Modeling and Optimal Control of Atmospheric Pollution Hazard in Nuclear and Chemical Disasters

Huang Shunxiang\textsuperscript{a,b,}\textsuperscript{*}, Liu Feng\textsuperscript{a,b,}\textsuperscript{†}, Zeng Qingcun\textsuperscript{b}
Hu Fei\textsuperscript{b}, Zhu Jiang\textsuperscript{b}, Wang Zifa\textsuperscript{b}

\textsuperscript{a}Institute of Chemical Defense, Beijing 102205, China
\textsuperscript{b}Institute of Atmospheric Physics, Chinese Academy of Sciences, Beijing 100029, China

Abstract

Nuclear and chemical disasters can cause heavy atmospheric pollution hazard and threat people’s lives and health. In this paper, theory and application for modeling and optimal control of such hazard is studied. The modeling is based on the simulation and visualization of atmospheric dispersion of pollutants, the source term estimation of nuclear and chemical disasters, and the risk evaluation of hazardous substances. The optimal control is based on Natural Cybernetics theory, effective and economic cost evaluation of control techniques, and optimization methods. Some applications and illustrations of modeling and optimal control are reported.

Keywords: atmospheric pollution hazard; nuclear and chemical disaster; modeling; optimal control; Natural Cybernetics

1. Introduction

Nuclear disasters and chemical disasters often cause leakage of radiological and toxic substances into the atmosphere and seriously contaminate air quality. These hazardous substances transport and diffuse with the motion of atmosphere and threat people’s lives and health and the environment in a vast area. There were several big nuclear
disasters happened in history. The 1986 Chernobyl nuclear plant accident (Zhou 1996, Stone 2006) of the former Soviet Union caused 31 deaths and tens of thousand people injured by high exposure dose of radiological rays. With the atmospheric dispersion and deposition, the radiological cloud affected the whole Europe and polluted over 200 thousand square kilometers land. The 2011 Fukushima Daiichi nuclear disaster in Japan caused by huge earthquake and flood released a lot amount of radiological substances and polluted atmosphere and ocean. There were many chemical disasters occurred in chemical industries, among which the most tragic one is the Bhopal chemical disaster in India, 1984 (Kleindorfer and Kunreuthe 1987, Boybeyi et al. 1995, Sharan and Gopalakrishnan 1997, Gupta 2000). In the accident, tons of toxic chemical gas caused over 3000 deaths and 300 thousand injured. Chemical weapons and chemical terrorism are threatening human lives in other approaches. During the World War I and II, thousands of lives were killed by chemical weapons. Now there are a lot amount of Japanese Abandoned Chemical Weapons (JACW) remained in China’s land in urgent need of destruction. Now in Syria, evidences show that chemical weapons were used to kill innocent civilians. Chemical terrorists attempt to cause chemical disasters by using chemical agents or attacking chemical facilities (Fitch et al. 2003, Huang et al. 2005). In the 1995 Tokyo subway chemical terrorism attack with sarin (Nagao et al. 1997), 12 people died and over 5000 injured and serious social chaos were caused. The nuclear and chemical disasters are all related with the atmospheric pollution by radiological or chemical hazardous substances, and cause massive casualties. The hazard of such a disaster was determined not only by the features and the leakage intense of the hazardous source, but also the weather conditions and social factors, such as human density, transportation and economic considerations (Huang et al. 2008). The motivation of this paper is to simulate the atmospheric pollution and evaluate the hazard of the nuclear and chemical disasters, and study optimal methods for control of the hazard based on simulation, evaluation and economic models.

In order to simulate the hazard of nuclear and chemical disasters, many elements that affect the hazardous sequence should be considered (Huang et al. 2004). First, it is needed to construct nuclear and chemical source term models to determine parameters such as release mass, release rate, plume rise height, etc. Second, atmospheric dispersion models should be constructed to simulate the transport, diffuse and deposition processes of nuclear and chemical substances in the atmosphere, and compute the spatial distribution and evolution. Third, evaluate the hazard, based on the concentration and dose (temporal accumulated concentration). Finally, the modeling and evaluation results can be displayed through a GIS (Geographic Information System) platform to aid decision makers to instruct the rescue and disposal of nuclear and chemical disasters.

On the basis of modeling, theories and technologies for controlling nuclear and chemical disaster hazard need to be developed. The control of hazard has two aspects: the prevention of risk and the reduction of hazard. The measures for prevention of risk include locating of nuclear and chemical facilities, planning the transportation of nuclear and chemical materials and the emergency respond resources, designing safer processes in nuclear and chemical industries, etc. Measures for reduction of hazard include the evacuation and protection of people, the disposal of hazardous sources, the decontamination of leaked hazardous substances, etc. The prevention and reduction of hazard is associated with natural factors such as weather condition and geographic conditions, and human factors such as sociality, economy and so on. In order to consider all these factors that affect the control of nuclear and chemical hazard, a new methodology need to be constructed to combine these macro and micro mechanisms and provide a scientific basis for the study of such control.

The theory of Natural Cybernetics, proposed by Zeng (1996), is such a methodology that studies the nature-society-economy complex huge system in a whole. It introduces two kinds of variables to describe natural and human factors respectively, and approach to an optimal state (optimal economic efficiency or optimal control effect) by adjusting some human factor variables to affect the evolution of the whole system. The Natural Cybernetics has been applied to several fields such as atmospheric environment, climate, hydraulic engineering, and safety science. This study was an application of the Natural Cybernetics in the field of optimal control of nuclear and chemical hazard.

This paper is arranged as follows. In section 2, the principals of modeling the nuclear and chemical disasters will be discussed. In section 3, optimal control theoretical frame and an example of application will be illustrated. A summary will be drawn in section 4.
2. Models for Nuclear and Chemical Disasters

In nuclear and chemical disasters, huge amount of hazardous substances may be released into the atmosphere and transport and diffuse with the motion of air stream. In order to correctly predict the hazard of the disasters, several kinds of models need to be investigated, the source term model, the atmospheric dispersion model, the meteorological field forecast model and the hazard evaluation model (Liu and Huang 2011). These models will be discussed later, and an illustration of application will be presented.

2.1. Source Term Models

Nuclear and chemical disasters were usually accompanied with explosion, high pressure jet, liquid evaporation and such phenomena, and the initial physical properties have complex features. The Thermodynamics and Mechanical effects can affect parameters of the hazardous sources, such as release rate, initial rise height, initial volume, etc. These source term parameters will affect the dispersion of hazardous substances in the atmosphere (Raskob and Ehrhardt 2007). By applying principles of explosion mechanics, fluid mechanics and Thermodynamics, the source term models for nuclear and chemical disasters were constructed to determine source term parameters. The models include: Church explosion model, gas leakage model (subsonic or sonic outlet), liquid leakage model (overheat or not), liquid pool evaporation model (natural evaporation or instantaneous evaporation), nuclear power plant source term model. All these models needed were integrated in a model system, and connected with nuclear and chemical substance database. In the model system, users choose accident category by menus and input condition parameters, and the source term parameters will be calculated to provide input data for further modeling.

2.2. Atmospheric Dispersion Models

The atmospheric dispersion models describe the transport of nuclear and chemical pollutants with the motion of air streams, their diffusion by turbulence, and their dry and wet deposition and transformation or decay processes (Lei et al. 1998). The atmospheric models are driven by source term data and meteorological data, modeling the concentration of nuclear and chemical pollutants and their time evolution for further hazard evaluation.

There are many kinds of atmospheric models. The classic Gaussian plume model is based on the assumptions that the weather conditions are homogeneous and steady, and the concentration obeys the Gaussian distribution. Although the Gaussian models are easy of implementation and widely applied in the field of environmental risk evaluation, the simplified and idealized assumptions make it unable to predict the dispersion of pollutants under complex weather and terrain conditions. While another kind of Gaussian model—the Gaussian puff model regards the accidentally released pollutants as a series of puffs, and tracks the center point of every puff in a Lagrangian way. Then the concentration can be calculated by adding the contribution of all these puffs released successively. The Gaussian puff model retained the Gaussian distribution assumption, and considered the winding of air streams caused by terrain effects. However, as the puffs enlarged and distorted by wind shear, the Gaussian distribution assumption no longer holds.

The popular atmospheric dispersion models are numerical models, which solve atmospheric dispersion equations with numerical methods. Because of different model equations or different means of description for dispersion mechanisms, there are Eulerian numerical models and random walk models. The Eulerian numerical model assumes that the pollutant concentration is a continuous function and its diffusion in the turbulent atmosphere is dominated by gradient transport mechanism. In this means, the mass conservation atmospheric dispersion equation is formulated and solved through numerically discrete algorithms (ENVIRON 2004). The random walk model, as opposite to Eulerian models, looks the pollutants as a lot of discrete random walk particles, which are tracked one by one to calculate their distribution probability (Liu et al. 2012). The concentration is then calculated, the higher probability of particles, the higher concentration will be.

We constructed the CDM model and the NDM model to predict the dispersion of chemical and nuclear substances respectively, as will be illustrated in section 2.5.
2.3. Meteorological Field Prediction Models

A meteorological field prediction model provides meteorological field data, such as wind, temperature, turbulent intense etc. The principle of such model is numerical solution of atmospheric dynamics equations, which are similar to Navier-Stokes equations in Fluid dynamics and considered unique features of atmospheric motion, such as rotation effect of the earth, atmospheric stratification effect, atmospheric radiation effect, terrain effect, etc. As for modeling nuclear and chemical disasters, the appropriate meteorological field prediction models are the meso-scale models, which simulate tens to thousands of kilometers.

There are several meso-scale meteorological models developed (Dudhia et al. 2000, Cotton et al. 2003), such as MM5, RAMS and ARPS. In this paper, the new generation meso-scale meteorological model, WRF, was adopted.

2.4. Hazard Evaluation Models

There are many kinds of nuclear and chemical substances, and it is needed that appropriate models be constructed for hazard evaluation based on their toxic or radiological mechanisms. The hazard evaluation is based on the following considerations, the toxicity of the hazardous substances, the concentration and dose of exposure, and the population density and protection measures. The hazard of nuclear and chemical substances is more often measured by dose rather than concentration, because dose reflects an accumulate effect. For instance, if exposed in a low concentration polluted environment for a long time, as the accumulated dose exceeds some threshold value, the harm will be irreversible.

The hazard evaluation models are integrated into the model system and connected with the nuclear and chemical substance database for input parameters.

2.5. An Application for Modeling Dispersion of Gases

- Comparisons between simulated and experimental data
  The field experiment was at early morning, and the wind direction was SSW. The meteorological fields was simulated with a meso-scale weather prediction model MESO, and the concentration and dose distribution was simulated with CDM model (Huang et al. 2011). The simulated results and the experimental results are shown in fig. 1(a) and fig. 1(b). It turns out that the hazardous zones and hazardous depth are very similar between the two figures. The relative errors of all compared data are within a factor of 2. The maximum error is -46.8%, the minimum error is 6.5%, and the mean error is 20.6%.

- Simulation of a Supposed Chemical Attack

Fig. 1. (a) Numerical simulation with CDM; (b) field diffusion experiment.
It was supposed that a chemical attack with sarin gas by terrorists was happened near the Bird’s Nest Gymnasium during the Beijing 2008 Olympic Games, and the hazard was simulated with CDM model (Huang et al. 2010). In fig. 2, it is shown that the simulated hazard zone is at the NE direction of the Gymnasium, and the hazard depth is over 8km. The hazard duration is shown in fig. 3, which means that the toxin cloud will stay near the Gymnasium for a long time over 200min.

According to the simulation results, the emergency rescue and monitoring forces should be deployed at the NE direction region to the Bird’s Nest Gymnasium under the weather conditions as supposed.

Fig. 2. The distribution of poisonous dose when a chemical accident occurred around the Bird’s nest

Fig. 3. The distribution of the risk duration when a chemical accident occurred at the Bird’s nest
3. Optimal Control of Nuclear and Chemical Disasters

A motivation for modeling nuclear and chemical disasters is to provide important information and support decision makers to take appropriate measures to control hazard. There may be many options in a decision making process, but an optimized control plan should be worked out by rational use of the limited resources available for emergency respond to control the hazard with the minimum cost.

3.1. Hazard Control Measures

The control of nuclear and chemical disaster hazard has two related aspects, the beforehand risk prevention, and the emergent hazard reduction.

The meaning of risk prevention lies in the proverb that an ounce of prevention is worth a pound of cure. Some predictable nuclear and chemical risks can be prevented or mitigated through prevention measures. For instance, the location of chemical plants or warehouses should consider their potential hazard to important zones such as political and economic centers, inhabitant zones and water resource to prevent destroyable hazard on such zones in case of accidents. Another example is to plan a reasonable route for transport of hazardous materials to reduce the risk to an acceptable level. Standing emergency respond forces are indispensible for a city or region to carry out fast respond missions when needed. Their scale, group, location and equipment will directly affect the respond efficiency, and need to be optimized.

Regardless of whether people are willing to see, when a nuclear or chemical disaster happens, fast and efficient measures must be taken to control the disaster to reduce the hazard on people and ecological environment. The control will be based on the information such as monitored or predicted spread range of nuclear or chemical substances, their concentration and dose distribution and time evolution, and the features of the disaster such as explosion, leakage, evaporation, etc. In order to mitigate the hazard, decision makers will evacuate the population in the hotspot, and set up guard region to stop unrelated people, and implement emergent decontamination. During these handling processes, there exist optimization problems, such as how to plan the evacuation, how to partition guard region, and how to plan emergency respond medical and decontaminating resources.

3.2. Models for Cost of Control

In every optimal control problem, there is an object function, or cost function. In the optimal control problems of nuclear and chemical hazard, the object function is the economic cost of all the control measures. The cost will be a limited value because of the constraints of resources. The relationship between economic cost and control measures can be revealed through consideration of each factors associated and comprehensive economic analysis. Different measures will have different effects and different economical costs.

3.3. Optimal Control Problems

Usually there may be a lot of measures of controlling hazard to be chosen, and the combination the measures can be a very big number. Furthermore, there may be various constraints, which make the problem more complex. Optimal control models should be set up for each problem, and appropriate optimization methods need to be developed for the solution. An optimal control problem minimizes or maximizes the object function by adjusting the values of control variables under certain constraints.

The control variables are variables that can be directly adjusted. In the control of nuclear and chemical disasters, the control variables include the sort and amount of emergency respond forces, the handling of hazardous sources, the area and means of evacuation, the area of guard regions, the area of decontamination, etc. The effects and cost of these measures are different and need to be optimized to provide the decision-making process a scientific basis.

The constraints are relatives and value limits associated with the variables. For instance, the atmospheric dispersion model is an important constraint, which describes the quantitative relations between control variables and hazard. Each control variable must be within a limited value range. The constraints make the optimal control problems difficult to solve.
The followings are typical optimal control problems in handling nuclear and chemical disasters.

- the optimal route problem for hazardous materials transport

It is supposed that there is tons of hazardous material to be transported from a chemical warehouse to a chemical plant for further processing, the problem is, to plan a route to minimize the risk to important protected zones along the route. It is assumed that probability of accident is very low, and the risk can be added together to get a total risk value along the route.

The problem is formulated as,

\[ \min J = \int_{L} R dl \]  \hspace{1cm} (1)

Where \( R \) is the hazard to important protection zones caused by an accident happened somewhere in the route. It is defined as a weighted integral of concentration in time and space.

\[ R = \int_{0}^{T} \int_{A} dt \int_{A} p CdS \]  \hspace{1cm} (2)

Where \( p \) is the weight factor, which reflects the importance of the protection zone. And \( C \) is the gas concentration and formulated by the atmospheric dispersion equation,

\[ \frac{\partial C}{\partial t} = F(C, V, T, ...) + Q(r_0) \]  \hspace{1cm} (3)

In the right hand of the equation, \( F \) denote the operator that formulates the effect of meteorological fields on the dispersion of gases, and \( Q(r_0) \) is the source intense, and \( r_0 \) is the position where an accident happens.

To plan an optimal route to minimize the risk, the risk caused by accident happens at every point along the route need to be calculated, this means that the atmospheric dispersion model need to be run many times to get enough information for the solution of optimal route problem. The computing cost will be very large and unaffordable. We introduced and developed the adjoint method, which can greatly reduce the cost of computing.

- the chemical hazard optimal control problem

It is supposed that there is a chemical accident happened and large amount of chemical gas released. To reduce the hazard, a source control handling plan is to be implemented. It is clear that, the faster the source be controlled, the less gas will release, and there will be lower cost on evacuation of population for security. However, this means more resources need to be invested for strengthening emergency forces and improving relevant technologies. The optimization is to find a critical point, which may compromise two parts of cost and make the total cost minimal. The optimal problem is formulated below.

\[ \min J = G_1(U) + G_2(C) \]  \hspace{1cm} (4)

\[ s.t. \quad \frac{\partial C}{\partial t} = F(C, V, T, ...) + Q(1 - U) \]  \hspace{1cm} (5)

Where \( U \) is the control variable, which ranges from 0 to 1. \( G_1(U) \) is the cost of control, which increases with \( U \), especially, when \( U \) approaches unity, the cost grow rapidly owing to nonlinear relationship between cost and effect. \( G_2(C) \) is the cost of evacuation, which depends on the concentration distribution, the hazarded area, population density and social factors.

- Decontamination of radiological polluted land

When a nuclear disaster occurred, radiological substances released into the atmosphere. With the dispersion process, they will eventually deposit and spread around the site. Because the radiological dust will remain in the land for a very long time before completely decay, it is a difficult problem to deal with the polluted land. Now there are mainly two kinds of approaches: to decontaminate the land and make it available, or let it be by isolating it permanently. The economic consideration may be the main criterion. If the techniques for decontamination of radiological pollution are cheap enough and below the loss of abandoning the land, it is worth doing, the choice will be worthy.

The mathematical formulation of the problem is as follows.

First, choose the most cost-effective plan for radiological decontamination, or to minimize the object function,
Where the economic cost $G(R_n)$ may be a segmented function of combination of multiple techniques, that is to say, multiple techniques may be applied successively till the radiological residual is below allowed value, $R_n$. Then compare the minimized economic cost with the expected profit of the land, and judge whether it is worthy of adoption, that is

$$G(R_n) \leq P \frac{1-r}{r}$$

Where $P$ is the expected profit of the land per year, and $r$ is the discount rate.

### 3.4. Optimization Methods

The optimization methods include a wide variety of methods for solving optimal problems. There are many kinds of optimal problems in the control of nuclear and chemical disasters, so it is needed to develop specific optimization methods.

Typical optimal problems are: linear programming, nonlinear programming, integer programming, route planning, etc. Relevant solving methods were developed for each kind of optimal problems. For instance, the simplex algorithm was designed for linear programming, and can get the optimal solution by finite times of iteration. A nonlinear programming problem was usually solved by algorithms based on gradients (Byrd et al. 1995), the key of which is to calculate the derivatives of object function respect to control variables (Zhu et al. 1999). However, in the control of hazard of atmospheric pollution, the constraints are complex, and the direct calculation of gradient is very difficult. In such problems, the adjoint method is introduced (Liu et al. 2004). By constructing the adjoint model of the atmospheric dispersion model, the gradient of the object function can calculated efficiently (Cacuci 1981, Marchuk 1994, Liu et al. 2007).

The optimal route problem is different from the above problems. It dose not search an optimal solution by varying the value of a set of variables. In contrast, it searches for an optimal route, and the methods of solution is unique. The classic variation method was successfully adopted to solve the famous Steepest Descent Curve problem. However, the modern optimal route problems are the consideration of graph theory. The Dijkstra algorithms, based on analytic solution principle, can guarantee the solution of shortest route from a source node to all other nodes after finite number of calculations. However, the computing efficiency is not satisfactory for large-scale problems. The genetic algorithms (Holland 1975, Loughlin et al. 2000), based on the analogue of evolution of creatures, has shown its successful applications in many fields.

### 3.5. An Application for Transport of Chemical Materials

The optimal route model is formulated as (Li et al. 2011),

$$R_n = 1 - \exp\{-\int P_n(l)dl[1+P(x)]\}$$

$$v_n(R) = \frac{R_n - R_{\min}}{R_{\max} - R_{\min} + \epsilon}$$

$$v_n(T) = \frac{T_n - T_{\min}}{T_{\max} - T_{\min} + \epsilon}$$

$$J_n = x_{ij} A_R v_n(R) + x_{ij} A_T v_n(T)$$
\[
\sum_{j=1}^{n} x_{ij} - \sum_{k=1}^{n} x_{kj} = 1
\]
\[s.t.\]
\[
\begin{align*}
\sum_{j=1}^{n} x_{ij} - \sum_{k=1}^{n} x_{ki} &= 0, \quad i = 2, 3, \ldots, n - 1 \\
\sum_{j=1}^{n} x_{ij} - \sum_{k=1}^{n} x_{ki} &= -1 \\
IR_i &< IR_{ij} \\
x_{ij} &\in \{0, 1\} \quad \forall (i, j) \in E
\end{align*}
\]

(12)

Where \(\lambda_R + \lambda_T = 1\), \(R_n\) is the risk of transport route \(l(x, y)\), \(P(x)\) is the penalty function, \(\epsilon\) is the arbitrarily small parameter, \(x_{ij}\) is the decision variable, which will be valued 1 or 0, denotes whether the road is chosen or not, i.e. \(R_{ij}\) is the risk value of the road \((i, j)\), and \(T_{ij}\) is the transport time (cost) of the road \((i, j)\). The constraints guarantee the continuity, the terminal, and the safety criteria of the route.

\[x_{ij} = \begin{cases} 
1, & \text{the road } (i, j) \text{ is chosen} \\
0, & \text{others}
\end{cases}\]

The transport net between the two positions are shown in fig.4, where there are 12 zones to be protected, labeled as black circles.

The predicted weather condition fields are used as input data to drive the adjoint model (Liu et al. 2005), and calculate the toxic dose distribution in the protected region, as shown in fig.5. On the basis of risk value calculations, the genetic algorithm is applied to solve the optimal route problem, and the divergence efficiency curve is shown in fig.5. The optimized route is determined, as shown in fig.6.
Fig. 5. The simulated toxic dose to the protected zones

Fig. 6. The optimized transport route
4. Summary

The modeling of atmospheric pollution hazard caused by nuclear and chemical disasters is associated with the investigation of a series of models: source term models, meteorological field prediction models, atmospheric models and hazard evaluation models. The models were integrated into a system for application in nuclear and chemical disaster emergency respond. Water tank and tracer gas experiments are carried on to verify the prediction of models, and there are good agreements between modeled and experiment data.

A main motivation of modeling the nuclear and chemical disasters is to take rational measures to control their hazard, i.e. to optimize the use of the resources to control the hazard. The optimal control of nuclear and chemical hazard includes the prevention of risk and the reduction of hazard. To formulate the optimal control problems, the Natural Cybernetics theory was introduced as the methodology to consider the associated natural factors and human factors into a whole system. The mathematical framework of optimal control problems is formulated based on the consideration of control measure effects and the corresponding economic costs, coupled with the atmospheric dispersion and hazard making processes. To solve the optimal control problems, relevant techniques, such as the adjoint method and the genetic algorithms are investigated. An example, the optimal route for transport of chemical materials is illustrated.

There are many problems in the modeling and control of nuclear and chemical disasters. For instance, the source term model is not satisfactory, and new methods need to be developed such as source inversion methods based on monitoring data. The economic cost of control measures and the cost of hazard need to be modelled and parameterized more precisely to make the optimization more realistic. High efficient optimization algorithms are needed for decision making.

Acknowledgements

Acknowledgements and Reference heading should be left justified, bold, with the first letter capitalized but have no numbers. Text below continues as normal.

This study was supported by the Natural Science Foundation of China (41375154, 40975089) and Special Fund for Meteo-scientific Research in the Public Interest (GYHY201106033).

References


