HEAT AND MASS TRANSFER AND MODELING AND PREDICTION OF ENVIRONMENTAL CATASTROPHES

A. M. Grishin

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Basic definitions and concepts of the physicomathematical theory of natural catastrophes are given. Possibilities of mathematical modeling of natural and technogenic catastrophes are discussed in the context of the theory of heat and mass transfer and the mechanics of reacting media. The importance of taking into account conjugate heat and mass exchange in modeling catastrophes is emphasized. A formula for evaluating the probability of a "collisional" catastrophe is given.

Basic Definitions and Concepts of the Physical Theory of Catastrophes. The problem of general regularities of the occurrence and development of catastrophes is still not clearly understood. At present, there is not even a general definition of an environmental catastrophe. In particular, the definition of a catastrophe is absent in [1, 2], while in [3], conversely, we have three formulations of an environmental catastrophe, namely:

(1) Natural anomaly (persistent drought, deaths of animals, etc.) often occurring as a result of direct or indirect action of human activity on natural processes and leading to acutely unfavorable environmental consequences or death of the population of a certain region.

(2) Accident at a technical device which caused unfavorable changes in the environment and, as a rule, mass death of living organisms and environmental damage.

(3) One of the states of nature.

In [4], by a catastrophe Ozhegov and Shvedova mean an event with tragic consequences (for example, railway accident or domestic incident) 0and also an "unexpected and extraordinary event in the history of the planet which affects its further existence."

None of the above definitions is comprehensive and constructive. The generic signs of a catastrophe are its detrimental consequences for people and the environment, including the fauna and flora. No physical meaning of a catastrophe is touched upon within the framework of such an approach and no concepts and methods of heat and mass transfer and continuum mechanics are used.

Therefore, in this work, a catastrophe denotes a relatively rapid and irreversible change in the parameters of state (state variables) of the environment which leads to a sharp deterioration of living conditions and to the death of vegetation, animals, and people. The term "relatively rapid" means that the characteristic time of a catastrophe t_c is much shorter than the average length of human life t_* .

There are natural and technogenic catastrophes.

By a natural catastrophe we mean a destructive phenomenon caused by geophysical factors that are not controlled by man (earthquakes, floods, eruptions of volcanos, forest fires, etc.).

If the comparatively rapid destructive changes in the environment are due to human activity or to the operation of man-made technical devices and industries, the catastrophe is referred to as technogenic. A technogenic catastrophe is also called an accident. An accident occurs, as a rule, because of violation of the rules and standards of operation of equipment.

Tomsk State University, Tomsk, Russia; email: fire@fire.tsu.tomsk.su. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 74, No. 4, pp. 41–47, July–August, 2001. Original article submitted July 17, 2000.

In Russia, there is a state standard [5] according to which by an accident is meant a "hazardous technical incident which brings a serious threat to the life and health of people at an object of a certain territory or aquatory and leads to the destruction of buildings, structures, equipment, and transport facilities, disruption of production or transport process, and damage to the environment."

The definitions (proposed in [5]) of a technogenic emergency situation, its source, and the damaging factor and damaging action of the source of a technogenic emergency situation can easily be modified for the description of natural catastrophes.

A natural emergency situation denotes a state of the environment in which normal conditions of the life and activity of people are disturbed in a certain territory of the earth and the property of people and the environment itself are damaged. In other words, a self-destruction hazard to the environment occurs in such a situation.

The sources of a natural emergency situation are those parts of the earth's space where natural catastrophes occur (earthquakes, impact of a meteorite on the earth's surface, snow avalanche, flood, etc.).

The damaging factors of a natural catastrophe are the concrete components of a sharp deviation of the state variables of the environment (temperature, pressure, concentration of the components in the atmosphere, concentration of toxins and bacteria in the air and soil) from normal (equilibrium) values.

The negative influence of one damaging factor or a set of them on the normal existence of people, animals, and plants that results in their death in the case where certain threshold values of these factors are exceeded will be called the damaging action of a natural hazard.

By analogy with the definition of a technogenic hazard, the concept of a hazard of natural catastrophes which is given in [6] can be presented as the state inherent in a concrete region on the earth and realized in the form of damaging actions of the source of a natural emergency situation on people, animals, and vegetation.

At present, the following forms of a natural hazard exist worldwide:

- (1) seismic hazard (hazard of earthquakes);
- (2) space or meteoric hazard;
- (3) forest fire hazard;
- (4) hazard of descent of a snow avalanche in mountains;
- (5) hazard of floods on plains in overflow of rivers;
- (6) hazard of the appearance of hurricanes and tornados on land and sea;
- (7) drought;
- (8) high-power lightning in the atmosphere;
- (9) magnetic storms;
- (10) biological hazard (invasion of injurious insects and epidemics).

A quantitative characteristic of both technogenic and natural hazards is the probability of the corresponding catastrophes, and the science which makes it possible to determine the probability of catastrophes is called risk analysis.

According to [7], catastrophes can be subdivided into three groups in scale: (a) local, (b) regional, and (c) global ones.

In the case of a local catastrophe, the quantity of released energy is $E \le 15$ ktons, which is sufficient for the destruction of an industrial object and the death of people in the territory of an industrial site.

In the case of a regional catastrophe, the quantity E varies within 16 ktons $\langle E \langle 1 \rangle$ Mton and the environmental consequences have an effect on the life of people at a distance of tens and hundreds of kilometers from the site of the catastrophe. The accident at the Chernobyl Nuclear Power Plant can be classified among regional catastrophes as well (1.7 mln ha of forest were contaminated with radionuclides in Belarus alone as a result of this accident).

A global catastrophe occurs when $E \ge 100$ Mtons. In explosion of a nuclear charge of such power, first comes a "nuclear" night and then a "nuclear" winter [8, 9]. As the evaluations show, a similar effect is obtained in collision of the earth with an asteroid of diameter $d \ge 1$ km [9].

Hazardous Space Objects (HSOs) and "Collisional" Winter. The term "hazardous space object" was introduced into catastrophe science in 1994 at the International Conference "Problems of Protection of the Earth against Collision with Hazardous Space Objects (HSOs)" [6]. By hazardous space objects we mean meteorites and comets. Meteorites are bodies of the solar system (fragments of asteroids) falling on the earth from interplanetary space. They can be iron, stony-iron, or stony. Comets are bodies of the solar system that consist of nuclei (laden with ice dust) 10–30 km in size and extended nonstationary atmospheres. Comets travel in strongly extended orbits. They differ in composition and size. The velocity of hazardous space objects varies from 11 to 72 km/sec. Therefore, during their fall many of them (micrometeorites) sublimate in dense atmospheric layers, since the temperature in the bow shock wave which emerges at the surface attains 6000° and "explosive," thermochemical destruction is realized as a result of sublimation and oxidation.

Large stony and iron meteorites collide with the earth's surface. This results in huge funnel-craters. The size of a crater in the USA (Arizona) is impressive: its diameter is 1300 m and its maximum depth is 170 m. By the size of the crater, scientists were able to evaluate the diameter of this iron meteorite (d = 24 m) and the velocity of entry into the atmosphere (v = 12 km/sec). The formation of the funnel is caused by the rapid (explosive) conversion of the kinetic energy of the meteorite to thermal energy in interaction with the surface layer of the crust. According to [10, 11], the energy released in this case has the same effect as an explosion of a million tons in TNT (trinitrotoluene) equivalent.

The theory of thermochemical destruction of meteorites in the earth's atmosphere for the case of their relatively low density (strong meteorites) was developed by S. S. Grigoryan [12]. In this case, part of the cosmic material falls out onto the earth, too, but the crater here is much smaller than upon the fall of iron meteorites.

Researchers have taken great interest in the Tunguska catastrophe. On June 30, 1908, a collision of a hazardous space object with the earth's atmosphere occurred. The lower part of the trajectory of the hazardous space object was located over the territory of Eastern Siberia. Witnesses say that a huge celestial body with a transverse dimension of 800 m moved at a certain angle to the horizon from east to west at a velocity of 1 km/sec [10, 11]. The flight ended with an explosion over the taiga in the region with longitude $\lambda = 101^{\circ}53'$ and latitude $\varphi = 60^{\circ}53'$ at 7 am local time. Light nights were observed for some time after the explosion.

The geophysical stations of Russia and other countries recorded air shock waves which traveled about the earth, while near the village of Vanavara where the explosion occurred one detected a powerful fall of forest 2000 km² in area. This suggests that the energy released during the explosion of the Tunguska meteorite exceeded the energy of an explosion of 1 mln tons in TNT equivalent. At the same time, no crater or considerable fragments of cosmic material were detected at the site of the fall. V. P. Korobeinikov et al. gave the most detailed analysis of the Tunguska problem. According to their evaluations [10, 11], the effective size of the given body was 50-76 m and the average velocity of its motion over the destruction zone was 1-2km/sec; the length of the explosion along the trajectory was 600 m. The Tunguska meteorite exploded at an altitude of 5–7 km above the ground, and the energy released in the explosion corresponded to 17.7–25 Mtons [10, 11]. The explosion resulted in the fall of forest and a forest fire in a radius of up to 9 km [10, 11], and the marks of burns on the trunks and branches of trees were observed at a distance of up to 16-17 km [10, 11]. The consequences of the explosion of the Tunguska celestial body are diverse. Works devoted to this problem are reviewed in [10, 11]. On this basis and as a result of his own investigations, Grigoryan has proposed a new hypothesis [11] that the Tunguska space body was the snow and ice nucleus of a small comet. The density of this nucleus was $\rho = 0.5$ g/cm³. The nucleus had the shape of a cylinder 38 m in radius and a mass of 115,000 tons.



Fig. 1. Relay mechanism of development of a "collisional" catastrophe: A_1 , A_2 , ..., A_9 represent the notation of the stages of the global catastrophe.

The rapid thermochemical destruction of this nucleus as a result of the sharp slowdown in dense atmospheric layers led to its explosion of 17.7 Mtons in TNT equivalent [5, 11], which is in agreement with the data of studies on the consequences of the explosion.

It should be said that collisions of the earth with celestial bodies are a constant so-called "meteor" or "space" hazard. According to the results of the latest investigations [9], the probability of a catastrophic collision of the earth with an asteroid during the nearest 100 years is 10^{-6} . When a constant service for astronomical observations is organized, mankind will be aware of such a collision one year ahead of this event [9].

In collision of space bodies with the earth, local, regional, and global catastrophes can occur depending on the size of the space bodies. In particular, the Tunguska catastrophe is regional. If the diameter of an asteroid is larger than 1 km, in the case of its collision with the earth first comes a "collisional" (cosmic) night and then a "collisional" (cosmic) winter. The mechanism of the occurrence of this catastrophe is as follows. When a crater is formed, more than 100 Mtons of energy is released and numerous very small particles of solid material are detected; these particles are removed to the stratosphere as a result of the formation of a powerful convective column – a jet of the heated air, disperse particles, and combustion products of various organic materials. The latter result from the massive fires that occur in the forests, cities, and villages located near the crater. Finally, a layer of sublimated disperse particles and triatomic gases that absorbs the solar radiation is formed in the stratosphere, causing the "collisional" night followed by the "collisional" winter to come. Thus, a relay mechanism of the development of this global catastrophe occurs (see Fig. 1).

The sequence of events A_1 , A_2 , ..., A_9 presented in the figure can be considered as a physical model of a "collisional" catastrophe, i.e., a set of cause-effect relationships of this complex phenomenon.

Mechanism and Stage of Development of Natural and Technogenic Catastrophes. Based on the mentioned publications and on the foregoing, it can be stated that the process of development of any catastrophe has three stages:

(1) induction period;

(2) rapid release of energy (elastic, nuclear, thermal, etc.) and its transformation to other types of energy;

(3) dissipation of the released energy in the environment.

By the induction period is meant the time of accumulation of destructive energy. During earthquakes this is the time during which the elastic energy of the strain of the earth's crust is accumulated, in the case of atmospheric tornados this is the time from the beginning of the thunderstorm till the formation of the funnel, and in the case of a collisional catastrophe this is the time during which the destructive kinetic energy of a killer asteroid is accumulated. The term "induction period" itself takes its origin in the theory of heat explosion (self-combustion) developed by Van't Hoff [13], Academician N. N. Semenov, Professor O. M. Todes, and Corresponding Member D. A. Frank-Kamenetskii [14]. Heat explosion is a typical catastrophic phenomenon which occurs in both nature (self-ignition of various substances) and engineering.

In the general case, any catastrophe occurs due to a deviation from an equilibrium course of natural or technogenic processes. For example, during an earthquake the equilibrium of the stress-strain state of the earth's crust is disturbed, which leads to its local rapid strain. During the explosion of a nuclear bomb, the equilibrium between the formation and destruction of neutrons is disturbed, which results in the nuclear chain reaction occurring in the nuclear bomb. As a catastrophe develops it is precisely in the second period that a disturbance of the equilibrium occurs in release of thermal, nuclear, electric, elastic, and any other type of energy.

It must be said that any global catastrophe has a cascade mechanism of development, i.e., at different stages of development it includes a multitude of local and regional catastrophes (see Fig. 1), among them massive forest fires, also [15]. There can be certain time intervals between them. As a result, after a series of catastrophes, at the last (third) stage a new thermodynamic equilibrium sets in on the planet earth.

The most complete study has been made of the physics and environmental consequences of a nuclear explosion. In [16, 17], the results of many years of investigation of this problem in the USSR and Russia are generalized.

The mechanism of catastrophes is closely linked with heat and mass transfer [18]. For example, in the case of a "collisional" catastrophe part of the kinetic energy of a moving hazardous space object is luminesced and falls onto the underlying surface, which results, as is shown in [18], in the zones of ignition of forest massifs in the vicinity of the epicenter of the explosion having the shape of ellipses whose larger axes coincide with the direction of motion of the Tunguska meteorite. It is only due to correct account for combined radiative-convective heat-exchange that we were able to propose in [18] a sufficiently accurate mathematical model for prediction of certain environmental consequences of the fall of hazardous space objects. Processes of heat and mass exchange play a major part at all stages of the development of various catastrophes, but their role is particularly great in the establishment of a new thermodynamic equilibrium.

Prediction and Mathematical Modeling of Catastrophes. The method of mathematical modeling based on computers is widely used at present for prediction of environmental consequences of catastrophes. The following types of mathematical models of catastrophes are used:

- (1) deterministic;
- (2) probabilistic;
- (3) mixed (deterministic-probabilistic);
- (4) simulation.

The most efficient tool of knowledge of catastrophes is the deterministic mathematical model.

A deterministic mathematical model of a physicochemical phenomenon denotes a set of differential, integral, integro-differential, transcendental, and algebraic equations and also corresponding boundary and initial conditions that adequately describe the motion, strain, and destruction of bodies and the fields of physical quantities (velocities, pressure, density, temperature, concentrations) for the catastrophic phenomenon under study. These equations express the laws of nature (laws of conservation of mass, momentum, energy, etc.).

Apart from the equations and boundary and initial conditions, a mathematical model also includes a database, i.e., a set of coefficients of derivatives and also functions and constants which describe the thermophysical and reaction properties of a continuous medium. A deterministic mathematical model reflects all basic cause-effect relationships in a short form coded using mathematical symbols. This definition reflects the methodology for solution of problems of heat and mass exchange and of the mechanics of continuous reacting media based on deterministic mathematical models which are commonly used in these scientific disciplines.

Mathematical modeling of catastrophic phenomena denotes a mathematical formulation of a problem, a numerical or analytical solution of a concrete system of equations with corresponding boundary conditions, and an analysis of numerical results and drawing of physically substantive conclusions.

In mathematical modeling of catastrophes, one has to use mathematical models for description of heterogeneous media and phenomena that cover nearly all divisions of modern physics, in different parts of space simultaneously. For this purpose, boundary conditions are required which express the laws of conservation of mass, momentum, and energy at the interfaces between media and are not contradictory to the second law of thermodynamics. Such conditions (boundary conditions of the fourth kind) within the framework of the theory of convective heat exchange were proposed for the first time by A. V. Luikov [19]. For a concrete problem of the convective heat exchange of a subsonic flow with a solid body, boundary conditions of the fourth kind are the conditions of conservation of thermal energy at the interface between the inert flow and the inert solid body. Subsequently they were extended to the solution of the problem of the ignition theory [20] and then [21] generalized to the case of thermochemical destruction of bodies in a hypersonic gas flow. A particular feature of all the above boundary conditions [19–22] is that they do not violate the second law of thermodynamics, whereas unjustified use of boundary conditions of the third kind leads to a negative value of the heat-transfer coefficient and violation of this law [19, 22].

The universal algorithm of mathematical modeling of catastrophes is presented in [10, 15], and the results of a numerical solution of the problem of ignition of combustible forest materials are given in [15, 18, 20].

According to [23, 24], by prediction of a catastrophe we will mean a scientifically substantiated conclusion of its site, time, and consequences with evidence of the reliability of this event.

By reliability of prediction we mean the evaluation of the probability of occurrence and environmental consequences of a catastrophe for the prescribed time interval. Aside from this term, use is often made of the concept "period of anticipation of prediction," which means the interval between the time of publication of the prediction and the time of occurrence of the catastrophe. Clearly, the longer the period of anticipation, the more time one has for conducting organizational measures aimed at decreasing the negative environmental consequences of a catastrophe. Furthermore, one often speaks of the accuracy of prediction. As a rule, this term is used for evaluating the error of predicted state variables of a medium, for example, the fields of temperature, moisture content, and concentration of the components, including radioactive ones. Clearly, in order to determine these fields, it is appropriate to use the basic concepts and mathematical models of the theory of heat and mass transfer [19] and the mechanics of multiphase reacting media [25]. Since different physicochemical phenomena occur at different stages of development of natural catastrophes, it is required that all of the mathematical models of heat and mass transfer and conjugate formulations of problems of heat and mass transfer and the mechanics of reacting media be used [19–21]. By using this approach, a simple procedure is developed in [26] for calculating the discharge of liquid radioactive waste from retention ponds.

According to the degree of coverage of the cause-effect relationships inherent in the phenomenon or the group of physicochemical phenomena under study, mathematical models are subdivided into general, particular, and optimum ones. The usefulness of general models lies in the fact that they represent an unusual kind of standard of accuracy of a physicomathematical description of the phenomenon, based on which, upon dropping terms of the equation insignificant for this problem, one is able to obtain simple models. Optimum models are those whose employment requires less computer time with preservation of the necessary accuracy of the predicted state variables of the problem under study. According to the character of the dependence of the solution of the problem on coordinates, mathematical models are subdivided into zero-dimensional (point), one-dimensional, two-dimensional, and three-dimensional ones.

In [27], for evaluating the probability of natural catastrophes it is proposed to use deterministic physical models of catastrophes and methods of the theory of probability [28]. In particular, by employing the rules of products of conditional probabilities for dependent and independent events we obtain the following expression for the probability of a "collisional" winter:

$$P(A_{1}, A_{2}, ..., A_{9}) = P(A_{1}) P(A_{2}/A_{1}) P(A_{3}/A_{1}A_{2}) ... P(A_{9}/A_{1}A_{2} ... A_{7}) + + P(A_{1}) P(A_{8}/A_{1}) P(A_{9}/A_{1}A_{8}).$$
(1)

It is easily seen that, all other things being equal, the probability of a multistage catastrophe is lower, the larger the number of dependent stages and higher, the more numerous the stages which are independent of each other.

Environmental-Mathematical Monitoring of Catastrophes and Accidents. At present, in setting up any industry and large industrial object, one creates a set of design plans and specifications; this set can be considered as a static model of the dynamic process of operation of this object. However, in connection with aging of the equipment, change in the socioeconomic situation, and action of natural and technogenic catastrophes, situations can occur which are not envisaged by the project and are capable of resulting in large-scale accidents. An example of such an accident can be provided by the accident at the Chernobyl Nuclear Power Plant. The probabilistic criterion of safety (PCS) used worldwide has the following drawbacks:

(1) no account is taken of all possible scenarios of catastrophes and the specific features of the location and technology which is used at a concrete object of the nuclear industry;

(2) no account is taken of the interactions of environmental and technogenic catastrophes (global warming of the climate, hazardous space objects);

(3) the probabilistic criterion of safety makes it impossible to envisage the development of catastrophic events and the entire set of negative consequences of a concrete catastrophe.

These drawbacks manifested themselves in full in connection with a forest fire in the vicinity of the city of Los Alamos (USA). According to [29], the fire lasted for a month (from May 5 to June 6, 2000). The velocity, first of a western wind and then of a southwestern one, reached 16 to 18 m/sec, the moisture content of the elements of combustible forest materials (pine needles, thin branches, and dry grass) was less than 10%, the temperature of the air was 22°C, and the air humidity was 23–28%. The area affected by the fire is a hilly terrain which contributed to the rapid spread of forest fires.

The cause of the fire was the so-called preventive burn-outs of the remains of the previous year's vegetation. This technology is widely used by the U.S. Federal Forest Service to prevent major forest fires. The decision to apply this technological method is taken in the USA at the local level – by a person who can be called a forester under the job nomenclature adopted in Russia.

The fire destroyed forests in a territory of 20,000 hectares. Five hundred houses were burned down in Los Alamos. About 18,000 people were evacuated. The activities of the Los Alamos National Laboratory (LANL) were practically stopped. Every day 1213 forest firefighters, 3–4 helicopters, and 10–15 fire engines took part in fighting the fire. The losses caused by the fire exceeded one billion two hundred million dollars. Therefore, it is necessary to carry out continuous environmental mathematical monitoring of potentially hazardous objects with account taken of changes in the environment and the society. In this connection, it is proposed to use the following algorithm of such monitoring:

(1) System determination of the boundaries of the studied region. Generalization of data on potentially hazardous objects on the basis of design plans and specifications and the changes in the society and the environment.

(2) Initial determination of the hazard involved in each of the natural catastrophes and in each type of activity for each hazardous state and creation of physical models of hazardous processes and objects.

(3) Ranking potentially hazardous objects and creating mathematical models of their operation using design plans and specifications of potentially hazardous industries as initial conditions and laws of conservation of mass, energy, and momentum.

(4) Evaluation of the hazard to the population in the case of normal operation of industries.

(5) Analysis and evaluation of the risk of major accidents, including the risk of toxic discharge and the risk of explosions and fires.

(6) Comprehensive evaluation of the prediction of the hazard of a potentially hazardous object with account taken of the features of the production technology, the age of the equipment, the conjugate heat and mass transfer with the environment, and the change in the state variables of the environment, as a result of technogenic and natural catastrophes.

(7) Creation of a procedure for assessing the environmental and economic damage caused by an accident or a natural catastrophe.

The creation of a system of environmental-mathematical monitoring should start with modeling of the operation of the most hazardous objects, as was done in [30] for the Siberian integrated chemical plant. At the same time, it is expedient to use rigorous mathematical models of the mechanics of continuous multiphase media [25] and of the theory of heat and mass transfer [19] and to use the so-called conjugate boundary conditions [19, 21] expressing the laws of conservation at the interface of media as boundary conditions. The advantage of these conditions is that when they are used the second law of thermodynamics is not violated.

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NOTATION

 A_1 , A_2 , ..., A_9 , events occurring in the case of a collisional catastrophe; $P(A_1)$, probability of the first event (collision of the earth with an asteroid or a comet); $P(A_2/A_1)$, probability of the second event (ignition of combustible forest materials (CFMs)) on condition that the first event has occurred; the remaining notation has an analogous meaning.

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