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Atmospheric dispersion modeling using Artificial Neural Network based cellular automata

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ABSTRACT

Forecasting atmospheric dispersion in complex configurations is a current challenge in fluid dynamics in terms of calculation time and accuracy. CFD models provide good accuracy but require a great computation time. Simplified or empirical models are designed to quickly evaluate the dispersion but are not adapted to complex geometry. Cellular Automata coupled with an Artificial Neural Network (CA-ANN) are developed here to calculate the atmospheric dispersion of methane (CH_4) in 2D. Efforts are made in reducing computation time while keeping an acceptable accuracy. A CFD simulations database is created and the Advection-Diffusion Equation is discretized to provide variables for the ANN. Neural network design is made thanks to best sampling selection, architecture selection and optimized initialization. The coefficient of determination is over 0.7 for most cases of the test set despite small errors accumulated through time steps. CA-ANN is faster than CFD models by a factor from 1.5 to 120.

1. Introduction

Industrial accidents involving atmospheric dispersion of flammable or toxic materials may generate extremely serious consequences. The disaster that occurred in *Bhopal*, India, in 1984 clearly shows the impact of toxic dispersion from a chemical industry. 40 tons of methyl isocyanate, or MIC, were released in 90 min from the Union Carbide fertilizer factory into the city of *Bhopal* after a cleaning operation. Sharan and Gopalakrishnan (1997) highlight the impact of topography and atmospheric conditions on the evolution of the plume. Especially, near field characteristics (in this case the presence of lakes near the factory) influenced directly the plume trajectory toward the city.

In case of flammable gas emissions, the consequences of a potential gas explosion depend especially on the plume size and on the concentrations before ignition. Therefore, the plume behavior just after the release is a key point to assess possible consequences. Brambilla et al. (2010) support the necessity to consider complex environment in specific cases. The Italian *Viareggio* train accident that occurred in 2009 led up to a liquefied petroleum gas transport tank leakage. The plume was dispersed in a specific manner because of the street configuration in the near field. The presence of buildings in the vicinity of the source is considered as the main important parameter in the plume dispersion.

The near field of the leakage, hence, appears to be significant for the pollution plume dispersion, and must be considered for forecasting this phenomenon.

To avoid such accidents, the risks analysis is currently performed with atmospheric dispersion models. Existing models currently distinguish two mechanisms, the wind flow and the dispersion process. Each model differs from the other, according to turbulence model. In terms of performance, two major criteria could be used: computational time and model accuracy.

The best model should be fast and accurate. Since this best model does not exist, available models are designed according to the goal to achieve, preferring accuracy or computation time. Nevertheless, attempts were made to combine both capacities. This study tries to make a step toward this objective using a method well known for its ability to represent any complex phenomena: neural networks. In order to take into consideration the spatial extension of the dispersion phenomenon, a new way of modeling is proposed combining cellular automata and neural network. The former represents the spatial dispersion of the phenomenon, the last implements the transition rule.

The case study proposes the horizontal 2D dispersion faced with a single obstacle but, as this approach is innovative and was not previously used for gas dispersion, several questions are addressed in this study:

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(i) the constitution and sampling of the database,
(ii) the design of the neural model,
(iii) the way to assess the quality of the model.

This paper is divided into six parts: after the introduction, a state of the art regarding dispersion modeling and neural networks modeling is proposed in parts 2 and 3. The proposed method is extensively described in part 4 addressing all the new questions as: database constitution, design of neural model, training and validation of the model. Part 5 proposes a presentation of the results and a discussion in relation with the ability of the proposed model to converge toward the targeted solution: CFD simulation. A conclusion is then proposed in section 6.

2. Atmospheric dispersion models review

2.1. Physics-based models

Usually, atmospheric dispersion modeling is done through the use of wind flow, calculated or determined, combined with dispersion modeling. In each model, turbulence is the main difficulty and has a major impact on the dispersion. Fig. 1 details turbulence modeling for several main modeling methods detailed in the following:

- Dispersion modeling in gaussian models is calculated by solving Advection Diffusion equation using turbulent diffusion coefficient or standard deviations determined empirically. These models consider the wind flow as homogeneous.
- Models from Computational Fluid Dynamics solved the Navier-Stokes equations to determine the wind flow. Turbulence is solved using closure equations of the system. These equations are transport equations of turbulent quantities. The turbulent diffusion coefficient is introduced in the advection-diffusion equation to model the dispersion. This parameter is directly linked to the variables of the closure equations.
- Intermediate simplified CFD models exist. Diagnostic wind flow models are capable of reconstructing a steady-state wind field from initial experimental data. They are based on simplified steady-state solutions of the Navier-Stokes equations.
- In Lagrangian models, the wind flow is determined from CFD eulerian model. Dispersion is realized by following the behavior of particles linked to initial conditions. Turbulence modeling is realized by adding fluctuation term to the mean velocity field in each particle position.

Gaussian models correspond to an analytical solution of the advection diffusion equation for idealized circumstances using Reynolds averaging. The main assumptions are:

- Gas dispersion is considered as passive
- Dispersion through turbulent diffusion is both isotropic and homogeneous
- Molecular diffusion is neglected
- Obstacles and relief are not considered so that wind field is considered as uniform in terms of time and space.

Therefore, Gaussian models are efficient in far field evaluation of atmospheric dispersion, for passive gas. They are mostly used to assess long term impact of industrial activities on the environment. Dispersion and physicochemical processes are included through specific parameterizations. These models require experimental dispersion coefficients calibrated from field experiments. Prairie grass (Barad, 1958) was one of the first campaign of field experiments. More recently, these coefficients were tested for urban environment using Indianapolis experiments (Hanna et al., 1999). These models are mainly adapted to operational purpose or emergency management due to the short computation time. However, complex geometries and site topology are generally not appropriately addressed. It notices that some modifications were proposed in the literature in order to adapt Gaussian models to non-passive gas dispersion. These integral models are based on properties conservation through the resolution of the fluid mechanics simplified equations. Atmospheric dispersion is split into different steps and specific models are applied for each one. For the final step, corresponding to the atmospheric dispersion modeling, the gas is considered as passive and Gaussian model is applied. This conservative approach also needs parameters defined by experiments and due to the use of a Gaussian model; integral models suffer from same limitations considering weather, complex geometries and site topology. Comparisons between Gaussian models and Lagrangian codes are well described by Caputo et al. (2003).

Diagnostic 3D wind flow models, also called kinematic models, generate a wind field by sustaining some physical constraints. In mass-consistent models, numerical solution of the steady-state three-dimensional continuity equation for the mean wind components is imposed. Parametric relations or wind data are used to consider momentum and energy equations which are not solved explicitly. In consequence, diagnostic wind flow models are specifically adapted to predict effects of orography (Castellani et al., 2015) but cannot take into account of thermal effects or effects due to pressure changing gradients.

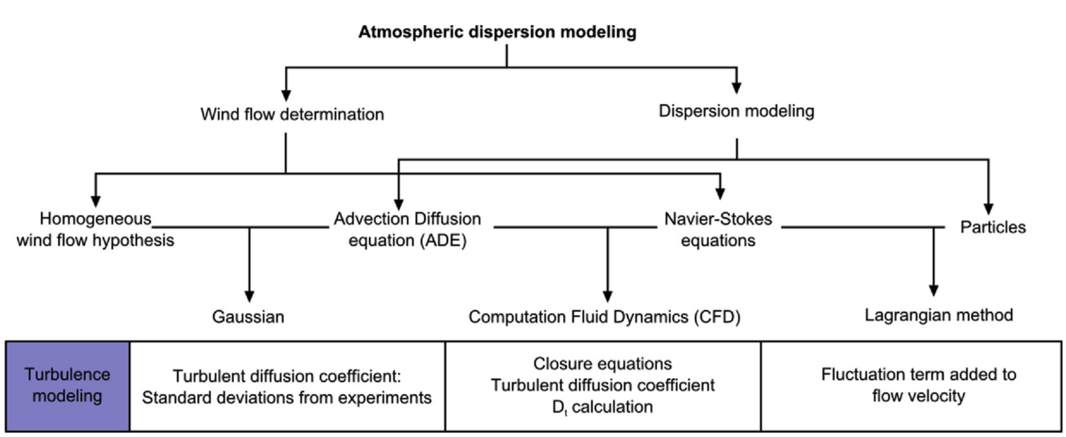

Fig. 1. Atmospheric dispersion modeling methods.