills by Boundary Suction

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Abstract: A method is presented for the control of chemical spills. The approach is based on real-time information provided by microsensors capable of monitoring instantaneous changes in the concentration of a chemical in solution or suspension. The method also utilizes current flow and transport data provided by a simulation model. Once a chemical cloud requiring control action is detected by the sensors, the model provides optimal directions to pre-installed boundary actuators capable of modifying the flow conditions in the system. The technique requires assimilation of data from the sensors to steer the model so the error between its current state and sensor measurements is minimized. The model also performs prediction simulations to determine the optimum set of actuator commands necessary to control the chemical plumes. Results of model control applications are shown to be capable of removing a chemical cloud from a flow through channel.

Key-Words: - Control; Channel Flow; Sensors; Actuators; Chemical spills; Pollution.

1 Introduction

The detectability and controllability of a chemical plume or cloud is of importance because of its threat to the quality of human life and property. This paper presents a construct by which a chemical spill can be detected automatically. The paper also presents a computer algorithm that can control flow and mass transport in man-made and natural channels by actuators that can eliminate the chemical cloud by blow and suction at the channel boundaries. The control process is based on a performance index that can be optimized in a period that is short enough to allow the implementation of the control function steps. This must include lag time in the system, feedback signal return and simulation time. It is obvious that adaptive control can only be achieved by an efficient algorithm that can perform numerous simulations of the system during the period of a single system response evaluation.

If a control mechanism is to be effective at all, both control and feedback signals must be transmissible in finite time. In other words, the process consists of two steps. First the boundary control function sends a signal to the output vector, i.e., the flow is changed by the actuator action, and in the following time increments, the characteristics of the flow are affected. Second, the differential change in the output vec-

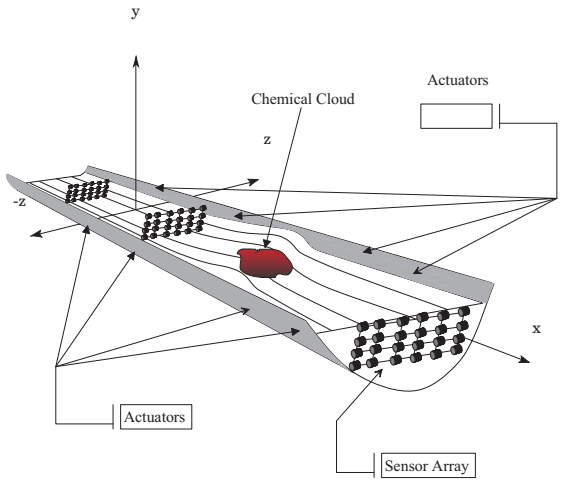

FIG. 1. Schematic of sensors and actuators

tor is sent back to the model, so it can sense the effectiveness of the signals transmitted and appropriately adjust its operation. The robustness of this closed-loop operation determines the success of the control action.

The alternative scenarios for the operation of the boundary controls can be determined by first calculating the sensitivity of the chemical cloud concentration to changes in the boundary controls. The tedious task of sensitivity calculation has been reduced by the use of equations which are adjoint to the governing equations [5]. Piasecki and Katopodes [9] have shown that control of contaminant plumes can be efficiently achieved using adjoint sensitivity analysis and Sanders and Katopodes [10] have demonstrated the control of multidimensional waves. The purpose of this paper is to apply the control process to determine blow and suction scenarios at the channel boundaries, so the elimination of a chemical cloud can be effected in real time.

2 Basic Equations

The basic hypothesis for real-time control is that a computer model is currently running and a sensor array has been installed in the prototype. The sensors are assumed to convey a continuous flow of data on all variables that are subject to simulation and control, as shown in Fig. 1. Since only a limited number of sensors is available, a background state $\mathbf{u}_b$ needs to be constructed to fill in the data voids. This is necessary in order to ensure that the model describes the current flow conditions as accurately as possible at all times. If necessary, the model is continuously adjusted to minimize the errors between computed and observed data.

A performance index $\mathcal{F}$ is constructed, based on two separate contributions. The first represents the distance between the measured vector of values $\tilde{\mathbf{u}}$ and the corresponding computed vector $\mathbf{u}$, based on the numerical model prediction. The second penalizes differences between the model's initial conditions $\mathbf{u}(0)$ and the background state $\mathbf{u}_b$. In general, the performance index can be written as follows

$$\mathcal{F} = \frac{1}{2}(\mathbf{u} - \tilde{\mathbf{u}})^T \mathbf{W}^{-1} (\mathbf{u} - \tilde{\mathbf{u}}) \qquad (1)$$

in which $\mathbf{W}$ is a weighting matrix that reflects the quality of the measurements, so measurements with large uncertainties contribute to the objective function to a lesser degree. The errors of various measurements are usually uncorrelated, so $\mathbf{W}$ is a diagonal matrix and thus easy to invert. Before any control action can be taken, the model must run through an assimilation period during which the initial conditions are optimized so the state predicted by the model agrees with the observations. The discrete dependent variables of the flow and transport equations can be written in the same vector form as follows

$$\frac{d\mathbf{u}}{dt} = f(\mathbf{u}, \alpha) \qquad (2)$$

in which the processes f include the spatial derivatives of the governing equations and any source terms, $\mathbf{u}$ is the vector of semi-discrete dependent variables and the vector α contains all other factors associated with the problem. In its most general form the parameter space includes initial and boundary conditions, resistance and mixing coefficients, feedback effects on parameters and, more importantly for the present study, the vector of the discrete values of the necessary actuator commands.

Adaptive control by history matching was first demonstrated by Chavent et al [6]. Control is achieved by an iterative method that optimally determines each value of the control action in a discrete time series by minimizing a user-selected objective function.

In order to assess the effect of a perturbation of a specific entry of the control vector, α, we introduce a functional of the corresponding output, which may be written as

$$\mathcal{F}(\mathbf{u}, \alpha, T) = \int_0^T \int_\Omega r(\mathbf{u}, \alpha, t)\, d\Omega\, dt \qquad (3)$$

where T is the time at which the effect is recorded, Ω is the solution domain and r is a user-specified response function, intended to establish a measure of the spatial and temporal distribution of the contaminant in the system. An estimate of the behavior of the response function due to changes in the loading vector is obtained by computing the total variation of Eq. (3). The present method uses the adjoint equations to compute all variations by a single run, so the optimization can be achieved in real time.

3 Direct Flow Model

As described in detail by Bradford and Katopodes [2], the model is based on the Reynolds averaged Navier-Stokes equations, i.e.

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}}{\partial x} + \frac{\partial \mathbf{g}}{\partial y} + \frac{\partial \mathbf{h}}{\partial z} = \mathbf{s} \qquad (4)$$

where $\mathbf{u} = (u \quad v \quad w)^T$ is the vector of fluid velocities in the x, y, and z directions, respectively, and $\mathbf{f}, \Delta g, \mathbf{h}$ are the flux vectors along these directions.

The term h represents the deviation of the free surface from the mean water level, $p = p_d/\rho_0$ where p_d is the dynamic pressure component. D_h and D_v denote the horizontal and vertical turbulence eddy diffusivities, respectively, and f is the Coriolis parameter. Several assumptions are implicit in Eqs. (4), which most notably include the Boussinesq approximation, Boussinesq eddy viscosity assumption, and constant atmospheric pressure. In addition, it has been assumed that turbulence anisotropy exists only between the vertical and horizontal directions.

In general, the free surface moves and therefore the domain of interest deforms with time. From a computational perspective, this can be handled by using a fixed numerical grid or a deforming grid with an upper boundary that moves with the free surface. The latter procedure is adopted in this study, which unfortunately prevents a direct calculation of the local fluid acceleration, $\partial \mathbf{u}/\partial t$. However, the Lagrangian fluid acceleration, $D\mathbf{u}/Dt$, can be computed and therefore the local acceleration may be determined as [1],

$$\frac{\partial \mathbf{u}}{\partial t} = \frac{D\mathbf{u}}{Dt} - w_d \frac{\partial \mathbf{u}}{\partial z} \qquad (5)$$

Note that it is assumed that the grid moves in the z direction only and w_d denotes the z component of the local velocity of the domain, i.e. $w_d = dz/dt$. This result can be substituted into Eq. (4) to yield

$$\frac{D\mathbf{u}}{Dt} - w_d \frac{\partial \mathbf{u}}{\partial z} + \frac{\partial \mathbf{f}}{\partial x} + \frac{\partial \mathbf{g}}{\partial y} + \frac{\partial \mathbf{h}}{\partial z} = \mathbf{s} \qquad (6)$$

In addition, the fluid is assumed to be incompressible, which is expressed as

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \qquad (7)$$

An expression for h is derived by integrating Eq. (7) in the z direction. Application of Leibnitz Rule, along with impermeable bottom and kinematic free surface boundary conditions, yields

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x}\left(\int_{-d}^{h} u dz\right) + \frac{\partial}{\partial y}\left(\int_{-d}^{h} v dz\right) = 0 \qquad (8)$$

Transport equations are solved for the fate and movement of scalars including buoyant plumes and turbulence quantities and an equation of state is used to relate the density of the fluid to scalars that may affect it [4].

4 Adjoint Equations

If A is a linear operator, the operator A^*, adjoint to A is defined by the Lagrange identity [7]

$$(Ah, g) = (h, A^* g) \qquad (9)$$

For the direct problem

$$A\phi(x) = f(x) \qquad (10)$$

we introduce an adjoint equation

$$A^*\phi^*(x) = r(x) \qquad (11)$$

where $r(x)$ is a user-defined function manifesting the difference between the direct model and the measurement of a sensor detecting a physical process. If we subtract the inner product of Eq. (11) and ϕ from the inner product of Eq. (10) and ϕ^*, we obtain

$$(A\phi, \phi^*) - (\phi, A^*\phi^*) = (f, \phi^*) - (r, \phi) \qquad (12)$$

Due to Lagrange's identity, the left-hand part of (12) is equal to zero. Then

$$(f, \phi^*) - (r, \phi) = 0 \qquad (13)$$

Therefore, to find the value of the functional $J_r = (r, \phi)$, we can alternatively solve $J_f = (f, \phi^*)$.

For the 3-D hydrodynamic and scalar transport equations (4), we can introduce a solution vector

$$\varphi = \begin{bmatrix} u \\ v \\ w \\ p \\ c \end{bmatrix}$$

and a nonlinear operator matrix

$$A(u) = \begin{bmatrix} \Lambda & -f & 0 & \frac{\partial}{\partial x} & 0 \\ f & \Lambda & 0 & \frac{\partial}{\partial y} & 0 \\ 0 & 0 & \Lambda & \frac{\partial}{\partial z} & 0 \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} & 0 & 0 \\ 0 & 0 & 0 & 0 & \Lambda \end{bmatrix}$$

where Λ is

$$\Lambda = \Lambda_1 + \Lambda_2 \tag{14}$$

$$\Lambda_1 = u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y} + w\frac{\partial}{\partial w} \tag{15}$$

$$\Lambda_2 = -D_h\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) - \frac{\partial}{\partial z}\left(D_v\frac{\partial}{\partial x}\right) \tag{16}$$

We can therefore rewrite governing equations (4) in the operator form, as follows

$$L\varphi \equiv B\frac{\partial \varphi}{\partial t} + A\varphi = 0 \tag{17}$$

where B is the matrix

$$B = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Then, Lagrange's identity leads to

$$(A(u)\varphi, \varphi^*)_{\Omega} = (\varphi, A(u)^*\varphi^*)_{\Omega} \tag{18}$$

For the nonlinear operator, if we assume that the solution of the direct problem is determined first and thus the function u can be consider as known. Then, by defining the following operators

$$\Lambda_1' u^* = -\left(\frac{\partial u u^*}{\partial x} + \frac{\partial v u^*}{\partial y} + \frac{\partial w u^*}{\partial z}\right)$$

$$\Lambda_1' v^* = -\left(\frac{\partial u v^*}{\partial x} + \frac{\partial v v^*}{\partial y} + \frac{\partial w v^*}{\partial z}\right)$$

$$\Lambda_1' w^* = -\left(\frac{\partial u w^*}{\partial x} + \frac{\partial v w^*}{\partial y} + \frac{\partial w w^*}{\partial z}\right)$$

and

$$A(u)^* = \begin{bmatrix} \Lambda^* & f & 0 & -\frac{\partial}{\partial x} & 0 \\ -f & \Lambda^* & 0 & -\frac{\partial}{\partial y} & 0 \\ 0 & 0 & \Lambda^* & -\frac{\partial}{\partial y} & 0 \\ -\frac{\partial}{\partial x} & -\frac{\partial}{\partial y} & -\frac{\partial}{\partial y} & 0 & 0 \\ 0 & 0 & 0 & 0 & \Lambda^* \end{bmatrix}$$

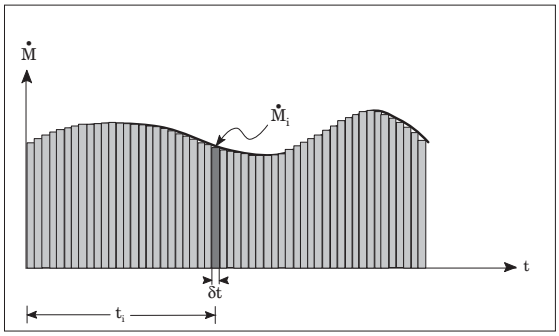

FIG. 2. History matching for actuators

where $\Lambda^* = \Lambda_1' + \Lambda_2$.

Then the adjoint problem becomes

$$-B\frac{\partial \varphi^*}{\partial t} + A^*\varphi^* = 0 \tag{19}$$

with initial conditions $\varphi^* =$ at $t = \bar{t}$ since the sensitivity should vanish at the end of the time of simulation of the direct problem.

A single solution of the direct problem, followed by a single solution of the adjoint problem, should then be sufficient to compute the objective function based on concentrations measurements of a chemical cloud. The functional $J((\varphi, r))$is completely equivalent to $J((f, \varphi^*))$, thus resulting in remarkable computational savings.

5 Sensors and Actuators

The sensor arrays are located either across the channel, as shown in Fig. 1 or along the side walls. Detectability studies carried out by Piasecki and Katopodes [9] indicate that the most efficient configuration from plum or cloud capturing consists of a series of arrays installed across the channel width. The sensor matrix is assumed to have no effect on the flow conditions. The miniature silicon-based chemical sensors that enable the monitoring of the plume are typically much smaller than conventional ion-selective electrodes or other chemical sensors. The primary advantage of small size is cost reduction. The sensors are mass-produced with hundreds of sensors on each silicon wafer.

Sensor miniaturization is directly advantageous, since with small sensors less calibration solution is needed, smaller samples can be used and signal-to-noise ratio can be enhanced [3]. Small size also makes arrays of sensors

very practical. In chemical plume monitoring, low cost and the benefits of arrays are the most compelling arguments for the use of microsensors [11]. Two types of electrochemical microsensors are used to detect the different analytes in this work. Potentiometric sensors are used to detect small ions such as hydrogen (pH) and potassium (K+). Amperometric sensors are used to detect analytes such as nitrate, cyanide and heavy metals [8].

Boundary control is implemented by blow and suction. Although arbitrary configuration of the actuators is possible, we consider only side wall actuators in this paper. This done both for practical reasons in the prototype, but also in anticipation for real applications, where blow and suction can only be effected easily at the channel side walls, as would be the case of using the ventilation system in a tunnel.

The actuators are simple orifices on the channel walls connected through tubes to a series of computer-controlled valves. A reversible pump attached to the valve manifold creates either suction or pressure depending on the feedback received by the computer code. The control calculations use a limited horizon, so valve instructions are obtained for only a few time steps, as prescribed by the operator. The amount of fluid mass sucked or pumped through each orifice and each time step represents the vector that needs to be optimized. Figure 2 shows a typical example of these parameters for one orifice. Once the time sequence of instructions is received, the valves execute the instructions over the control horizon and a new set of concentrations is collected by the sensors. The control process is run once again, and the procedure is repeated.

6 Control Results

Model control results are obtained by constructing a virtual prototype within the computer model. Sensor arrays are assumed to exist over several cross sections of the channel, and selected grid points act as information gatherers during a direct simulation of the transport of a chemical cloud. In this fashion, the detectability of the system is exact albeit available at a limited number of discrete data points. Next, a series of virtual actuators is placed on the channel walls and the control algorithm is asked to identify their operation pattern. Thus, once the sensors detect the chemical cloud, the most

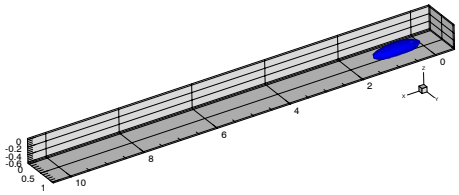

FIG. 3. Chemical cloud control; t=1

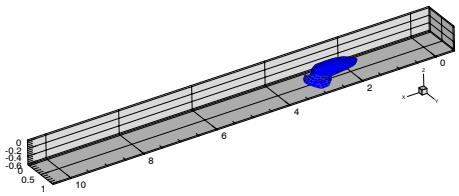

FIG. 4. Chemical cloud control; t=2

influential actuators begin to suck fluid (and chemical)out of the system attempting to minimize the chemical concentration at the sensor location. Preliminary results from a hypothetical cloud are presented in Figures 3 through 12. The simulation corresponds to flow of water in a rectangular channel with a free surface. The flow is steady and uniform in the longitudinal direction and the contaminant source is located near the inlet. There is no boundary flow prior to the control action. Once flow is initiated, it is limited to suction only to simplify the flow pattern. Furthermore, suction velocities are limited to values that correspond to the hypothetical pump and valve capacity.

As shown in Figs. 4-6, the cloud propagates in the longitudinal direction due to advection. Once it is detected, wall orifices are activated and a significant part of the cloud is eliminated within a short period of time. These preliminary results serve to demonstrate the ability of the wall suction to intercept the cloud, but since no real feedback and time delay are used, the success of the model should be viewed with caution.

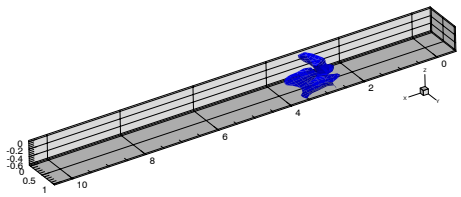

FIG. 5. Chemical cloud control; t=3

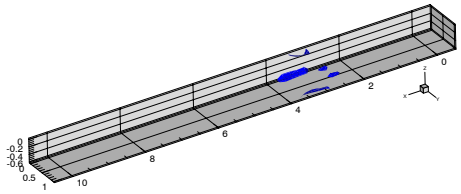

FIG. 6. Chemical cloud control; t=4

6 Conclusion

A mathematical model for simulation and control was presented that is capable of determining control strategies for mitigating a hazardous chemical release in a channel. Adjoint equation theory was used to obtain gradient information for the computation of sensitivities of the control parameters. This makes the method very efficient, as only two simulations are needed to increment the control action over a limited time horizon. Sensor arrays can detect a contaminant cloud and wall suction can be optimized both in spatially and temporally, so the cloud is removed in the most efficient way. Preliminary results demonstrate that the approach shows a lot of promise although application to a real system is needed to validate the real-time controllability of the flow and transport processes. If successful, this model could become a powerful tool in the mitigation of hazardous chemical releases in channels in real time. The model could be used for both air and water systems and any chemical or biological agent.

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