 ICCES, vol.15, no.1, pp.19-25

Risk simulation of nanomaterials pollution in power engineering

A.A.Bayramov[1]

Summary

As we know, anthropogenic activities of Power Engineering create wastewater and air pollution, lead to aerosol attenuation of solar radiation and to growth of entropy on the Earth and, as result, climate change. The human Power activities disturb heat and entropy balance and impair ecology. Also, this leads to greenhouse effect and, as result, to climate change. Wastewater in river and sea basins as well as air pollution can influence an exchange of energy between sunlight on the Earth and long-wave radiation leaving in space.

In the paper the role of nanomaterials pollution in Power Engineering is analyzed. We have carried out the procedure of risk analysis and vulnerability of territories to Power Engineering pollution, specifically, nanomaterials impact on an environment. The mathematical methods of simulation of the individual risks are considered for the purpose of nanomaterials risk reduction and remediation. At last, we have carried out researches at a plant of polymeric materials (and nanomaterials), located near to Baku. We have made assessment the individual risk of person affection and constructed the map of equal isolines and zones of individual risk for a plant of polymeric materials and nanomaterials.

Keywords: pollution, models of risk analysis, nanomaterials, simulation

Introduction

Nanotechnology can be defined as the control and restructuring of matter below 100 nm in size in order to create materials, devices, structures and functional systems. Simply put, nanotechnology is the direct manipulation of matter at the level of atoms and molecules [1]. Restructuring nature at the nanoscale leads to materials with novel and exotic properties. The novel properties of nanomaterials make them attractive for use in industrial processes.

The concepts of risks and vulnerability of territories to natural and anthropogenous impacts as Power Engineering pollution have fundamental sense in ecological researches [2,3]. With their help it is possible to reveal potentially dangerous situations and objects, quantitatively to estimate a degree of weight of possible consequences of catastrophic events [4,5]. Thus it is necessary to consider a wide spectrum of cooperating processes on long intervals of time in areas various scales

[1] Institute of Physics Azerbaijan National Academy of Sciences, Baku, Azerbaijan

at uncertainty of sources of disturbances. It demands, that models of processes and the data of supervision were shared in a mode of straight and reverse [7].

Various aspects anthropogenous (in particular, nanomaterials) impacts as result of Power Engineering are directly taken into account in models through the parametrical description of sources of heat, a moisture and polluting impurity and changes of a surface of the Earth on the large areas. Researched processes are described by models of hydro thermodynamics in climatic system, models of transfer and transformation of the moisture, polluting impurity in gas and aerosol states.

Let assume, that all elements of a complex can contain uncertainty and a mistakes. Let's consider models, which are directly connected to processes of carry of heat, a moisture above mentioned nanomaterials.

$$L_{\varphi} \equiv \frac{\partial \pi \varphi_i}{\partial t} + div\pi\left(\varphi_i u - \mu_i grad\varphi_i\right) + \pi\left(H\left(\varphi\right)\right)_i - \pi\left(f_i\left(x,t\right) + r_i\right) = 0, \quad i = \overline{1,n} \tag{1}$$

Here: φ ={$\varphi_i(\boldsymbol{x},t)$, $i = \overline{1,n}$}$\in Q(D_t)$ is state vector-function. Components φ_i describe potential temperature, humidity in an atmosphere, concentration of polluting impurity in gas and aerosol state of nanomaterials; D_t is the range of change space coordinates and time; $\boldsymbol{f}$ = {$f_i(\boldsymbol{x},t)$, $i = \overline{1,n}$} is a function of sources of heat, moisture and impurity; $\boldsymbol{r}$ = {$r_i(\boldsymbol{x},t)$, $i = \overline{1,n}$} are the functions described uncertainties and mistakes of models; $\boldsymbol{u}$ = (u_1,u_2,u_3) is a vector of velocity; μ_i= $(\mu_1,\mu_2,\mu_3)_i$ are the factors of a turbulent exchange for a substance φ_i in direction of $\boldsymbol{x}$ = {x_i, i = 1,2,3} coordinates; $H(\varphi)$ is a nonlinear matrix operator described local processes of transformation of corresponding substances. It does not contain derivatives from functions of states on$x$ and$t$. If the processes of nanomaterials creation and their transformation are taken into account in model then one more variable that is the size of particles is added. u, μ_i, f_i functions and input data of initial and boundary conditions are included in set a component of a vector of parameters $\boldsymbol{Y}$ belonging to range of allowable values *R(Dt)*.

Initial conditions at$t$ = 0 and parameters of model can be written down as

$$\varphi^0 = \varphi_a^0 + \xi\left(x\right), \quad \Upsilon = \Upsilon_a + \zeta\left(x,t\right) \tag{2}$$

Here: φ_a^0 and $\boldsymbol{Y}_a$ are given aprioristic assessment of initial fields φ^0 and vector of parameters $\boldsymbol{Y}$; $\xi(x)$, $\zeta(x,t)$ are mistakes and uncertainty of initial fields and parameters.

Boundary conditions for closure of model are defined by the physical contents of an investigated problem. Proceeding from the form advective-diffusion operators in (1) for convenient they are presenting as

$$\mu_n = \frac{\partial \varphi_i}{\partial n} + \alpha_i \varphi_i - g_i = 0, \quad i = \overline{1,n} \tag{3}$$

Here: $\alpha_i = \alpha_i(x,t,\varphi)$ are functions determining behavior of streams of substances on borders, including modes of their interaction with a surface of the Earth., and g_i are functions of sources, set on borders$\Omega_t$areasD_t.

All methods of the decision of tasks are under construction with use of variational principles [8]. For these purposes the variational formulation of a complex of models (1)÷(3) put down as integrated identity

$$I(\varphi, Y, \varphi*) \equiv \int (L(\varphi), \varphi*)\, dDdt = 0 \tag{4}$$

Here: φ* belongs to space $Q*(D_t)$, conjugate relative to $Q(D_t)$. The integrated identity (4) is transformed subject to of boundary and initial conditions so that at substitution φ*=φ from it we have the ratio of balance of energy of researched system. Proceeding from this condition having executed all necessary transformations in (4) for model (1)-(3), we shall finally receive integrated identity

$$I(\varphi, Y, \varphi*) \equiv \sum_{i=1}^{n} \left\{ (\Lambda\varphi, \varphi*)_i + \int_{D_t} \left[(H(\varphi))_i - f_i - r_i \right] \varphi_i^* \pi dDdt \right\} = 0 \tag{5}$$

Here:

$$(\Lambda\varphi, \varphi*) \equiv \left\{ \int_{D_t} \left[\frac{1}{2} \left(\left(\varphi * \frac{\partial \pi\varphi}{\partial t} - \varphi \frac{\partial \pi\varphi*}{\partial t} \right) + (\varphi * div\pi\varphi u - \varphi div\pi\varphi * u) \right) + \right. \right.$$

$$\left. \left. + \pi\mu grad\varphi \cdot grad\varphi * \right] dDdt + \frac{1}{2} \int_{D} \varphi\varphi * \pi d\, D|_0^t + \int_{\Omega_t} \left(\frac{\varphi u_n}{2} + \alpha\varphi - g \right) \varphi * \pi d\Omega dt \right\}_t \tag{6}$$

Here: u_n is a normal to boundary component of velocity vector. The variational formulation (5) and (6) is used for construction of discrete approximations of model.

In [8] authors used the variational organization of models that on their basis to construct the combined methods of direct and inverse modeling for the problems of higher system level connected to questions of ecological safety and quality management of an environment. These methods include algorithms of calculation of sensitivity functions to variations of the input data, parameters and sources. All these algorithms are generated by corresponding variational principles in which integrated identity of a kind (4) is the key role.

Assessment of ecological risks and vulnerability of territories to anthropogenous nanomaterials impacts - one of typical problems of ecological forecasting. For problems of this class we use combined methods of direct and inverse modeling, methods of the theory of models sensitivity and the generalized characteristics of quality of an environment.

Simulation of risk assessment of nanomaterials

The analysis of nanomaterials manufacture shows, what even at normal functioning, the influence of such objects on an environment is connected both to social - psychological influence on people, and with the potential danger of pollution of an atmosphere and territory dangerous substances [9÷13]. Therefore, the model of risk should reflect all essential factors on which functioning system to the greatest degree depends should be taken into account.

Output parameters of mathematical model of risk determine a mathematical expectation of amount of the affected people living in area of industrial object [14]. We shall consider possible analytical approaches to the decision of a problem. The mathematical expectation (risk R) of amounts of affected people can be determined dependence

$$R_= \int_{\varphi=0}^{2\pi} \int_{l=0}^{\infty} r(\varphi,l)\cdot P(\varphi,l)\, d\varphi \cdot dl,$$

Where: $r(\varphi,l)$ is a distance from a plant up to the person in polar coordinates (the beginning of coordinates is superposed with plant); $P(\varphi,l)$ is a probability of affection of the person in a point with (φ,l) coordinates.

The probability of affection $P(\varphi,l)$ is defined as follows:

$$P(\varphi,l) = P_0(\varphi)\cdot P_l(l,\varphi_0),$$

Where: $P_0(\varphi)$ is a probability of that at the moment of emission the direction of wind $\varphi = \varphi_0$ will be realized; $P_l(l,\varphi_0)$ is a probability of affection on distance l from a place of emission in direction φ_0.

As a pollution is equiprobable at any moment then $P_0(\varphi)$ should be defined on the basis of a wind rose in the given zone or region. If to neglect differences in characteristics of an underlying surface on each of directions of possible distribution of harmful emission and to enter concept of the average characteristic it is possible to simplify essentially a problem, having divided variables:

$$R_= \int_{l=0}^{l=\infty} P(l) \int_{\varphi=0}^{\varphi=2\pi} r(\varphi,l)\cdot P(\varphi)\, d\varphi \cdot dl$$

This approach to calculation of risk criterion is one of possible variants of an analytical method of assessment. In practice of risk assessment the following approaches to mathematical modelling risk are considered by us.

Modelling of individual risk. Individual risk is probability of the person affection in the course of year from the certain reasons in the certain point of space. Results of the analysis of individual risk are displayed on a map of the plant as the closed lines of equal values (isolines). [15-16]

The construction of isolines of individual risk is carried out under the formula (10)

$$R_i\left(x,y\right) = \sum_{m \in M} \sum_{l \in L} P_{Q(x,y)} F\left(A_m\right) \tag{7}$$

Where:$P_{Q(x,y)}$ is a probability of influence on the person in a point with coordinates *(x, y)* of the damaging factor Q with the intensity corresponding to affection of the person (healthy man of 40 years) under condition of realization of A_m event (pollution); $F_{(Am)}$ is frequency of occurrence of A_m event per year; M is a set of indexes which corresponds to considered events; L is a set of indexes which correspond to the list of all damaging factors arising at considered events.

We have carried out researches at a plant of polymeric materials (and nanomaterials), located near to Baku. Isolines of equal risk and zones of individual risk are resulted on figure 1 for this factory.

We can see from figure 1, that near of plant (zone 1) the individual risk of person affection is high, R=10^{-4}. In zone 2 R=10^{-5} (the individual risk of person affection is acceptable). At last, in zone 3 R=10^{-6}, i.e. the individual risk of person affection is low.

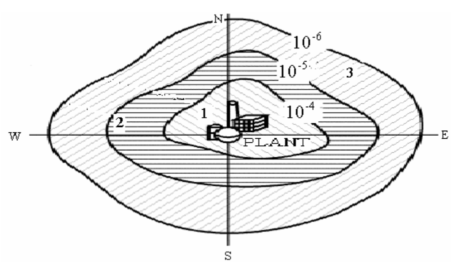

Figure 1: Construction isolines of equal risk and zones of individual risk for a plant of polymeric materials (and nanomaterials): 1, 2, 3 are zones of accordingly high, acceptable and low risk.

Conclusion

So, we know that anthropogenic activities of Power Engineering create wastewater and air pollution, lead to aerosol attenuation of solar radiation and to growth of entropy on the Earth and, as result, climate change. The human Power activities disturb heat and entropy balance and impair ecology. Also, this leads to greenhouse effect and, as result, to climate change. Wastewater in river and sea basins as well as air pollution can influence an exchange of energy between sunlight on the Earth and long-wave radiation leaving in space. In the paper the role of nanomaterials pollution in Power Engineering is analyzed. We have carried out the procedure of risk analysis and vulnerability of territories to Power Engineering pollution, specifically, nanomaterials impact on an environment. The mathematical methods of simulation of the risks are considered for the purpose of nanomaterials risk reduction and remediation. At last, we have carried out researches at a plant of polymeric materials (and nanomaterials), located near to Baku. We have made assessment the individual risk of person affection and constructed the map of equal isolines and zones of individual risk for a plant of polymeric materials and nanomaterials.

References

1. **Nordan & Holman** (2005) "A prudent approach to nanotechnology environmental, health and safety risks" *Industrial Biotechnology,* vol. 1,, p 146.
2. IPCC. (2007) *Contribution of Working Group I to the Fourth Assessment.* **Solomon, S., D. Qin, M. Manning** (eds.) Report of the Intergovernmental Panel on Climate Change.
3. **Grandel J.** (1992) "*Aspects of risk theory*". N. Y.: Springer-Verlag.
4. **Bayramov A.A., Hashimov A.M., Qurbanov K.B.** (2009) Environmental risk of entropy growth and climate change. Proc. 2nd Int. Conference "Energy and Climate Change", Athens, Greece, p.67
5. **Bayramov A.A.** (2008) Power Engineering and environment entropy growth. Proc. of IV Int. Conference on Technical and Physical Problems of Power Engineering, Piesti, Romania, V-29-33
6. **Penenko V.V., Cvetova E.A.** (2004) "Mathematical models for research of risks of environment pollution". *Applied Mech. And Theor.Phys.*, v.45, #2, pp.136-146.
7. **Penenko V.V., Cvetova E.A.** (2002) "Methods and models for research environment and ecological risk assessment". *Optics of atmosphere and ocean*, v. 15, pp. 412–418.
8. **Arius Tolstoshev** (2006)*Nanotechnology*. Earth Policy Centre. Australia.

9. **Bayramov A.A.** (2005) "*About some albedo features of the Caspian surface in the clouded conditions*" Proc. VIII Int. Congress "Energy, Ecology, Economy", Baku, pp.155-156.

10. **Bayramov A.A.** (2008) "*Wasterwater and aerosol attenuation of solar radiation above sea basins*". Proc. US/EU–Baltic Int. Symposium, Tallin Estoniya, # 080121-001.

11. **Hamilton AJ, Stagnitti F, Boland A, Premier R.** (2005) "*Quantitative microbial risk assessment modelling for the use of reclaimed water in irrigated horticulture*" C Brebbia, V Popov, D Fayzieva (eds) WIT Trans on Biomedicine and Health, 9, pp.71–81.

12. **Hamilton AJ, Stagnitti F, Premier R.** (2007) "*RIRA: A tool for conducting health risk assessments for irrigation of edible crops with recycled water*". Computers and Electronics in Agriculture. v.57,is.1.

13. *Global Ozone Research and Monitoring Projects-Report* 16,1985, WMO, Atmospheric Ozone, v.1.

14. **Bayramov A.A.** (2009) Environmental Risk Assessment of Nanomaterials. *Nanotechnology Risks and Benefits. NATO Science for Peace and Security Series C: Environmental Security* Igor Linkov, Jeffery Steevens (Ed.-s), p.317-325, Springer, Dordrecht / Boston / London.

15. **Bayramov A.A.** (2008) Environmental risks of polymeric nanomaterials. *Risk Analysis: The Science and the Art*, SRA Annual Meeting, Boston, USA, p.42.

16. **Bayramov A.A., Safarov N.A.** (2008) Organic-Silicon Sensors and Risk Assessment of Organic Nanomaterials. Jour. "*Scientific Israel - Technological Advantages*" vol.10, No.4, pp.138-146.