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Near Field Atmospheric Dispersion Modeling on an Industrial Site Using Neural Networks

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Assessment of likely consequences of a potential accident is a major concern of loss prevention and safety promotion in process industry. Loss of confinement on a storage tank, vessel or piping on industrial sites may imply atmospheric dispersion of toxic or flammable gases. Gas dispersion forecasting is a difficult task since turbulence modeling at large scale involves expensive calculations. Therefore simpler models are used but remain inaccurate especially in near field of the gas source. The present work aims to study if Neural Networks and Cellular Automata could be relevant to overcome these gaps. These tools were investigated on steady state and dynamic state. A database was designed from RANS k-ε CFD and Gaussian plume models. Both methods were then applied. Their efficiencies are compared and discussed in terms of quality, real-time applicability and real-life plausibility.

1. Introduction

Major industrial accidents entailing atmospheric dispersion are leading concerns for risk prevention research because of the huge consequences involved. Bhopal disaster sadly illustrates the impact of dispersion of a toxic gas such as methyl isocyanate (MIC) inside and beyond an industrial site. Sharan (1997) showed the importance of both atmospheric conditions and topography. Indeed, local characteristics such as presence of lakes near Bhopal had a major contribution in transporting the MIC into the city area. Flammable gases emissions are also in the studied area because of the UVCE possibility. The Viareggio is a tragic example of LPG dispersion. Brambilla (2009) reported the requirement for taking account of congested environments in such cases.
Industrial sites are defined by various configuration areas. Process buildings, storages or free spaces influence in different ways the atmospheric dispersion because of wind field modifications. Important losses of confinement mainly occur on storages so this study is focused on this type of obstacles.
Models allowing predictions of gas dispersion are abundant. The main strategies are Computational Fluid Dynamics (CFD), semi-empirical and empirical models. CFD models attempt to solve the Navier-Stokes equations using different kinds of refinement depending of the goal to achieve. Duration of computing, numerical convergence and required expertise (especially for the choice of appropriate turbulence modeling) are the drawbacks of such fineness. Moreover, in several cases, experiments are needed in order to calibrate coefficients. Semi-empirical models such as integral approaches are designed from theory with some assumptions in order to simplify the use of such models while keeping physical soundness. It results in faster modeling and relatively accurate results, especially on simple cases. This explains why their use is widely spread in the industry. Empirical models are based on experiments. From those, correlations are made and can provide accurate results in the range of the experiments database. Beyond this range, the results are not ensured. Gaussian models are one of those. While empirical models can provide inaccurate concentrations, semi-empirical ones preserve consistent results even if the error margin could be important. In any cases, it is crucial to confront models and experimentations (Meroney, 2004).

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Starting from this description of the atmospheric dispersion modeling landscape, the proposed approach includes data obtained either by simulation or experiments. It consists in using Machine Learning tools such as Artificial Neural Networks (ANNs) and Cellular Automata (CA). The training database consists in simulation results instead of *in situ* experiments to first design the methodology. Experimental database could be used in second place, to ensure the model to better fit reality.

1.1 Artificial Neural Networks

Artificial Neural Networks (ANNs) came from the original idea to emulate the structure and behavior of the brain (Minsky, 1969). It consists of several mathematical functions, termed as neurons, which are linked in a network. ANN are powerfull non-linear statistical data modeling tools. They are generally used when the process to model is not fully known thanks to two essential properties: first the universal approximation (Hornik, 1989), and second the parsimony (Barron, 1993). Thanks to these properties ANNs are able to predict efficiently future behaviors on never encountered situations. ANNs can be used in classification, in text recognition for example (Dreyfus, 2004). They can also be used to forecast physical phenomenon, presenting powerful models (Siou, 2011, Toukourou, 2011). The information about the non-linear phenomenon to simulate or forecast must be provided using a database. As previously presented, ANNs act generally like a black-box: the physics cannot be extracted from the results.

A neuron is a nonlinear, parameterized, bounded function. Variables are assigned to the inputs of the neuron. Output of a neuron is the result of nonlinear combination of the inputs, weighted by the parameters and using an s-shaped function like a sigmoid. A neural network is the composition of several neurons. Parameters calibration is done through application of an algorithm using the training database and designed to decrease the model error (in this work the Levenberg-Marquardt method (Hagan, 1994). The function realized by the ANN is continuously tested on a disjoined set of examples, namely the validation set. This last set is employed to avoid overtraining using early stopping (Sjöberg, 1995). Lastly, performances of the model must be measured on another set, never used during training or stopping: the test, or validation set.

ANN have already been used in atmospheric dispersion. Prevision of concentrations of tracers in complex terrain have been made by training an ANN using databases of values coming from various sensors spatially distributed (Podnar, 2002). In this case, the output variable is the predicted concentration at a specific point. Moreover, these studies are based on chronic pollution instead of accidental pollution, which is the topic of the present work. Cao (2007) gives an example of the use of neural networks to model the evolution of an aerosol plume. The database has been made especially for the study. It results that the neural networks forecasted more accurate estimations than a Gaussian model. Despite these good results, it appears the difficulty to apply this model in real life situations because of the difficulty to collect inputs information for the neural network.

1.2 Cellular automata

Cellular automata (CA) are tools used for modeling physical phenomena in discrete space-time coordinates. Initially, Von Neumann was interested in seeking logical abstraction of the self-reproduction mechanisms seen in many life-based processes. He adopted a discrete approach for the time, the space and others dynamical variables. He made up a self-replicating theoretical machine, a two dimensional cellular automaton able to reach 29 different states. Since then, CA have been used in simulating various physical phenomena. For instance, Avolio (2006) models volcanic eruption pyroclastic flows using CA whereas differential equations systems and shows good agreements with observations of the real event. The impact of local interactions on the evolution of the phenomenon is an important feature that promotes the use of CA. From this statement, Wolfram (1983) designed systematic local rules to study different influences from direct neighborhood. Conclusions of his work were that from simple local rules, it is possible to observe very complex phenomena such as biological systems evolution or structure and patterns development in the growth of organisms. He demonstrated that CA can emulate specific behavior of biological or physical phenomenon observed in real life. Itami (1994) formalized cellular automata, defining Q, as the global state of the system:

$$Q = \langle S, N, T \rangle \tag{1}$$

S represents the discrete states accepted for the cellular automaton. *N* represents the neighborhood of cells providing input values for the transition rules. Depending on the aim of the study, different neighborhoods can be set such as Moore or Von Neumann type. The transition rule *T* defines how a cell

changes his state from the current time step to the next. A large number of quantitative mathematical techniques can be used.
As in classical numerical simulations, the system is defined on a domain. Dimensions and shapes of the cells are determined depending on the phenomenon to model and the acuteness requested.
The transition rule updates synchronously the states of each cell between each time step. According to classical methods, some stability criteria have to be described before using the CA to ensure limitations of numerical errors.
Marin (2000), based on the work of Guariso (1992), identified the different phenomena involved in atmospheric dispersion in order to determine transition rules. Calibration parameters were determined by using measurements from three petrochemical complexes. Comparisons with field measurements gave good agreements and the importance of parameters calibration was strongly underlined. Sarkar (2006) specified a similar method based on simplification of the advection-diffusion equation and developed a model to assess consequences of a loss of confinement on an industrial site, taking account the particular configuration (storage, buildings, type of the area). Vick (2007) gave guidelines to model multi-physics complex processes through CA. These studies pointed out the importance of the determination of the calibration parameters to better fit measurements and the accuracy increase with time step shortening.

In this work, the aim is to check relevance of coupled ANN and CA to predict concentrations of several case studies. The ANN ability to take over large amount of data and to extract a specific behavior is engaged through static and dynamic modeling of atmospheric dispersion.

2. Methodology

2.1 Artificial Neural Networks for stationary modeling

Industrial site observation allows defining various areas corresponding to various pollutant behavior. Indeed, process buildings, storages or free spaces interact in different ways with atmospheric dispersion because of wind field modification. To gradually increase the difficulty, we initially consider a stationary source term. A database is built from CFD, using resolution of the Reynolds Averaged Navier-Stokes equations by adding equations of turbulent kinetic energy k and its dissipation rate ε. The accuracy of such a model and development of all the parameters used are not discussed here, since the objective of this study is to establish a consistent method. We will consider in the future using ANNs with an experimental database. A loss of confinement of gaseous methane into air is modeled. The simulations were set in steady state. The dispersion is modeled in two dimensions. The mesh is composed of 401 301 nodes, with greater density near the methane source. The wind direction is parallel to the ejection direction of the gas. The mix of air and methane is done on a free field of 40 m long and 20 m large. Symmetry conditions are applied at the half of the two meters diameter source. The input of air is set as velocity inlet. Mass flow inlet represents the methane input with a volume fraction of 1. The domain output is set as pressure outlet. In order to simulate correctly the different behavior of the plume, a range from 0.5 to 5 $kg.s^{-1}$ is considered for the methane. The velocity range for the wind input is included between 2 and 10 $m.s^{-1}$.

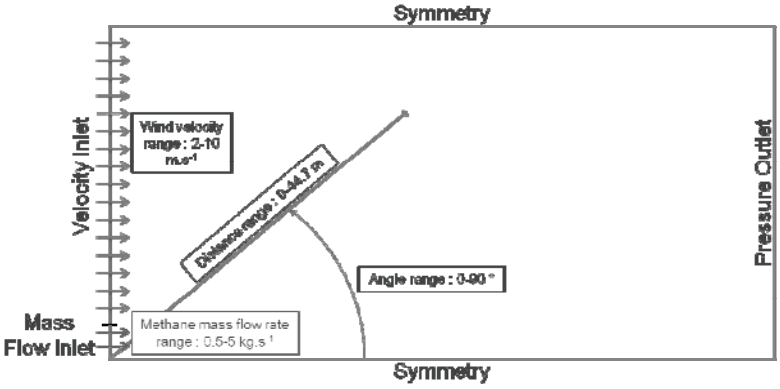

Fig. 1: Configuration used for the simulation.

The database was built from 46 experiments with variations within these ranges. It contains the inputs used by the neural network: the distance (m) and the angle (°) from source to the point to be evaluated, the wind velocity ($m.s^{-1}$) and the methane mass flow rate ($kg.s^{-1}$). The output, or target in training phase, is the methane concentration ($mol.m^{-3}$).

In order to optimize the computational time, a selection of several data is done instead of taking the wholeness of the >18 000 000 values for each variable. For each case, 20 concentration intervals were created. 50 points per interval including coordinates and concentrations were saved. 36,800 points formed the training set. 4,599 points were used as validation set.

2.2 A Cellular automaton with neural network transition rule

The goal was to model the evolution of the concentration of a pollutant from a source term (point or surface) over time. CA is thus used with ANN transition rule (CA-ANN). As seen above, CA are mostly used with discretization and simplification of physics laws. ANN are used to forecast variables evolution of a phenomenon based on interpolation of a representative database describing it.

First, it is important to define the time step and the dimensions of the cells. According to classical numerical methods, Courant–Friedrichs–Lewy condition (CFL condition) has to be fulfilled. This number corresponds to a threshold over which instability of calculation is observed, growing quickly at each time step. It appears if cells dimensions are less than the distance travelled by the faster wave of the phenomenon during one time step. The minimum time steps and cell dimensions are thus linked by the equation:

$$\frac{u\Delta t}{\Delta x} \leq CFL_{max} \tag{2}$$

u is the faster wave velocity, Δt and Δx are the discrete time and distance steps.

To elaborate and evaluate the method, Gaussian puff model is used to create a database. In a first time, we only consider the wind direction dimension. These models are based on the resolution of the advection-diffusion equation (ADE) with several assumptions not described here:

$$\frac{\partial C}{\partial t} + \frac{\partial U_i C}{\partial x_i} = D\frac{\partial^2 C}{\partial x_i^2} \tag{3}$$

As neural networks need relevant variables to work efficiently, the discretization of this equation is done using an explicit scheme. The CFL number is set to one. Consequently, setting the cell dimension Δx and knowing the maximum velocity u gives the time step Δt to be used.

The neural network inputs correspond to cell variables: concentration parameters (C_i^t, C_{i-1}^t, C_{i+1}^t) are collected from gaussian model database. First and second discretized derivative are calculated from those data for each cell i considered. The output, or target in training phase, is the concentration ($g.m^{-3}$) at time t+1 in the cell i considered. Before training, the database is normalized. The learning algorithm is then applied (Levenberg Marquardt). Validation sequence is applied on non-trained data. Fig. 2 sums up the sequence.

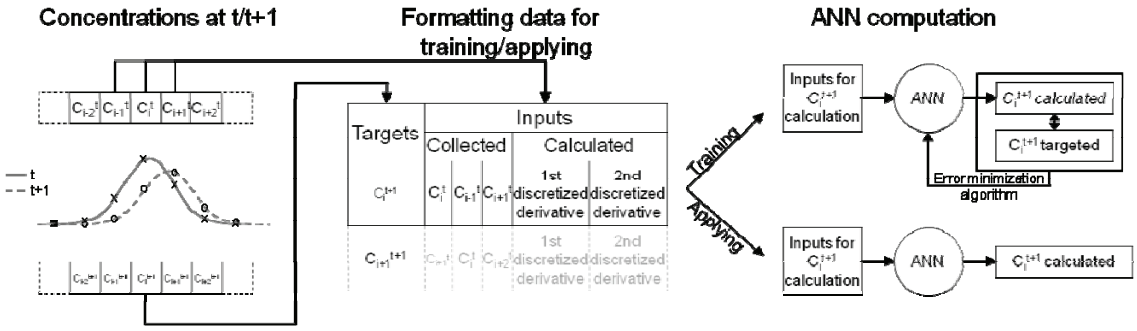

Fig. 2: Logical steps to compute cell concentration à time t+1.

In order to evaluate the relevance of such a method, a non-learned example is presented to the cellular automaton and compared to the solution of the Gaussian model.

3. Results

3.1 Artificial Neural Networks

In order to prevent overfitting, early stopping is applied. Results are shown on figure 3 and 4. It provides good performance in generalization. The error graph points out a correlation coefficient R^2 of 0.99. Figure 3 shows that an important number of points are well predicted. Few are less correctly predicted and seem to be isolated cases. Figure 4 compares results from the CFD software and neural network method. Good global agreements are shown. However, several types of error can be identified, such as overestimations for high gradients or negative concentration. The latter requires a correction step to insure physical soundness, but this problem is inherent to empirical modeling.

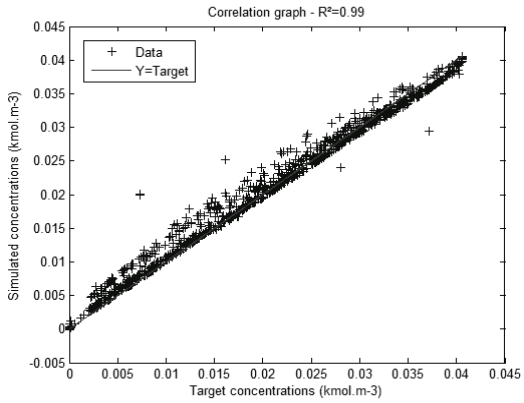

Fig.3: Correlation graph between CFD data and ANN simulation.

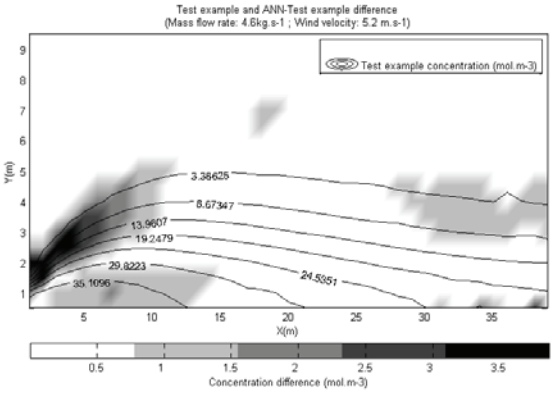

Fig. 4: ANN simulation relative error.

3.2 Cellular automata with neural networks transition rules

The training phase gives satisfying results with a correlation coefficient R^2 near to one. This outcome was expected due to non-linear fitting skills of ANN on equation based data. A validation example is tested with present method. CA is initialized with t_0=40 s concentration distribution from a Gaussian puff model. Rating the CA is done by confronting results from both models. Good agreements are obtained for the first time steps of the modeling. As the iteration number increases, the correlation between CA-ANN model and Gaussian plume model data decreases as seen on Figure 5. It can be explained because of the error propagation with iterations. The first steps are well modeled but few differences appear and grow. A divergent behavior is observed after 32th iteration. The error made during each time step is expanded.

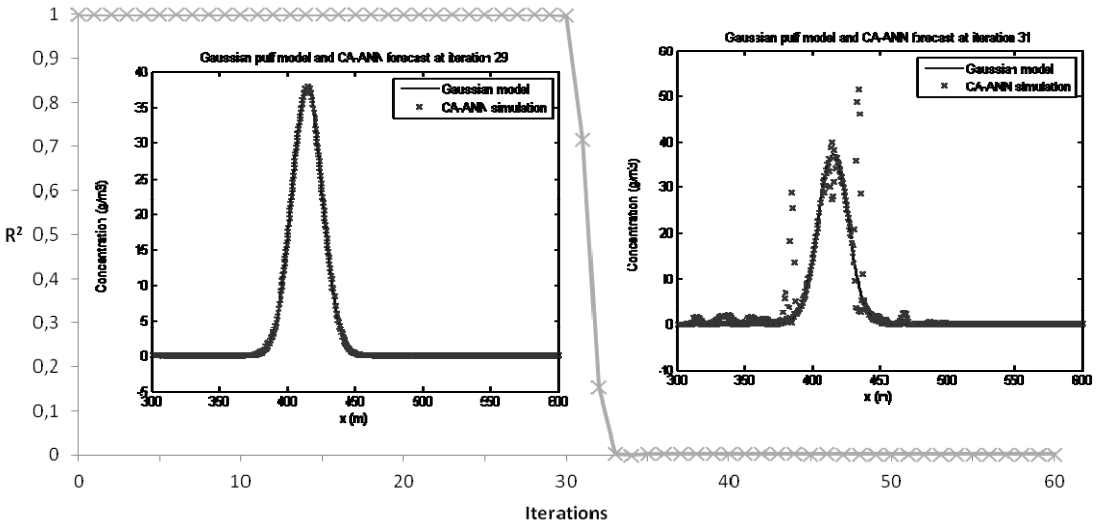

Fig.5.: Decrease of correlation coefficient (between gaussian model and CA-ANN) with iteration number.

4. Improvements

Several improvements can be made on the ANN stationary part. In addition to some errors fixing, special care will be taken in submitting single obstacle to ANN atmospheric modeling. Several different configurations will have to be considered like the position, the shape, and the dimensions of the obstacles. The next step will be to aggregate such different cases according to geometry observed on industrial sites. To ensure realistic results on the CA with ANN transition rules, a two-dimension CFD database will be created using adequate CFL conditions. Perspectives of this work will be obstacle consideration by adding cell environmental characteristics.

5. Conclusion

Existing forecasting models in atmospheric dispersion have the drawback of being slow but accurate or fast but not enough appropriate. Two methods both using machine learning have been developed and compared to existing models to forecast atmospheric dispersion in open terrain. The stationary ANN model gave good agreement with CFD software with the advantage of faster processing. The 1-D dynamic CA-NN model shows hopeful trends in modeling dynamic atmospheric dispersion and has to be implemented with a 2D CFD learning database to better assess its potential.

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