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# The real-time estimation of hazardous gas dispersion by the integration of gas detectors, neural network and gas dispersion models

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## HIGHLIGHTS

- The approach works with scenario simulation, gas detectors, and neural network.
- The approach bypasses the source terms needed by traditional models.
- A rough analysis of optimal gas detector placement is demonstrated.
- We analyze the reliability of the prediction results of the new approach.

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## ABSTRACT

Release of hazardous materials in chemical industries is a major threat to surrounding areas. Current gas dispersion models like PHAST and FLACS, use release velocity, release elevation, meteorological parameters, and other related information as model input. In general, such information is not always available during an on-going accident. In this paper, we develop a fast prediction approach which could bypass the input parameters that are difficult to obtain and predict the released gas concentration at certain off-site location using parameters that could be obtained easily. The new approach is an integration of gas detectors, artificial neural network (ANN) and one of the aforementioned gas dispersion models. PHAST is applied to simulate numbers of release scenarios and the results containing the spatial and temporal distributions of released gas concentration are prepared as input and target data samples for training the neural network. The approach was applied to a case study involving a hypothetical chlorine release with varying release rates and atmospheric conditions. The results of the approach that are concentration and dispersion time profiles in the environmental sensitive locations were validated against PHAST. The validation shows highly correlations with PHAST and convincingly demonstrates the effectiveness of the proposed approach.

## 1. Introduction

Accidental release of toxic/flammable chemicals and its accompanying vapor cloud dispersion are worthy of concerns in industrial safety and social security. Several models are currently available for simulating the hazardous gas discharge, dispersion, and for evaluating the influence to the surrounding environment. Source information, though difficult to acquire in emergency situation, is essential to all the existing gas dispersion models which are Gaussian models, integrated models (PHAST etc.) and computational fluid dynamics (CFD) models. The computing time also varies from one model to another; the simplest Gaussian model can estimate long-term passive dispersion for simplified continuous release scenarios or the ground level heavy-gas dispersion within seconds [1]. When decision maker requires more convincing results that terrain effect cannot be neglected or the phase transitions in the release are involved, Gaussian model is no longer suitable [2]. The integrated models are capable of simulating the transitions between different stages of dense-gas dispersion, including slumping, creeping, phase transition, and passive dispersion. These models could give credible results in few minutes, however, terrain effect is still not considered in the integrated models [3,4]. When it comes to simulation involving complex geometry, CFD model is the only option because the influence of surface roughness is significant [5–11]

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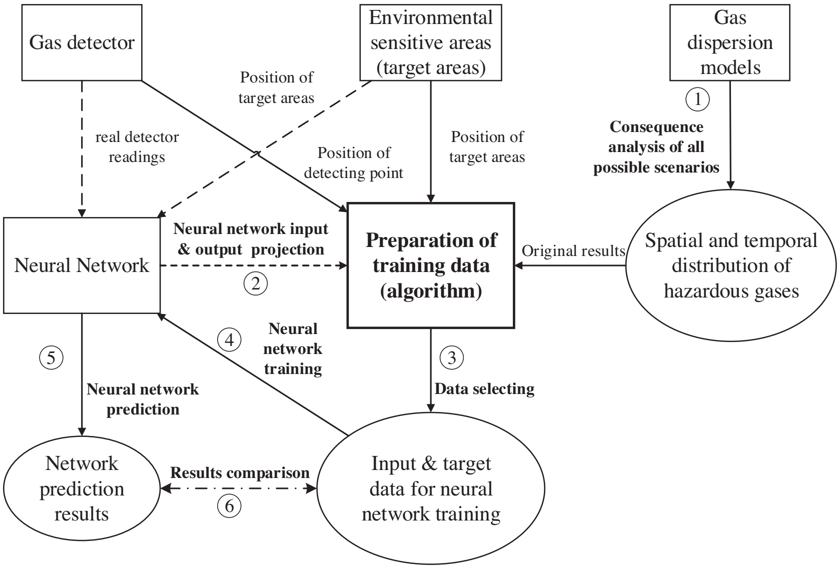

**Fig. 1.** The architecture of the integrated model.

and cannot be neglected. CFD allows the wind velocity to be completely resolved compared with the integrated models in which the wind velocity is a single value or a function of height. When well prepared, CFD models will give detailed time-dependent, 3-dimensional concentration profiles of released substance in complex terrains. Cases that chlorine and LPG released in urban areas were studied [12,13]. The price of giving detailed simulation results using CFD is complex model configuration and hours of computation, which limits the application of CFD models in emergency response.

In the past few years, several major accidents with strong off-site influences have aroused wide public concerns, efforts have been taken to study the off-site influence of certain chemical storage or transportation failures [14–18] and the research emphasized the importance of source information in pursuing accurate results. However, the unavailability of certain source information and the time-consuming simulation limited the implementation of these models in emergency situation. Therefore, a thought of using the results of pre-simulated release scenarios for emergencies has been putting forward. A previous study demonstrated a technique of estimating the hazardous gas release rate using optical sensor and neural network [19,20]. In that approach, the release rates estimated by the neural network were validated by a commercial software, PHAST, and the validation results showed acceptable deviations. But that approach did not predict the future influences to distant places.

This paper demonstrates an alternative real-time prediction approach that estimates the influence of hazardous gases to off-site locations. The approach is an integration of gas detectors, artificial neural network and gas dispersion simulations. In the approach, PHAST is used to simulate large numbers of release scenarios that could possibly cover most of the situations [21–23] and the neural network is used to correlate the simulation results with the concentrations detected by gas detectors in specific locations. If the neural network is well trained, the approach will then provide real-time prediction results of gas concentration at distant locations without source information.

In the PHAST simulation, storage status, release rate, weather conditions are considered except the terrain effect [24]. An algorithm is developed to generate input and target data samples from PHAST results to train the neural network. The approach is verified using a case study of hypothetical chlorine release.

## 2. Methodology

### 2.1. Workflow of the integrated model

The integration of gas detectors, artificial neural network, and gas dispersion model for predicting the real-time gas dispersion contains 6 steps, as shown in Fig. 1.

a Identification and consequence analysis (mainly the gas dispersion simulation) of release scenarios that should cover nearly all possibilities. Results containing temporal and spatial concentrations data are stored in a database.
b The input and target data used to train the artificial neural network are essential in predicting the real-time dispersion of leaked gases. The input data should be easy to acquire in emergency situation and the target data can either be the concentration at distant areas or the expected evacuation time for the distant areas.
c A data preparation algorithm is developed to generate the input and target data samples. The location of gas detectors and environmental sensitive areas are taken in to consideration.
d The neural network is trained using some (about 75%) of the input-target data samples generated in step 3.
e The remaining 25% of the input-target data samples that the network has never seen are used to calculate the designed results.
f The performance of this approach is evaluated by comparing the network predictions with the associated targets data generated by the data preparation algorithm from PHAST simulation results.

### 2.2. General scenario

A general leak scenario consists of several components: (1) source conditions (release material and location, release velocity); (2) weather conditions (wind speed, wind direction, temperature, pressure, humidity, and solar radiation); (3) diffusion areas (facility layout). By varying the value of these components between their upper and lower bounds that could be decided through risk analysis, scenarios will be generated. The coverage of these scenarios is determined by adjusting the upper and lower bound of the aforementioned components.

A top view of the general scenario is demonstrated in Fig. 2. The *x*-axes of the coordinate system is the same as the prevailing wind direction and its perpendicular direction lies the *y*-axes. The