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**NUMERICAL SIMULATION OF INDUSTRIAL AND ACCIDENTAL
RELEASE FORMATION AND TRANSPORT**

Analytical report on Task Order 006 of Subcontract No 0002P0004-95 between
the University of California and VNIIEF (IEP)

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CONTENTS

	Page
Introduction.....	3
1. General description of accident conditions whose consequences are to be represented by the models developed	4
1.1. Accident explosion conditions	4
1.2. RM combustion in fire and industrial release formation.....	5
1.3. Summary of the techniques used and their application to the Task	7
Order purposes	7
2. Description of computer models, phenomena included, and their development, and the results of comparisons against closed form solution ..	10
2.1. "Jet" and "Cloud" techniques	10
2.2. EGAK code package	16
2.3. COND and COAG techniques	22
2.4. Engineering method	29
2.5. "Prognosis" technique	34
2.6. INM RAS - VNIIEF technique	40
3. Analysis of specific experimental data to calibrate the source term parameters and of these parameters on the calculated dispersion and deposition of contamination	43
3.1. Data on the particle size distribution in the source of release	43
3.2. Data on buoyancy dynamics of explosion cloud	46
3.3. Data on release jet formation	51
3.4. Data on ground and ground air pollutions resulting from accidental and industrial releases	54
References	60

INTRODUCTION

Among diverse possible emergencies and incidents involving industrial releases, the most serious threat to the environment and public are accidental and industrial releases of hazardous materials into the atmosphere. Firstly, pollutants transport in the atmosphere involves processes so much dynamic, that these releases generally have immediate impacts. Secondly, atmospheric releases cause pollution of the ground air layer and underlying surface (i.e. soil, water, vegetation), thus resulting directly in the environmental pollution and high risks of hostile materials intake by the human body and animals.

In turn, of atmospheric releases the most hazardous are technogenic type effluents of radioactive materials (RM) resulting from events such as nuclear tests, nuclear weapons or reactor accidents, authorized and unauthorized releases from nuclear power stations (NPS).

Unfortunately, today it is virtually impossible to conduct directly RM atmospheric releasing experiments because of highly negative response of the public whatever adequate environmental safety measures might be provided with their efficiency proved. For previous accidents involving RM release, it was not a frequent possibility to credibly characterize the source of release, atmospheric and terrain conditions at the accident time, and also the dynamics and general pattern of pollutants. This all makes invaluable the results of earlier methodological experiments using RM; and thus, what is extremely topical is the comparison of these experimental data with the calculations, and verification of numerical techniques as required.

It is the key goal of this work under Task Order 006 to make a comparison between the data calculated using VNIIEF-developed theoretical models and numerical techniques and those available in literature, and also LANL-furnished experimental data on industrial and accidental releases into the atmosphere. We have chosen to describe and discuss the following experiments:

Experiments to simulate accidental RM release into the atmosphere following dummy nuclear warhead explosions in the open ground and RM (plutonium, uranium) combustion in fire.

Experiments to study and simulate industrial releases of chemically toxic materials through ducts.

Section 1 of this report is essentially a summary. It describes a general understanding of physical phenomena contributing to the formation and transport of industrial and accidental releases, and also includes the list and descriptions of the numerical techniques used. Section 2 will give a more detailed description of the numerical techniques and their resulting updating and adaptation in terms of Task Order 006. The following informations are given for each numerical technique described in Section 2:

- technique description;
- technique updating to Task Order 006;
- technique applications for the purpose of Task Order 006;
- methodological or verification calculations and results.

Section 3 will summarize experimental data. While the details of the above-mentioned experiments can not be all simulated numerically, the analytical study has been made to pick the results either used as input data for calculations, or subject to comparisons with numerical data. The experiments are arbitrarily broken down into groups accounting for certain accidental and industrial release conditions. Each group has the following information described thereon:

- experiment description;
- most critical experimental data;
- possible use of the results for comparison with the calculations.

1. GENERAL DESCRIPTION OF ACCIDENT CONDITIONS WHOSE CONSEQUENCES ARE TO BE REPRESENTED BY THE MODELS DEVELOPED

1.1. Accident explosion conditions.

An accident explosion involving dispersion of RMs contained in a nuclear weapon (NW) may be caused by abnormal environments such as lightning stroke, ignition and the following detonation of high explosives (HE) in fire, HE impacted by falling NW, and also unauthorized personnel activities or sabotage.

Open-ground NW accident explosion represents the most dangerous threat such as ground contamination by dispersed RM. Nuclear yield is virtually impossible for this accident explosion, so we are not going to take it into consideration. Three phases of the accident explosion evolution can be distinguished. For the first and most dynamic one, there occur both initial distribution of RM in space and size distribution of primary RM particles (particles' spectrum). In the second, or intermediate phase, there forms a dynamic distributed source of particles as a result of the explosion cloud uprising with soil particles of the underlying surface entrapped thereinto. The final, third phase, has RM particles transported by directed atmospheric flows, particulate cloud dissipated by atmospheric turbulent diffusion, and particles deposited in the gravitation field (sedimentation).

Phase 1 of accident explosion.

When HE detonates, a part of its energy goes into the internal RM energy of a nuclear weapon, thereby causing RM partly to vaporize and melt. This is followed by RM expansion which results in their dispersion into fine particles (aerosols) due to the following phenomena:

- RM vapor condenses to form submicron-size aerosols;
- RM liquid phase disintegrates into droplets of $\sim 1\mu\text{m}$ size typically;
- RM solid phase disintegrates into fragments of millimeters' size.

Explosion products (EP) expansion is retarded due to energy transmission to the surrounding air, so for HE energy $E \sim (100-5000)$ MJ the EP pressure would become equal to the atmospheric over the time $\sim (0.1-1)$ s [1]. Along with that, the EP cloud stabilizes to have lower density and higher temperature $\sim 1000^\circ\text{C}$, and radius $R \sim (5-20)$ m. Fine particles smaller than $\sim 10\mu\text{m}$ undergo abrupt deceleration in the EP cloud and then almost completely follow the way gases move within the cloud. Larger fragments of $\sim 1\text{mm}$ size escape from the EP cloud at several kilometers per second velocity, decelerate, partially burn and further fragmentize, thereby forming a secondary cloud of very fine RM aerosols with typical radius $\sim (100-500)\text{m}$.

Thus, following the first phase of accident explosion a fraction of RM (up to 30%) falls out as larger fragments in the local vicinity to the explosion point. The rest of RM exist as finer RM particles in the primary cloud of hot EP ($R \sim 5-20\text{m}$), and additionally form a secondary RM cloud ($R \sim 100-500\text{m}$) due to larger fragments' combustion. There are no data available on the distribution balance of RM aerosols between the primary and secondary clouds. The predominant chemical form of RM existing in aerosols is dioxides having about $11\text{g}/\text{cm}^3$ density. The secondary cloud of RM particles is located in the atmosphere not disturbed by the accident explosion (clearly, excluding the cases where explosion is followed by a large-scale fire) and later the transport of RM particles within this cloud depends on the atmospheric behaviors (see phase 3 of the accident explosion).

Quantitative description of any conditions existing in the first phase of explosion accident is beyond the purposes of Task Order 006, however, the above given general description may help perform the analysis of experimental data and properly specify the initial characteristics of the source of RM particles.

Phase 2 of the accident explosion

Phase 1 is followed by a hot cloud of low-density EPs ascending in the atmosphere due to Archimedes buoyant force, at about 10 m/s velocities; as the cloud is ascending it

produces a toroidal vortex ring (TVR) and forms a field of flows that draws into the cloud the soil particles from the ground air layer and the underlying surface, RM particles precipitate on the entrapped soil particles in the cloud to form composite particles through binary collisions, or coagulation. These particles represent a complex pattern both morphologically and chemically, with density $\sim (3-5) \text{ g/cm}^3$, and particle size distribution is ranging broadly within $d \sim (0.1-1000) \mu\text{m}$ [2] (where d is the equivalent aerodynamic diameter, i.e. calculated diameter for which the measured sedimentation velocity is related to the particle density $\rho = 1 \text{ g/cm}^3$). The larger particles of the spectrum sediment more rapidly and thus have time to fall out on the ground during the EP cloud ascension. Small size fraction rises up with the EP cloud, and when the cloud has become stabilized in altitude it is to set the contamination pattern of the ground at distances $\sim (10-100) \text{ km}$ from the explosion location.

There is a specific feature in accident explosions having the above-mentioned energies $E \sim (100-5000) \text{ MJ}$, which lies in that turbulent fluctuations in the ground air layer have specific energies comparable to EP energies. As a result, atmospheric turbulence phenomena substantially contribute to the cloud ascension dynamics and diffusion in the atmosphere. Eventually, over the time of several minutes the EP cloud (together with the RM particles it carries) slows down and stabilizes at an altitude of hundreds of meters having characteristic size of tens to hundreds of meters. The cloud stabilization in altitude completes the second phase of the accident explosion.

Phase 3 of the accident explosion

Following its stabilization, the primary EP-RM cloud, like the secondary RM cloud after phase 1, is subject to atmospheric behaviors only. The RM particle size distribution remains virtually the same, and the following conditions are dominating:

- RM particles are transported by directed atmospheric flows,
- particulate cloud dissipates due to atmospheric turbulent diffusion,
- particles sediment in the gravitation field.

The final ground contamination pattern is formed in the times related to the distance from the explosion location. For kilometers' distance these times are around ~ 10 minutes, and about 24 hours for hundreds of kilometers. These are about the same times for RM intake by the human body through inhalation, given the cloud traveling. These data will be addressed in more detail in the pertinent calculations. Later and long-term intake of RMs by the human body is due to RMs being brought to the ground air layer by secondary dust erosion mechanisms, and this is what restricts one's access to and operations directly in the contaminated area.

1.2. RM combustion in fire and industrial release formation.

Sources of radioactive releases to the atmosphere include radioactives combustion in fires that may possibly result from events such as nuclear weapons or power reactor accidents [1,2,3].

Testing for ignition and oxidation of fissile materials was conducted by field experiments and laboratory investigations [4].

Uranium and plutonium easily adsorb oxygen to form a thin oxide film on their surfaces. Oxygen diffusion through the oxide film when it is not torn off by air flow, is what determines the later oxidation rate. To describe the oxidation rate following the oxide film formation, the Arrhenius law is generally used:

$$\frac{dW^n}{dt} = A \cdot p^a \cdot \exp\left(-\frac{E}{R \cdot T}\right), \quad (1.2.1)$$

where

- n , A and a are the constants,
- R - universal gas constant,
- E - activation energy,
- T - temperature,
- p - pressure.

The kinetics of uranium and plutonium oxidation are well described in refs. [5,6]. Ref. [7] gives the Arrhenius law's parameters that are used to calculate high - temperature oxidation of the scattering uranium and plutonium fragments.

Initially, oxidation in pure and doped plutonium proceeds parabolically ($n = 2$). For later times representing fire environments, the reaction becomes near linear function of time.

Ref. [7] reports, that the oxidation rate of scattering fragments increases by an order of magnitude or more when the heating temperature goes as high as the melting point and the oxide film is removed by the air flow. The oxidation rate in air proved virtually constant for all metals tested, and this indicates that the process is dependent on the oxygen diffusion through the boundary layer rather than oxygen adsorption by metals. The oxidation rate value for a series of experiments was about $1720 \text{ mg/cm}^2 \text{ min.}$ as average.

High pyrophoric capacity makes uranium, plutonium and their alloys self - heat with slow temperature growth [8,9,10]. Ignition temperature depends on test sample shape and mass. Thick uranium samples ignite at $\sim 600^\circ \text{C}$, α - phase plutonium samples at $\sim 500^\circ \text{C}$, and for δ - phase plutonium samples active heat release starts at $\sim 400^\circ \text{C}$.

During combustion, the oxide film tends to crack and damage, while convective air flows stir the oxide aerosols all through the space covered by the fire [11 - 18]. These aerosols may partly enter the environment. The most important threat for the human health is plutonium aerosols of $\leq 10 \mu\text{m}$ typical size, i.e. the so - called respirable size fraction. Aerosols resulting from uranium combustion have average diameter smaller than for plutonium combustion. This observation is supported by laboratory and field measurements (Vixen A, 1959, Australia). It has been shown by electron microscopy investigations, that larger particles have numerous finer particles on their surface. There were individual cases, where chain - like aerosol clusters were observed. The summarized data from numerous measurements of plutonium size fractions transforming to respirable aerosols are described in [4]. As average, about $6 \cdot 10^{-4}$ of the total mass goes into respirables. In some cases, respirable plutonium fraction in combustion is smaller than 10^{-5} and, alternatively, is percents for other cases. The above mentioned experiment Vixen A observed at 1% level for plutonium and $\sim 6\%$ for uranium.

Currently, there is no clear understanding of how different effects contribute to aerosol fraction percentage in fissile materials combustion, though some effects have been studied by laboratory experiments. For example, inert sand dust [13] existing during aerosol formation may reduce the amount of respirable material by about a factor of 5. Next, small inert material admixtures may also change both the combustion rate and aerosols percentage by an order of magnitude. The various effects contributing to the amount of volatile aerosols need additional experimental study, this being illustrated by ref. [16].

The most hazardous for humans are ultrafine aerosols resulting from burning plutonium drops falling in the air [13,15,17]. These aerosols include chains of ultrasmall cubic particle crystals ($4 - 100\text{nm}$) and a few nearly spherical particles of $0.5 \mu\text{m}$ size or smaller. They have active median aerodynamic diameter $1 - 2 \mu\text{m}$ and higher solubility. As shown by experiments for various droplet sizes, 10 - 40% of plutonium and 20 - 60% of uranium go into aerosols during droplet combustion at $\sim 2000^\circ \text{C}$. Uranium and plutonium drops have different combustion behaviors. As the plutonium drop is falling, it is continuously losing the surface oxide while monotonously producing aerosols, their amount slightly increasing with the droplet exploding towards the end of the reaction. As it is falling down, the uranium droplet increases in weight due to oxidation, and much less contributes to aerosol producing from the surface than plutonium drop. Major amounts of aerosols produced are those by the droplet explosion. The experiments described used the methodology to investigate metal droplet combustion, as developed in [19, 20].

It can be concluded in general, that under extreme conditions about 10 to 40% plutonium (and 20-60% uranium) may go into respirable fraction. Combustion at temperatures $\leq 1000^{\circ}\text{C}$ representative of common fires makes no more than 1% of plutonium, and 6% of uranium, go into respirable fraction.

The works [1, 2] were conducted to simulate accident conditions for sodium - cooled reactors. A vessel of $\approx 850 \text{ m}^3$ volume was used to observe sodium oxide aerosol forming during the combustion of sodium heated up to 600°C . In this experiments, about 22 - 26% of oxidized sodium went into aerosol fraction.

The above information provides understanding of the earlier development of the source of release with RM existing and burning in fire. The next stage is governed by the dynamics of combustion products jets forming and uprising and the flow dynamics in the fire area. The third stage is associated with the processes including atmospheric transport, turbulent diffusion and sedimentation of aerosols.

Another more common source of anthropogeneous pollution of the environment is industrial releases to the atmosphere [21,22]. Among the major pollution sources associated with human activities is combustion process which is basic in power and transportation industries. For example, coal combustion produces particles basically including carbon, silicon dioxide, aluminum oxide, iron, sulphur and organic oxides. Gaseous effluents include sulphur dioxide, carbon oxide, hydrocarbons and iron oxides. Automobiles generate lead dioxide aerosols having very harmful effects on the human body. Power and transport industries are responsible for about 2/3 of the total aerosols resulting from human activities.

Other aerosol sources include metal industries, where aerosols result from ore roasting and smelting productions and contain metal oxides. Construction materials production, particularly, cement industry have fine mineral particles" dust produced. Various aerosols exist in process and vent duct wastes, and chemical industries.

Industrial releases, followed by pollutants transport by winds may be significantly contributed by chemical reactions and interaction physics. Gases may react photochemically, chemically and catalytically with other pollutants. They may either join the atmospheric natural components, such as oxygen, carbon dioxide, water vapor, or produce other gases or particles. Solid particles may chemically react with gases or between each other as subjected to solar radiation, and also undergo transformations physically, such as integration with other particles to form large aggregated particles.

1.3. Summary of the techniques used and their applications to the Task Order purposes.

1.3.1. The techniques titled "Jet" and "Cloud" [1] are intended to calculate the dynamics of a release like jet or cloud as it moves in the atmosphere with the wind velocity and temperature fields specified. It is assumed, that the jet has uniform parameters in its sectional plane. How jet gases will mix with the surrounding air, depends on the apex angle of the jet which is a function of the rate of effluence and other external conditions. The cloud gases mixing with the surrounding air is to be described by introducing the cloud mass value m as a function of external parameters.

For the purpose of the Task Order, these techniques are used to calculate the dynamics of jet-like industrial releases, phase 2 of accident explosion clouding conditions, and also serve as dynamic distributed source model involved in "Prognosis" technique.

1.3.2. EGAK code package is to be used for computer simulations of 2D multi-flows [2]. What can be considered for these flows is large deformations including the occurrence of multiply connected regions and flow transitions to turbulent conditions.

This code package incorporates the methods capable of calculation gas- and hydrodynamic flows, and flows in terms of viscosity, thermal conductivity, detonation of high explosives, turbulent mixing, phase transitions and finely distributed pollutants existing.

The package employs a continual approach to every flow component and continuous representation of flows through the computational cell boundaries. In so doing, it uses a method of concentrations to avoid unclear boundaries between the components. Basically, this method implies the calculations of flows from mixed cells using a specific algorithm to define the amounts and sequential flows of components based on the analysis of the field of concentrations.

With the gasdynamic techniques as incorporated in EGAK package, unsteady flows including turbulent can be directly simulated [3]. This can provide quite correctly some turbulent flow characteristics being quite correct, which exist due to large-scale fluctuations.

To simulate small-scale turbulent effects, the package has implemented a two-parametric semi-empirical turbulent mixing model. Accordingly, there may be an approach to simulate turbulence resulting from both gravitational and tangential instabilities.

Within the scope of this Task Order, the techniques involved in this package can be used to simulate earlier accident conditions, such as jetting, and pollutants cloud formation and buoyancy, allowing for gravity. The calculations are made using a semi-empirical model both with and without turbulent mixing included. Gasdynamic techniques are used as basic models to include into EGAK package the condensation and coagulation kinetics block involving split physical phenomena technique.

1.3.3. COND and COAG techniques.

COND techniques [4] are designed to numerically simulate the kinetics of oversaturated vapor condensation and the way thermodynamic parameters of the two-phase system will change due to the condensation.

The numerical model incorporates a kinetic equation for size distribution function of condensed droplets, equations for variations in thermodynamic quantities, and equations for a source of critically sized particles and the growth rate of an individual particle. The numerical model involves Smoluchovsky's equation for particles concentrations and size distributions and also uses the frequencies of binary collisions (coagulation kernel) as specified by the given coagulation behaviour.

COAG techniques are intended for numerical simulations of the kinetics of aerosol coagulation accounting for aerosol size distribution and concentration changing as a result of binary collisions. The numerical model involves Smoluchovsky's equation for particle concentrations and size distributions and also uses the frequencies of binary collisions (coagulation kernel) as specified by the given coagulation behavior.

The numerical simulation algorithm is based on the multigroup approach used to solve Smoluchovsky's equation. Moreover, a set of equations describing particle concentrations in groups is obtained using an integration and interpolation method, thus providing the numerical technique with balancing features as required.

COND and COAG techniques are independent blocks to be incorporated in EGAK package for calculations made jointly with gasdynamic codes using split phenomena technique. Also, for the purpose of the Task Order, COND techniques will be used to predict variations in the aerosol size distribution near the source of release and determine the composite particles' activity.

1.3.4. Engineering methods to estimate environmental pollutions by industrial and accidental releases of hostile materials into the atmosphere.

These methods are intended for applications where urgent prediction of ground pollution by hazardous materials is required. They are based on a semi-empirical transport and diffusion model with Pasquill dispersion parameters. The model accounts for: weather conditions; ground wind velocity distribution in altitude and velocity variations with distance; pollution source distribution in altitude and size fractions differing in the underlying surface absorption or sedimentation rates; precipitation effects with washout factor introduced; and underlying surface roughness.

The model can calculate ground contamination by fission products, plutonium, uranium and other radiation sources. Within the Task Order, it is used for calculations and comparison against experimental data on ground contamination following RM explosion and fire accidents.

1.3.5. "Prognosis" technique.

"Prognosis" is a technique to calculate ground pollution density and ground level concentrations of particles following industrial and accidental releases into the atmosphere. Pollutants transport in the atmosphere is described using a 3D turbulent diffusion equation. Pollutant releases are considered as distributed sources having specific particle size distributions. The underlying surface absorbing properties are reproduced by specifying the relevant boundary conditions. The atmospheric turbulent diffusion tensor is assumed as diagonal. The tensor components and wind velocity field are time and height dependent. Horizontal diffusion coefficients are to be calculated according to [5], while vertical diffusivity and wind velocity field calculations are made in terms of the atmospheric boundary layer model [6].

Turbulent diffusion equation is numerically solved using Monte-Carlo method. To make this method more efficient, the solution involves an integral representation [7] to factorize the solution as a function of horizontal coordinates. This factorization provides the solution through modeling the diffusive wandering of particles in a single coordinate i.e. height. Moreover, it helps minimize stochastic noise in predicting the ground pollution density. The resulting calculated data can be read out by either display or printer as pollution charts for any time station and surface grid, similar charts for ground level concentrations, contamination profiles in any direction, and the rates radionuclides enter the human body through inhalation with the contaminants cloud passing over the ground surface.

In terms of the Task Order, the technique is used for calculations to be compared with experimental data for ground contaminations from explosion accidents. The technique is being added by dynamic distributed source considerations as mentioned in paragraph 1.3.1, so that it will be useful to describe the accident explosion conditions continuously through phase 1 and 2.

1.3.6. INM RAS-VNIIEF techniques [8].

With this procedure, the dynamics of atmospheric flows and turbulent diffusion can be described taking into account complex terrain features, heat and mass transfer in the near-Earth layer, formation and evolution kinetics for various pollution components.

The atmospheric hydrothermodynamics model has been implemented in two versions, such as hydrostatic approximation - to define the general pattern of mesoscaled atmospheric flows, and nonhydrostatic approximation - to describe the dynamics for clouding and atmospheric flows with considerable vertical velocities. Atmospheric turbulence characteristics are determined using Reynolds' viscous stress tensor and equation for turbulent energy balance. The Earth's surface temperature is found from the thermal balance in terms of heat and moisture exchange in soil.

Pollutant transports are described by solving hydrodynamics equations simultaneously with the turbulent diffusion, condensation and coagulation kinetics equations for aerosols, as well as the equations for chemical and photochemical reaction kinetics.

For the purpose of the Task Order, the technique has been updated to provide calculations of distributed source formation in the vicinity of release location, this requiring correct account of compressibility in the basic equations and optimized calculation algorithm using nonstandard grid around the source. The technique is used for calculations and comparison with experimental data on industrial releases spreading in complex terrain environments.

2. DESCRIPTION OF COMPUTER MODELS, PHENOMENA INCLUDED, AND THEIR DEVELOPMENT, AND THE RESULTS OF COMPARISONS AGAINST CLOSED FORM SOLUTION

2.1. "Jet" and "Cloud" techniques.

Hydrodynamic vortex ring model (HVRM method)

This method is to describe an earlier uprise stage of a buoyant vortex ring resulting from the evolution of initial buoyant region with its density much lower than the surrounding one, and near-spherical shape. Specifically, this region may be generated as a result of an explosion or a short-term release of some bulk heat.

For small explosions (or releases), the uprise altitude $H1$ for the earlier stage of interest is low relative to the nonuniformity parameter Δ of the atmosphere, and thus the latter can be considered as uniform incompressible liquid. It is also expected, that the uprise stage in question is not sufficient for turbulent mixing effects to show themselves.

Let at some initial time $t = 0$, there be a spherical cloud forming in nonviscous atmosphere of infinitely low density ($\rho_0 \rightarrow 0$), having radius $R0$. Given $R0 \ll \Delta = p_{e0}/\rho_{e0}g$, the density ρ_e and pressure p_e of the undisturbed atmosphere can be assumed approximately constant in altitude: $p_e \approx p_{e0}$, $\rho_e \approx \rho_{e0}$, and therefore one can neglect the cloud expansion ($\text{div } u = 0$). Further, assume $R0/g = \rho = 1$.

While it is assumed, that the cloud has clearly shaped edge, and diffusion processes, turbulent included, are negligible, the vorticity w is concentrated on its outside.

Hydrodynamics equations, with the above-listed assumptions, can be used to derive therefrom the equations for the major parameters of the buoyant vortex ring.

The equation for $R1$ diameter of the vortex ring is:

$$R1 = [4(t + u1) / 3\Gamma]^{1/2} \quad (2.1.1)$$

For $t > t_0$, the circulation $\Gamma = \int R^2 w d\sigma$ (where $d\sigma$ is the element of the ring section produced by the plane crossing the axis of symmetry OX , and R - distance from the axis), is taken at the time the vortex ring generates, t_0 , when the maximum value $\Gamma = \Gamma_0$ is achieved, which further remains unchanged. Based on two-dimensional calculations such as in [1], we take $\Gamma_0 = 5$ and $t_0 = 1.6$.

Formula (2.1.1) appears nearly the same as the similar equation [2], however, the constructions [2] are further made on the assumption that $a1/R1$ is constant.

For the vortex ring having circular cross-section ($a1$ is sectional radius) and surface vorticity distribution, the ring velocity can be written to the order of $a1/r1$ [3] as

$$u1 = \frac{\Gamma_0}{4\pi R1} \cdot \left(\ln \frac{8R1}{a1} - d \right), \quad d \approx 1/2 \quad (2.1.2)$$

Given $u1$ changing slightly at the stage where $t \approx u1$, the formula (2.1.1) may assume $u(t) = u(t_0) = u_0$.

The incompressibility ($R1 a1^2 \approx \text{const}$) and no vorticity diffusion conditions result in the expression for the vortex ring sectional radius $a1 = [2/\pi R1]^{1/2}$. For $t < t_0$ we assume, that the spherical cloud will be rising as $H1 = t^2/2$.

For $t > t_0$, $H1$ can be analytically expressed as

$$H1 = 2a_m [\sqrt{\tau}(\ln \tau - 2) - \sqrt{\tau_0}(\ln \tau_0 - 2)] + 2b_m (\sqrt{\tau} - \sqrt{\tau_0}) + t_0^2/2 \quad (2.1.3)$$

where $\tau = t + u_0$, $\tau_0 = t_0 + u_0$, $b_m = a_0 [\ln(8c_m^{3/4} \cdot \sqrt{3\pi/2}) - 1/2]$, $a_m = 3 a_0 / 4$, $c_m = 4/3\Gamma$, $a_0 = \Gamma/4\pi\sqrt{c_m}$. Here, $R1 = \sqrt{c_m \tau}$.

Calculations for the above set of equations were made as applied to the test [4], where a "hot" vortex ring was produced by firing a spherical vessel (of the radius $R = 5\text{m}$) containing methane-air mixture.

Release jet formation model ("Jet").

Let us consider the dynamics of hot gas jet released into the atmosphere, which is described by altitudinal distributions of wind velocity $\vec{V}$, temperature T and pressure P . For the effluence point, the data to be defined are the jet initial overheat, and effluent gas velocity magnitude and direction.

Consider a jet element of a "second's" mass (fig. 2.1.1) which is expressed as

$$m = \rho' S u, \quad (2.1.4)$$

Fig. 2.1.1. Problem geometry and notation.

where ρ' is the jet air density, S - cross-section perpendicular to the jet axis. Assume, that S section in the plane perpendicular to u is represented by a circle of R radius. Assume also, that all jet-defining quantities are constant in the cross-section S plane.

As it moves, the jet element will be subject to buoyancy. In addition, the jet element will tend to mix with surrounding air and thus have its mass changing. Therefore, Meshchersky dynamics equation for variable mass body [5] must be used to express the jet element motion. In our case, this equation will be given as

$$\frac{d\vec{u}}{dt} = -\vec{g} \frac{T' - T}{T} - (\vec{u} - \vec{V}) \frac{1}{m} \frac{dm}{dt}, \quad (2.1.5)$$

where $\vec{u}$ and T' are the jet gas velocity and temperature, respectively, $\vec{V}$ and T - atmospheric air velocity and temperature, respectively, m - "second's" mass (2.1.4), $\vec{g}$ - gravitational acceleration. The first term in eq. (2.1.4) represents the acceleration resulting from the buoyancy force, the second - the acceleration due to jet gases mixing with the surrounding air. The "second's" mass increment is expressed as

$$\frac{1}{m} \frac{dm}{dt} = -\frac{1}{T'} \frac{dT'}{dt} + \vec{Z} \frac{d\vec{u}}{dt} + \varphi, \quad (2.1.6)$$

where

$$\vec{Z} = \frac{\vec{u}}{u^2} \quad \text{and} \quad \varphi = \frac{2}{R} \frac{dR}{dt} + (\vec{g}\vec{u}) \frac{\mu}{R_g T}, \quad (2.1.7)$$

Substituting eqs. (2.1.6) and (2.1.7) into (2.1.5) yields

$$\frac{d\bar{u}}{dt} = -\bar{g} \frac{T' - T}{T} - (\bar{u} - \bar{V}) \left[-\frac{1}{T'} \frac{dT'}{dt} + \bar{Z} \frac{d\bar{u}}{dt} + \varphi \right] \quad (2.1.8)$$

Let us derive gas temperature equation for the jet element. It can be obtained from the element enthalpy equation $H = E + P\Omega$:

$$\frac{dH}{dt} = \frac{dQ}{dt} + \Omega \frac{dP}{dt}, \quad (2.1.9)$$

where H is the jet element enthalpy, Q - heat quantity and Ω - gas volume in the jet element. Assuming adiabatic jet motion, then $dQ/dt = 0$. Here we ignore the condensation heat of water vapor that may exist in the jet. This is reasonable in the case, where water vapour has low concentration or the jet has relative humidity lower than 100 %. The jet element enthalpy will change due to both the jet gas temperature variation and its mixing with the surrounding air. Thus,

$$\frac{dT'}{dt} = -(T' - T) \frac{1}{m} \frac{dm}{dt} + \frac{(\bar{g}\bar{u})}{C_p} \left(\frac{T'}{T} \right), \quad (2.1.10)$$

where the first term accounts for the jet mixing with the surrounding air, and the other - for the jet cooling adiabatically by during the ascent. When eq. (2.1.6) is substituted into eq. (2.1.10), the jet element temperature equation will finally take the form

$$\frac{dT'}{dt} = -\frac{T'}{T} (T' - T) \left[\bar{Z} \frac{d\bar{u}}{dt} + \varphi \right] + \frac{(\bar{g}\bar{u})}{C_p} \left(\frac{T'}{T} \right)^2. \quad (2.1.11)$$

What is now left to do is substitute eq. (2.1.11) into the equation of motion (2.1.8). This substitution will result in the equation of motion expressed as

$$A_k \frac{du_k}{dt} = \left\{ -\bar{g} \frac{T' - T}{T} - (\bar{u} - \bar{V}) \left(\frac{T'}{T} \right) \left[\varphi - \frac{(\bar{g}\bar{u})}{C_p T} \right] \right\}_i, \quad (2.1.12)$$

where

$$A_k = \delta_k + \left(\frac{T'}{T} \right) (\bar{u} - \bar{V})_i Z_k. \quad (2.1.12a)$$

The equation for the jet element radius vector is given as

$$\frac{d\bar{X}}{dt} = \bar{u}. \quad (2.1.13)$$

The set of eqs. (2.1.11), (2.1.12) and (2.1.13) describing the jet dynamics is not complete. For its closure, an equation for jet element sectional radius R variation is required. If we introduce an apex half-angle of jet α , then it can be written for dR/dt , that

$$\frac{dR}{dt} = utg\alpha \quad (2.1.14)$$

It is impossible to define this half-angle only based on section-average quantities. Therefore, empirical relationships have to be used for this purpose. Let us distinguish two

phases in the jet, active and passive. The active phase typically shows the jet turbulence significantly exceeding the atmospheric. This is the case where there is a submerged turbulent jet with $\alpha = \text{const}$ [6]. For the passive phase, atmospheric turbulence should be taken into account. In [7], the following equation has been obtained for the jet apex half-angle tangent in passive case:

$$\text{tg } \alpha = \frac{2A^2 D}{R |\bar{u}|} \quad (2.1.15)$$

Thus, the set of jet dynamic equations will have the following form:

$$\begin{aligned} \frac{dR}{dt} &= u \text{tg } \alpha \\ A_* \frac{du_k}{dt} &= \left\{ -\bar{g} \frac{T' - T}{T} - (\bar{u} - \bar{V}) \left(\frac{T'}{T} \right) \left[\varphi - \frac{(\bar{g}\bar{u})}{C_p T} \right] \right\}_i \\ \frac{dT'}{dt} &= -\frac{T'}{T} (T' - T) \left[\bar{Z} \frac{d\bar{u}}{dt} + \varphi \right] + \frac{(\bar{g}\bar{u})}{C_p} \left(\frac{T'}{T} \right)^2 \\ \frac{d\bar{X}}{dt} &= \bar{u} \end{aligned} \quad (2.1.16)$$

Cloud rise model ("Cloud").

The next practically important problem to be considered is hot gases' cloud dynamics. The same as for the jet case, the cloud motion should depend on the temperature difference between the cloud gases and the ambient air, and also on its mixing with the air. We only restrict the consideration to the case where temperature and density are uniformly distributed within the cloud. Assume the cloud is shaped as the ball of R radius. The equation of cloud motion is written as (2.1.5) where $\bar{u}$ is the cloud center velocity, T' - cloud gas temperature, $\bar{V}$ and T - atmospheric air velocity and temperature, respectively, m - cloud mass, and g - gravitational acceleration. The cloud mass equation is expressed as

$$m = \rho' \Omega, \quad (2.1.17)$$

where ρ' - is the cloud air density, Ω - cloud volume. The cloud temperature equation has the form of (2.1.13).

The cloud mass equation is defined in terms of turbulent mixing behaviour of the cloud gases and the ambient air. As a first approximation, it can be assumed that m equation has the form similar to that used in [8]:

$$\frac{1}{m} \frac{dm}{dt} = F_m, \quad (2.1.18)$$

where $F_m = \text{const}$. Generally, F_m is the function related to the cloud temperature, density and rise velocity.

The set of equations to describe hot gas cloud dynamics is the following:

$$\frac{dT'}{dt} = -(T' - T) F_m + \frac{(\bar{g}\bar{u})}{C_p} \left(\frac{T'}{T} \right)$$

$$\frac{d\bar{u}}{dt} = -\bar{g} \frac{T' - T}{T} - (\bar{u} - \bar{V}) F_m \quad (2.1.19)$$

$$\frac{dR}{dt} = \frac{R}{3} \left[\frac{1}{T'} \frac{dT'}{dt} - (\bar{g}\bar{u}) \frac{\mu}{R_g T} + F_m \right]$$

$$\frac{d\bar{X}}{dt} = \bar{u}$$

Note, that the cloud rise model for instantaneous release case is also applicable, if slightly modified, to the case considering long-term gas effluence at low-velocities (such as for jets forming in combustion). All to be done for this purpose, is select the value of constant of eq. (2.1.17) from experimental data and provide for the jet element $m \sim R^2$.

Updating the technique.

Updating the calculation technique for explosion cloud dynamics consists in modernising the second equation (2.1.19) and defining the value of F_m .

Consider the cloud uprising by Archimedes buoyancy force as ellipsoid with the ratio D_v/D_h accounting for its oblateness, where D_v and D_h are vertical and horizontal cloud diameters, respectively. Experimental data indicate, this ratio is smoothly decreasing with time. This is rather well approximated by $D_v/D_h = \text{const.}$

As it moves, there occurs interaction between the cloud and the air mass per unit time

$$\frac{dm}{dt} = \rho S_1 |\bar{u} - \bar{V}|, \quad (2.1.20)$$

where ρ is the atmospheric air density,

$$S_1 = \frac{\pi D_h^2}{4} \frac{|u_z|}{\sqrt{u_z^2 + |u_x - V_x|^2}} \left(1 + \frac{D_v^2}{D_h^2} \frac{|u_x - V_x|^2}{u_z^2} \right)^{1/2}, \quad (2.1.21)$$

is the cross-section of the elliptic cylinder which is tangent to the ellipsoid of revolution with the generatrices parallel to relative velocity vector of the cloud (i.e. this cross-section is perpendicular to the velocity vector). It is assumed here that D_v is the dimension in z-axis, and D_h - in x-axis.

The portion of air the cloud is interacting with goes into the cloud, and the other portion does not intermix following the interaction and thus takes away the momentum. Then we rewrite the second equation in (2.1.19) as

$$\frac{d\bar{u}}{dt} = -\bar{g} \frac{T' - T}{T} - (\bar{u} - \bar{V}) \cdot F_m - \frac{d\bar{p}_a}{dt}, \quad (2.1.22)$$

where $\bar{p}_a$ is the momentum of the air having interacted with but being outside the cloud. Let k be the air fraction which intermixes with the cloud, then

$$\frac{1}{m} \frac{dm}{dt} = \frac{k}{\rho' \Omega} \rho S_1 |\bar{u} - \bar{V}|, \quad (2.1.23)$$

where $\Omega = \pi D_v^2 D_h / 6$ - is the volume of the ellipsoid of revolution.

Rewrite eq. (2.1.23) as follows:

$$\frac{1}{m} \frac{dm}{dt} = \frac{3k}{2(D_v/D_h)} \frac{|u_z|}{\xi D_r} \left(1 + \frac{D_v^2 |u_x - V_x|^2}{D_h^2 u_z^2} \right)^{\frac{1}{2}}, \quad (2.1.24)$$

where ξ - is the density ratio of the fire flash material to the ambient air.

$$\frac{d\vec{p}_a}{dt} = \alpha (\vec{u} - \vec{V}) (1 - k) \rho_a S_{\perp} |\vec{u} - \vec{V}|, \quad (2.1.25)$$

Here, α account for the air fraction that following its interacting but not intermixing with the cloud may move at a mean relative velocity different from $\vec{u} - \vec{V}$.

Using eq. (2.1.24) and (2.1.25), rewrite the law of conservation of momentum (2nd equation in (2.1.19)) in the following way:

$$\frac{d\vec{u}}{dt} = -\tilde{g} \frac{T' - T}{T} - a(\vec{u} - \vec{V}) b \frac{|u_z|}{\xi D_h} \left(1 + \frac{D_v^2 |u_x - V_x|^2}{D_h^2 u_z^2} \right)^{\frac{1}{2}}. \quad (2.1.26)$$

The terms introduced here are $a = 1 + \alpha \frac{1-k}{k}$, $b = \frac{3k}{2(D_v/D_h)}$.

Thus, the proposed model has the function F_m of (2.1.18) expressed as

$$F_m = b \frac{|u_z|}{\xi D_h} \left(1 + \frac{D_v^2 |u_x - V_x|^2}{D_h^2 u_z^2} \right)^{\frac{1}{2}}, \quad (2.1.27)$$

The solution of the set of cloud dynamics equations (2.1.19) requires, firstly, that the vertical to horizontal diameter ratio of the cloud be defined. Based on the reviewed experimental data available, we can take this ratio constant as equal to $D_v/D_h = 0.65$ during the cloud rise.

Secondly, weather conditions must be specified, i.e. air temperature and wind velocity as functions of altitude.

And finally, initial conditions should be specified. High explosive detonation on the ground surface is followed by a fire ball generated due to the thermal portion of energy, its generation being completed by the time t_0 . The fire ball diameter can be estimated assuming that explosion products will be expanding until the in-ball pressure equals the atmospheric P :

$$D_0 = \left(\frac{6 \gamma - 1}{\pi \gamma} \frac{Q}{P} \right)^{1/3} \quad (2.1.28)$$

For $\gamma = 1.4$ and heat released by high explosive detonation $Q = 4520$ kJ/kg [9], $D_0 = 2.91 m_{he}^{1/3}$, where m_{he} is the effective high explosive mass. The resulting equation for fire ball diameter agrees well with the expressions given in [6], given that the temperature achieved in detonation is 5000 K.

Based on the estimates of [10], one can obtain $t_0 = 0.03 m_{HE}^{1/3}$. For high explosive masses ranging within 10 - 1000 kg, t_0 is less than 0.03 s., this value being much smaller than the cloud stabilization time 2 - 5 min. Therefore, we take $t_0 = 0$.

16
Consider the density relation of the fire ball substance to the ambient air:

$\xi = \frac{m_{fb}}{\pi/6 D_{fp}^3 \rho} = 0.063 \frac{m_{fb}}{m_{HE}}$. Typically, $m_{fb} = m_{HE}$, thus allowing $\xi=0.126$ to be taken at initial time.

Now a and b terms have to be selected. For this purpose, we make use of the data from refs. [9,11]. Ref. [11] suggests expressing the cloud top stabilization altitude in the quiescent and still atmosphere having standard temperature gradient as $H = 86.4 m_{HE}^{1/4}$ meters.

It is assumed in [9], that stabilization time for any non nuclear explosion is 2 min. Based on the regression analysis of test data for effective HE mass range 53.5 - 1270 kg, the expression $H = 92.5 m_{HE}^{1/4}$ meters has been suggested for the cloud top altitude. Standard geometric deviation of altitude for 22 tests analysed is 1.23.

We believe, it would be reasonable to take the following parameters: $a = 1.5$ and $b = 1.4$. Calculations using this parameters provide the description of the cloud rise dynamics in standard atmosphere as follows. Two minutes after the explosion the cloud top is at the altitude of $H = 86 m_{HE}^{1/4}$ meters. In 3.5 minutes, when the cloud substance becomes equal in density to the ambient air, the cloud top is at $H = 110 m_{HE}^{1/4}$ meters. In about 6 minutes the cloud velocity becomes opposite in sign. This occurs when the cloud top is at $H = 123 m_{HE}^{1/4}$ meters.

Note, that the solution of the set of equations is affected by the initial cloud density variations insignificantly. Thus, the density reduction by a factor of 2 results in about 1.2% increase of the above altitude.

The cloud rise height is more susceptible to initial cloud volume variations. For the volume changing by a factor of 2, the cloud rise height will change by 1.2 times.

The use of the methods in the project and their calibration.

"Prognosis" techniques are intended to predict distributed dynamical sources of release forming as jet and cloud. The basic calculation formulae are reported in ref. [12], and the selection of parameters a and b in eq.(2.1.26) has been made under this Task Order with the calibration against the data of refs. [9,11]. The data from these calibrations are detailed in paragraph 3.2.

2.2. EGAK code package.

2.2.1. General description of the package.

EGAK code package [1] is intended for numerical simulations of nonsteady two - dimensional multiflows featured by large deformations, turbulized flows included.

The code modules incorporated in the package help account for a wide range of physical phenomena including those typical of the flows considered in this work, namely:

- gas - liquid - vapor media dynamics;
- flow turbulence;
- diffusion (molecular and turbulent);
- distributed particles dynamics;
- detonation of explosives and combustible mixtures.

The package successively employs a subiterative method which provides combinations of individual modules to simulate particular flow types, and also involve in or omit from consideration some selected phenomena.

The package uses quadriangular computational grids which are movable as desired and flow adaptable. There are capabilities of specifying both internal and external (as

related to the computational field) boundary conditions, which can provide simulations of flows in intricately configured including multiply connected regions.

2.2.2. Calculation techniques for gas-liquid-vapor flows.

For the purposes of gas-liquid-vapor flow calculations, the package implements some explicit and implicit (in wave transport) Eulerian [2,3] and combined Lagrangian - Eulerian [4,5] methods. These methods are essentially distinguished by continual representation of any flow components that can be described by the following set of thermodynamic parameters: mass and volume concentrations, and specific energies. To define their interfaces, a concentrations method is used [6], thus virtually avoiding computational diffusion at the boundaries which is typically inherent in Eulerian and Lagrangian - Eulerian techniques.

With the above-listed methods, flows can be simulated for a wide range of Mach numbers. The validation and applications of these methods are summarized in [2-6].

2.2.3. Semiempirical turbulence model.

There are techniques involved in the package, which can sometimes provide direct (with no turbulence models used) modeling of turbulent mixing. The results of some calculations of this kind are included in refs. [7-9]. In addition, the explicit - implicit Lagrangian - Eulerian gasdynamic method [4] is used by the package as a basis to implement an original $\kappa - \epsilon$ turbulence model. What specifically features the model is that it allows calculations to be made for turbulence generated by either gravitational or tangential instability individually as well as their combined effects.

2.2.4. Disperse phase flow simulation.

Descriptions of disperse component flows are made using interpenetrated continua approximation which provides for discriminating groups of particles different in size. Each group is represented as continuum with its velocity, density, temperature and particle size fields. It is assumed, that the particle concentration is low, so that particle interactions can be neglected. The particles are bound up with the carrier, or gas - vapor phase by both the momentum exchange due to velocity nonequilibrium and energy exchange due to temperature nonequilibrium.

2.2.5. Some benchmark calculations.

To verify potential uses of the EGAK package models and techniques to simulate phenomena representative of accident explosions or releases, calculations have been made for the flows previously studied experimentally and theoretically. Further, we will describe briefly the calculation procedures and results.

Problem 1. Thermic climbing in the atmosphere.

The problem is stated as follows (fig. 2.2.1). There is a thermic, i.e. spherical region ($R=4.7\text{m}$) having temperature $T=1000^\circ\text{C}$, in the equilibrium exponential atmosphere, with its temperature varying with altitude as shown by table 2.2.1.

Table 2.2.1. Temperature profile for problem 1.

Z(m)	0	100	300	400	1000
T, °C	15	15	20	18	12

Fig. 2.2.1. Problem 1 geometry.

The thermic pressure is taken equal to atmospheric. The equation of state of the atmosphere and thermic is $P=(\gamma-1)e$ with $\gamma=1.4$.

Section 2.1. describes the hydrodynamic vortex ring model (HVRM) which is useful to account for the thermic buoyancy behavior. Two calculations have been made to compare data between HVRM and EGAK calculations, different in the computation grid size ($h=1\text{m}$ and $h=0.5\text{m}$). Some calculated data are given in figs. 2.2.2 and 2.2.3. Clearly, the theoretical and both calculated curves for thermic climb vs. time show good agreement.

Fig. 2.2.2. Velocity field in the thermic climb problem for mesh $h=1\text{m}$.

Fig. 2.2.3. Thermic altitude from time.

Problem 2. Effluence from tank.

The calculation has been made for nitrogen effluence into the air at Mach $M=3$ ($U=1020$ m/s), using the $\kappa - \epsilon$ turbulent mixing model. This problem was experimentally studied in [10]. The hole diameter was $D=1.25$ cm, the effluent jet and air densities were taken the same, $=0.00125$ g/cm³. The equations of state of gases were $P=(\gamma-1)\rho$, with $\gamma=1.4$. Fig. 2.2.4. shows volume concentration isolines for nitrogen calculated for three times. Clearly, the jet is undergoing rather strong diffusion, and the apex angle of the jet at its fixed portion is near experimental value ($\text{tg } \alpha \sim 0.09$). The initial portion of the jet also has the length nearly the same as the experimental value, $L - 14D$.

Fig. 2.2.5. gives the nitrogen volume concentration profile across the section $x/D=21.6$ at the final time ($t=28$ ms). Also given here are the experimental data for the cross-section $x/D=19.2$.

Generally, it should be noted that the calculated data for the fixed flow length well agree with experimental data.

Problem 3. Shock wave in dust-gas medium.

Simulation has been made for the experiments [11] investigating shock waves in dust and gas media. The experiments were performed using a shock tube 2m long and 0.15m in diameter. The tube was filled with air-suspended quartz sand. The shock wave was initiated by an explosive charge at the bottom end of the tube. At the mid-section of the tube, oscillographic records were taken for pressure and illumination intensity of the photodetector by UV light through the medium.

Fig. 2.2.4. Nitrogen concentration isolines at times 8, 16 and 28 ms.

Fig. 2.2.5. Volume concentration profile of nitrogen at 28 ms.

The calculations were made in one-dimensional approximation using a uniform fixed grid with 1cm mesh size. The calculation procedures and results are detailed in [12]. Figs. 2.2.6. and 2.2.7. compare the experimental and calculated data for single-disperse mixture. The data show good agreement in pressure profiles. The troughs in the photodetector illumination virtually coincide with the density peaks of the dust-gas medium.

Fig. 2.2.6 Photodetector illumination (experiment), relative density (calculation) at tube mid-section.

Fig. 2.2.7. Tube mid-section pressure.

2.2.6. New developments on the Contract topic.

1. The turbulent mixing calculation technique (section 2.2.3) was added by the capability to account for air turbulence background as resulting from the wind and temperature gradient which can not be directly considered due to the relevant problem being three-dimensional.

2. The flow model for poly-disperse medium (section 2.2.4.) is integrated with the models for vapor component coagulation and heterogeneous condensation on disperse phase particles, as described in paragraph 2.3. The droplet distribution in size is described by defining a number of groups of particles each represented as continuum having its velocity, density, temperature and size fields. In doing so, split phenomena method at physical processes is employed. Currently, selected code modules have been optimized and are undergoing general proof-testing, and the data base on material properties is under development.

2.2.7. Potential developments.

This section outlines potential ways to improve and develop the EGAK models and methods for industrial accident simulation applications.

1. Extend the EGAK models and methods available to a 3D case. To date, the gasdynamic module and basic service codes have been implemented.

2. Develop improved turbulence models accounting for, particularly, the turbulence nonisotropy and boundary layers existing at stiff walls.

3. Involve a semiempirical turbulence model for polydisperse media flows.

4. Include a combined multicontinual and discrete model for polydispersed medium, providing for some size fractions of disperse phase to be represented as continual (multivelocit) approximations, and others - discretely. With this model, one will be able to describe components where the use of continual approximation is unreasonable, such as size fractions having few particles, though their effects on the phenomenon in question are important.

2.2.8. Potential EGAK package applications in accident simulation efforts.

The code modules incorporated in EGAK package can be used to look at some events typical of industrial accidents, such as:

- any kinds of explosions (involving high explosives, combustible mixtures, overheated fluids, etc.), including detonation considerations;
- jet effluents from pipes;
- accident explosion, release and jet impacts on the nearest locations;
- generation of gas-vapor, (gas)-droplet-vapor and dust-gas clouds and their evolution in the proximity to the accident location;
- fall-out of large-size accident products.

2.3. COND and COAG techniques.

Earlier in the formation of distributed sources of accidental or industrial releases there are important phenomena taking place which are responsible for particle size distribution.

Vapor condensations on atmospheric pollutants and aerosol components are important effects for releases of gaseous and vaporized materials. Condensation phenomena may be significant not only in the problems for close neighborhood of the source of release, but also in distant transport problems (e. g. acid rain formation).

Another important phenomenon which influences particle size distribution is coagulation, which means particles enlargement through binary collisions and merging. Coagulation is basically significant for the close vicinity of the source, since binary collisions are rather frequent only for concentrated aerosol releases. Later, the release

cloud is very much subject to washing out by atmospheric turbulent diffusion, and thus the coagulation decreases.

Coagulation description is also important to define the composition pattern of particles. Thus, open-ground explosions have the explosion cloud entraining a great number of finely dispersed ground particles, and the resulting particle spectrum not only incorporates release components but also particles having complex composition pattern. Eventually, these spectrum and composition spectrum are what determine the pollution behavior for the underlying surface and atmosphere in accidental and industrial releases, since these are what aerosol gravity sedimentation velocity, and fallout chemical and radioactive compositions, etc. all depend on.

Numerical simulation of condensation and coagulation is carried out based on phenomena splitting scheme and using COND and COAG codes, respectively.

Numerical model implemented in COND code, incorporates:

- continuity equation for distribution function $C(g, t)$ of particles in size g .

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial g} (v_g C) = J \delta(g - g_c(t)), \quad (2.3.1)$$

where v_g is the rate for drop size change in condensation, J - flow (source) of particles to larger-size region, g_c - number of molecules in a critical drop. The right-hand-side of eq. (2.3.1) describes random occurrence of obit-critical particles tending to further growth. By solving the kinetic equation (2.3.1), one can evaluate the condensation level $x(t)$ and resulting number of drops $v(t)$.

$$x(t) = \int_0^{\infty} g C dg, \quad v(t) = \int_0^{\infty} C dg.$$

- equation accounting for liquid and vapor temperature T changes:

$$\frac{d}{dt} [T(a c_b + (1-x)c_r + x c_x) - \lambda_1 x / k] = -T(1+a-x) \frac{d \ln(V/V_0)}{dt} \quad (2.3.2)$$

Here c_b is the dimensionless heat capacity of the gas medium where condensation occurs, c_r, c_x - specific heat capacities of vapor and liquid for constant volume, λ_1 - condensation heat, k - Boltzmann's constants, a - term dependent on condensing medium and gas initial densities. The right-hand-side of eq. (2.3.2) accounts for the temperature change due to the system volume variation.

The following equation is used to define the vapor saturation temperature T_p with the given vapor pressure P :

$$P_v(T_p) = P \quad (2.3.3)$$

Numerical simulation considers vapor as ideal gas.

Detailed equations for v_g, J, g_c and also interpolation relationship for $P_v(T_p)$ function are given in [1]. The forms of eqs. (2.3.1) through (2.3.3) are of no basic importance for developing the numerical algorithm.

Particles method is used as a basis to numerically solve eq. (2.3.1). This method has the distribution function $C(g, t)$ over the time interval $[t'', t'' + \Delta t]$ expressed as

$$C = \sum_{i=1}^N v_i(t) \delta(g - g_i(t)) + v_{N+1}(t) \delta(g - g_{N+1}(t)) \quad (2.3.4)$$

with $v_{N+1}(t^n) = 0$. Based on this representation of $C(g, t)$ and using eq. (2.3.1), the following set of equations can be obtained for V_i, g_i [1]:

$$\frac{dv_i}{dt} = 0, \quad 1 \leq i \leq N \quad (2.3.5)$$

$$\frac{dg_i}{dt} = v_s(g_i), \quad 1 \leq i \leq N+1 \quad (2.3.6)$$

$$v_{N+1}(t^{n+1}) = \int_{t^n}^{t^{n+1}} J dt \quad (2.3.7)$$

Eq. (2.3.5) implies that the weights v_i of model particles which have existed in the system by the time $t = t^n$ are unchanged over the step Δt . The weight v_{N+1} of a model particle injected into the system at this step, should be selected, according to (2.3.7), such that would properly render the number of real particles produced by the source in between the times $[t^n, t^{n+1}]$.

Eqs. (2.3.6) are solved by the 2nd order Runge-Kutta scheme

$$g_i^{n+1/2} = g_i^n + \frac{\Delta t}{2} v_s^n, \quad g_i^{n+1} = g_i^n + \Delta t v_s^{n+1/2} \quad (2.3.8)$$

where superscript indicates the time the value refers to, and $t^{n+1/2} = t^n + \Delta t / 2$. The injected particle weight is initially calculated by the formula:

$$v_{N+1}^{n+1} = J^{n+1/2} \Delta t.$$

As soon as it becomes possible to determine J^{n+1} this weight value is to be revised:

$$v_{N+1}^{n+1} = \frac{1}{2} (J^{n+1} + J^n) \Delta t.$$

This approach allows to improve significantly the algorithm accuracy.

Initial size of the particle injected at time $t = t^{n+1/2}$ is assumed equal to $g_{N+1}^{n+1/2} = g^{n+1/2}$, and its size at $t = t^{n+1}$ is calculated by the formula:

$$g_{N+1}^{n+1} = g_{N+1}^{n+1/2} + \frac{\Delta t}{2} v_s^{n+1/2}$$

While particles generate at each Δt step, their number N may appear too large to conduct the calculations efficiently. Therefore, COND code provides for the following procedure to reduce model particles: when their number N has exceeded any specified value, then each two particles having numbers $(2i, 2i-1)$ are made to form one particle of i number, with its weight v_i , and size g_i equal to:

$$v_i = v_{2i-1} + v_{2i}, \quad g_i = (g_{2i-1} v_{2i-1} + g_{2i} v_{2i}) / v_i$$

This procedure maintains the number of drops $v = \sum_{i=1}^N v_i$, and condensation level

$$x = \sum_{i=1}^N g_i v_i.$$

According to scheme (2.3.8), eq. (2.3.2) is to be solved twice for Δt step: for the intervals $[t^n, t^{n+1/2}]$ and $[t^{n+1/2}, t^{n+1}]$. This involves the use of centered schemes in the 2nd order of accuracy.

Eq. (2.3.3) is calculated using Newton iteration process.

COND code has been developed as an independent module and validated by benchmarks [1], and now can be used to simulate vapor condensation behaviors as part of gasdynamics software used to calculate atmospheric transport of industrial effluents [2].

COAG code has been developed as part of the project activity to simulate coagulation behaviors.

Numerical simulation of coagulation phenomena as offered by COAG code, is based on numerical solution of Smoluchovsky's equation for the distribution function $C(g, t)$

$$\frac{\partial C}{\partial t} = S(C; g, t), \quad (2.3.9)$$

where S is Smoluchovsky operator,

$$S(C; g, t) = \frac{1}{2} \int_0^g k(g-n, n) C(g-n) C(n) dn - C(g) \int_0^\infty k(g, n) C(n) dn \quad (2.3.10)$$

(to make writing shorter, we have omitted some arguments at C and k functions). Here, $k(g, n)$ - is the coagulation kernel (occurrence of g - and n -sized particles coalescence).

The numerical technique for eq. (2.3.9) as implemented in COAG code, is similar to that described in [3] and proceeds as follows.

In terms of variable g , consider a grid with nodes $g_1=0, g_2, \dots, g_I$ and define the number of particles N_i in between (g_i, g_{i+1})

$$N_i = \int_{g_i}^{g_{i+1}} C(g, t) dg \quad (i=1, 2, \dots, I-1)$$

By integrating eq. (2.3.9) over the interval (g_i, g_{i+1}) and using quadrature formulae where the function $C(g)$ for each interval (g_k, g_{k+1}) is replaced by the average value

$$\bar{C}_k = N_k / (g_{k+1} - g_k),$$

it would be possible to obtain a set of the following ordinary differential equations for N_i values:

$$\frac{dN_i}{dt} = \sum_{j=1}^i \sum_{k=1}^{i-j} a_{jk}^i N_j N_k - N_i \sum_{j=1}^{I-1} N_j b_{ij} \quad (2.3.11)$$

where a_{jk}^i, b_{ij} coefficients are given through the integral of coagulation kernel by formulae such as

$$b_{ij} = \frac{1}{(g_{i+1} - g_i)(g_{j+1} - g_j)} \int_{g_i}^{g_{i+1}} dg \int_{g_j}^{g_{j+1}} k(g, n) dn$$

$$a_{jk}^i = \frac{1}{(g_{j+1} - g_j)(g_{k+1} - g_k)} \int_{g_i}^{g_{i+1}} dg \int_{g_j}^{g_{j+1}} \int_{g_k}^{g_{k+1}} k(g, n) dn$$

$\alpha_j(g), \beta_j(g)$ are some linear functions of g .

To solve numerically eq. (2.3.11), COAG code uses an implicit scheme of the 2nd order of accuracy, i.e. of the form

$$\frac{N_i^{n+1} - N_i^n}{\Delta t} = F_i(N_1^{n+1}, \dots, N_{i-1}^{n+1}) \quad (2.3.12)$$

Nonlinear set of algebraic equations (2.3.12) is solved using Seidel iteration technique.

The coefficients a_{jk}^i, b_{ij} are calculated involving quadrature formulae with the function $k(g, n)$ substituted by the constant $k(\frac{g_{j+1} + g_j}{2}, \frac{g_{k+1} + g_k}{2})$.

The solutions of Smoluchovsky's equations are specifically featured by their displacement towards higher g values with time t . Therefore, COAG code involves the procedure to extend the grid in g variable followed by interpolation to a new N_i matrix. Moreover, the interpolation algorithm is based on the requirement that the total mass of particles in the system be unchanged.

Let there be at a certain time t a grid of nodes g_i with N_i particles in the intervals (g_i, g_{i+1}) and a new grid $\tilde{g}_i$, $(i=1, 2, \dots, I)$ built having the same number of nodes, where $\tilde{g}_1 = g_1$; e.g., it may be assumed that

$$\tilde{g}_i = g_i + g(g_i - g_1), \quad i > 1.$$

Let us find the number $\tilde{N}_i$ of particles in the interval $(\tilde{g}_i, \tilde{g}_{i+1})$ of the new grid, so that the particles mass $\tilde{m}_i$ within this interval be equal to the total mass of particles contained within the intervals (g_k, g_{k+1}) of the older grid, which fall within the interval

$(\tilde{g}_i, \tilde{g}_{i+1})$. (By definition, $\tilde{m}_i = \int_{\tilde{g}_i}^{\tilde{g}_{i+1}} g C dg$).

For this purpose, we tentatively calculate the values

$$M_k = \int_{g_k}^{\tilde{g}_i} g C(g) dg = \sum_{i=1}^{j-1} \int_{g_i}^{g_{i+1}} g C dg + \int_{g_j}^{\tilde{g}_i} g C dg$$

where g_j is selected on the assumption $g_j \leq \tilde{g}_i < g_{j+1}$ using quadrature formulae of the form

$$\int_{g_i}^{g_{i+1}} g C dg = \frac{N_i}{g_{i+1} - g_i} \cdot \frac{g_{i+1}^2 - g_i^2}{2}.$$

Then, it will be easy to evaluate the mass values $\tilde{m}_i$:

$$\tilde{m}_1 = m_1; \tilde{m}_i = m_{i+1} - m_i, \quad 2 \leq i \leq I-1.$$

and also new $\tilde{N}_i$ values

$$\tilde{N}_i = 2 \cdot \tilde{m}_i / (\tilde{g}_i + g_{i+1}).$$

COAG code has been validated against two benchmark problem types: problems having analytical solutions and those where self-similar solutions for Smoluchovsky's equation are available [4].

Two spectrum characteristics were considered in comparing numerical and analytical data: number N_i of particles in the interval (g_i, g_{i+1})

$$N_i(t) = \int_{g_i}^{g_{i+1}} C(g, t) dg$$

and cumulative mass of particles $M(g, t)$ as a function of their size

$$M(g,t) = \int_0^g gC(g,t)dg$$

Analytical solutions to Smoluchovsky's equation for the function $C(g,t)$ have been only obtained for coagulation kernel being constant values $K(g,n)=a=\text{const}$. In this case, the total mass of particles

$$M = \int_0^\infty gCdg$$

remains constant, while the number N of particles in the system

$$N(t) = \int_0^\infty Cdg$$

is varied as required

$$N(t) = \frac{N_0}{1 + N_0 a t / 2},$$

where $N_0 = N(t=0)$.

For problems with coagulation kernel being constant, the technique implemented in COAG code has provided sufficient accuracy in applications even with small number of grid nodes g ($I \approx 20 - 30$).

To illustrate the capabilities of this numerical technique as applied to variable coagulation kernel, let us consider a problem for Brownian coagulation of particles under diffusion conditions [4]. In this case, the kernel (in dimensionless form) is given as

$$k(g,n) = (g^{1/3} + n^{1/3})(g^{-1/3} + n^{-1/3})$$

Smoluchovsky's equation has the following analytical solution for this kernel:

$$C(g,t) = \frac{N^2}{M} \Psi\left(\frac{gN}{M}\right)$$

where M , N are the particles' mass and number in the system, respectively. Here, $M=\text{const}$,

$$N = N(t) = \frac{N_0}{1 + 2.208 N_0 t}$$

and $\Psi(x)$ is some tabular specified function ([4], p. 120). Fig.2.3.1 compares the analytical and numerical solutions (curves 1 and 2, respectively) at time $t=10$ where the solution of Smoluchovsky's equation may be expected to become self-similar. The results have been obtained for the following parameters

$$N_0 = 1, \quad M = 1.5$$

Initial profile $C(g,t=0)$ is selected of the form

$$C(g,t=0) = \begin{cases} 0, & g < 1 \\ N_0, & 1 < g < 2 \\ 0, & g > 2 \end{cases}$$

The calculation has been made for stepping $\Delta t = 0.2$, and initial (nonuniform) grid of g nodes has been specified for the interval $0 \leq g \leq 30$ and included $I=46$ nodes. Clearly, the self-similar and numerical solutions show good agreement between each other.

If there are particles in the release cloud, that are different in chemical and size distributions, then their coagulation will result in particles representing composite mixtures.

Fig.2.3.1. Comparison the analytical and numerical solutions (curves 1 and 2, respectively) at time $t=10$

Generally, the generation of these particles must be described by solving a kinetics equation [5], which is more complicated than (2.3.9). However, it is most important for many practical problems to evaluate only the addition of chemically toxic or radioactive impurities to the particles making up the major release fraction, while the impurities and the major fraction have sharply different size distributions: impurities are normally very small-size particles, but the major fraction has wide distribution range.

To solve these problems numerically in the frame of COAG code, it is suitable to have impurity particles lying in the range $g_1 \leq g \leq g_2$, and take the major fraction size distribution specified for $g > g_2$. In doing so, the following three chains in coagulation behaviors may be identified:

- impurity particle coagulate themselves;
- major fraction particles coagulate with composite particles;
- impurity particles coagulate with composite-mixed particles and major fraction particles.

The second chain effects are either very small, or may be determined using COAG code to make calculations for the major fraction individually. The first and third chains are most important, and they can be easily calculated in terms of the allowed agreement in size distribution conditions. Moreover, we neglect coagulation behaviors within the major

fraction, therefore eqs. (2.3.11) will have but b_{ij}, a_{ji}^i coefficients not equal to zero, thereby making the calculations easier. Impurity particles in each composite-mixed particle are easily quantifiable from equations for N_i allowing for the relevant coalescence mechanism.

Defining coagulation kernels is a separate problem. Coagulation in the cloud (or jet) earlier in the accidental release formation is specifically featured by the gas having higher temperature and lower density, and also substantial turbulent mixing. According to estimates Brownian coagulation is what dominates for particles having sizes $r < 0.1-0.5 \mu m$, and turbulent coagulation - for the larger. These mechanisms are additively effective, therefore it may be assumed that

$$k = k_{\text{brown}} + k_{\text{turb}}$$

Equation for k_{turb} over intermediate particle sizes $0.5 < r < 10 - 30 \mu m$ was derived in [6] allowing for particles being entrapped by the medium and inertial effects. Under the Task Order, we have obtained an equation for k_{turb} expressed in general. For $r > 30 \mu m$, is written as

$$k_{\text{turb}}(r_1, r_2) = \pi \varepsilon^{1/2} (r_1 + r_2)^2 [\tau_{\text{rel}}(r_1) + \tau_{\text{rel}}(r_2)]^{1/2}, \quad (2.3.13)$$

where ε is the turbulent fluctuation energy, τ_{rel} - velocity relaxation time for particles moving through the medium. Note ref. [7] addressing a similar problem to define the coagulation kernel with particles moving in a turbulent medium.

2.4. Engineering techniques.

Pollutant released by a source is to be transported and dispersed in the atmosphere, where large-scale flows such as wind are responsible for moving the pollutant amounts as a whole, while small-scale turbulent fluctuations make the pollutant disperse by intermixing it with the surrounding air.

The propagation pattern of the pollutant is substantially dependent on wind velocity and the vertical temperature profile of the atmosphere associated with solar radiation flux, terrestrial heat flow, atmospheric humidity and cloudiness, etc.

In calculation practice, the pollutant dispersal situations are classified by stability categories of weather conditions. Currently, the classifications by Pasquill [1], Pasquill-

Gifford [2,3], Turner [4], Uhlig [5], Smith [6], Luna and Church [7] and others are used to categorise weather conditions.

The weather classification system which has become most commonly accepted is that by Pasquill [1-2,10,12]; it provides for six stability classes for atmosphere in the increasing order from A through F.

Two model types are used to describe concentration fields and surface pollutants: those based on semiempirical turbulent diffusion equation solved with various ways to specify diffusivity factor and average wind velocity (K model), and on the Gaussian model with various relationships for cloud or jet dispersal (statistical model) [6,8-13]. More frequently used is the Gaussian model which requires minimum set of input data.

For this model, the dilution factor (i.e. concentration/intensity) in a short-term release is:

$$G(x,y,z) = \frac{F(x)}{2\pi\sigma_y\sigma_z U} \exp\left[-\frac{y^2}{2\sigma_y^2}\right] \quad (2.4.1)$$

where x, y, z are Eulerian coordinates of the point in space, U - wind velocity, h - release cloud altitude over the ground, $F(x)$ - pollutant cloud depletion function, σ_y, σ_z - standard deviation of release cloud pollutant distributions in the respective axes (Pasquill parameters).

The dilution factor at the ground level $z = 0$ and the cloud axis $y = 0$:

$$G(x,0,0) = \frac{F(x)}{\pi\sigma_y\sigma_z U} \exp\left(-\frac{h^2}{2\sigma_z^2}\right) \quad (2.4.2)$$

Maximum dilution factor at the ground level is:

$$G(x_{\max},0,0) = \frac{2F(x_{\max})\sigma_z}{\pi\epsilon U h^2 \sigma_y} \quad (2.4.3)$$

and $x_{\max}$ is to be found from the equation:

$$\sigma_z = \frac{h}{\sqrt{2}} \quad (2.4.4)$$

The concentration N and surface pollution S are respectively:

$$N(x,0,0) = \frac{Q}{T} G(x,0,0) \quad (2.4.5)$$

where Q is the total amount of material in the release, T - release duration and

$$S(x,0,0) = N(x,0,0)WT \quad (2.4.6)$$

where W is the dry sedimentation velocity of the pollutant. This value does not mean kinematic velocity. Typically, $W = 1 - 2$ cm/s for particles posing respiration hazards.

Pollutant depletion in the cloud due to the particles dry fall out on the ground surface is described by the function:

$$F(X) = \exp \left[-\sqrt{\frac{2}{\pi}} \int_0^X \frac{1}{\sigma_z} \exp \left(-\frac{h^2}{2\sigma^2} \right) dx \right] \quad (2.4.7)$$

The cloud depletion resulting from wet precipitation due to rain drops or snow flakes trapping aerosols is generally represented by the exponential law:

$$F_{\omega}(x) = F(x) \exp \left[-\Lambda \left(\frac{x}{U} - \frac{x_0}{U} \right) \right] \quad (2.4.8)$$

where x_0 is the distance from the source where precipitation started, Λ - aerosol wash-out efficiency.

$$\Lambda = 10^{-5} k I \quad 1/s \quad (2.4.9)$$

I is the precipitation intensity, mm/hour,

k - relative wash-out efficiency of precipitations:

rain:	1.0
snow	3.0
thunderstorm rain	1.1
drizzle	4.5
snow and rain	2.4
fog	5.0
pouring rain	2.8

Surface pollution in the trace axis with wet precipitation of pollutants is:

$$S(x,0,0) = N(x,0,0) T \left(W + \sqrt{\frac{\pi}{2}} \sigma_z \Lambda \exp \left(\frac{h^2}{2\sigma^2} \right) \right) \quad (2.4.10)$$

Currently, there are several versions for standard deviations σ_y and σ_z of pollutant distributions in the release cloud. Generally, they are found by comparing measurements of pollutant concentrations in the air and the data calculated by dispersal model based on any weather conditions classification. Moreover, different terrains and release conditions result in different data. In this way, the data are accumulated, the later developments normally involving the previous experimental information which is stored by international and national data banks.

Currently, the most well developed and commonly used are the formula by Smith-Hosker [6;14], with the lateral and vertical variances σ_y and σ_z expressed thereby as:

$$\sigma_y(x) = \frac{ax}{\sqrt{1 + 0.0001x}} \quad (2.4.11)$$

$$\sigma_z(x) = \begin{cases} f(z_0, x) g(x) & \text{for } \sigma_z(x) \leq \sigma_z^{\max} \\ \sigma_z^{\max} & \text{for } \sigma_z(x) > \sigma_z^{\max} \end{cases} \quad (2.4.12)$$

where

$$f(z_0, x) = \begin{cases} \ln[bx^c(1+dx^e)] & \text{for } z > 10 \\ \ln\left[\frac{bx^c}{1+dx^e}\right] & \text{for } z_0 \leq 10 \end{cases}$$

$$g(x) = \frac{fx^h}{1+kx^l}$$

$\sigma_z^{\max}$ is the σ_z limit for the given stability class, m.

z_0 - roughness height of the underlying surface, cm.

x - distance from the source of release, m.

The function $f(z_0, x)$ accounts for the ground microrelief through the roughness height, z_0 , which is represented for different microrelief types by the following values:

Snow, lawn 1 cm high	$z_0 = 0.1$ cm
Mown or small grass, 15 cm high or lower	0.6 - 2
High grass up to 60 cm	4 - 9
Non-uniform ground with	
grass, shrubbery and other features	10 - 20
Park or forest up to 10 m high	20 - 100
City constructions	100

The tables 2.4.1 and 2.4.2 summarise numerical values of the parameters included in Smith-Hosker's formulae.

Table 2.4.1 Values for Smith-Hosker's formulae.

Pasquill stability	$\sigma_z^{\max}_M$	a	f	h	k	l
A	1600	0.22	0.112	1.06	5.38 E-4	0.815
B	920	0.16	0.130	0.95	6.52 E-4	0.750
C	640	0.11	0.112	0.92	9.05 E-4	0.718
D	400	0.08	0.098	0.889	1.35 E-3	0.689
E	220	0.06	0.0609	0.895	1.96 E-3	0.684
F	100	0.04	0.0638	0.783	1.36 E-3	0.674

Table 2.4.2 Values for Smith-Hosker's formulae.

z_0 cm	b	c	d	e
1	1.56	0.048	6.25 E-4	0.45
4	2.02	0.0269	7.76 E-4	0.37
10	2.73	0	0	0
40	5.16	-0.098	5.38 E-2	0.225
100	7.37	-0.0957	2.34 E-4	0.60
400	11.7	-0.128	2.18 E-5	0.78

The formation of release gas-fume jet or explosion cloud depends very much on the processes involved.

The engineering techniques consider three potential sources of release.

1. Explosion.

The maximum uprise height h and diameter D of the cloud will be estimated in this case from the empirical relationship:

$$h = 93E^{0.25} \text{ m} \quad (2.4.13)$$

$$D = 37E^{0.25} \text{ m}$$

E is the explosion yield in kg TNT.

2. Fire.

For atmospheric stabilities of classes A through D (unstable and neutral), the cloud uprise above the ground surface [15] is

$$h = \frac{16\Phi x^{\frac{2}{3}}}{U} \text{ m} \quad (2.4.14)$$

$$\Phi = 3.710^{-5} Q_T \text{ m}$$

where U is the wind velocity in m/s, x - distance from the source of release, m, and Q_T - heat release rate, cal/s.

For stable atmosphere (E - F classes)

$$h = 2.9 \left(\frac{\Phi}{UB} \right)^{\frac{1}{3}} \text{ m} \quad (2.4.15)$$

$$B = \frac{g}{t} \left(2 \frac{\Delta t}{\Delta z} \right) 1/s$$

where g is the gravitational acceleration, $g = 9.81 \text{ m/s}^2$, t - absolute ground air temperature, $\frac{\Delta t}{\Delta z}$ - potential temperature gradient (difference between the measured and absolute temperature gradient).

3. Release through high smokestacks.

The maximum height the release jet reaches for neutral conditions [11-12] is

$$h = 3 \frac{dV}{2U} + 400 \frac{\Phi}{U^3} \quad (2.4.16)$$

$$\Phi = 4.35 10^{-5} Q_T$$

where d is the stack outlet diameter, m, V - effluence velocity from stack, m/s.

For stable conditions in windy weather

$$h = 1.5B^{-\frac{1}{6}} \left(\frac{Vd}{2\sqrt{U}} \right)^{\frac{2}{3}} + 2.6 \left(\frac{\Phi}{UB} \right)^{\frac{1}{3}} \quad (2.4.17)$$

and for stable conditions in still situation:

$$h = 5.1\Phi^{\frac{1}{4}} B^{-\frac{3}{8}} \quad (2.4.18)$$

It is approximately assumed that $B = 8.7 \cdot 10^{-4}$ for E class, and $B = 1.75 \cdot 10^{-3}$ for F class.

The Gaussian turbulent diffusion model has been programmed at VNIIEF together with three sets of standard deviations σ_y and σ_z as given in the forms by Smth-Hosker mentioned above, Pasquill-Gifford [2-3] and Briggs [15].

During the contract activities, the code was added by new capabilities. The model involved in the code can account for:

- distribution of N point sources of release in altitudes with wind velocities specified for each;
- distribution for N point sources in altitudes, with ground wind velocity ($h=2m$) specified and wind velocity distributed in altitude as required by Pasquill-Gifford model:

$$U(H) = \left(\frac{H}{2} \right)^p \cdot U(H=2)$$

where p is the factor related to the atmospheric stability class.
The values of p are given in table 2.4.3.

Table 2.4.3. Factor p values for Pasquill-Gifford model.

Pasquill stability	A	B	C	D	E	F
p	0.07	0.07	0.10	0.15	0.35	0.55

The code provides for the use of standard deviations σ_y and σ_z as

$$\sigma_{y1}(x) = \sigma_y(x) + r$$

$$\sigma_{z1}(x) = \sigma_z(x) + r$$

where r is the characteristic cloud size at the source altitude, this form allowing for initial spacial smearing of the source.

Any source of release may include m size fractions differing in their percentage and sedimentation velocity W. Thus, the calculation is made for Nm components each additively contributing to the total concentration and surface pollution.

While describing the explosion cloud travel, the code can go over from dry to wet precipitation conditions and reversely, and also vary the ground wind velocity at a certain distance from the source of release.

The engineering model is suitable for release calculations of plutonium and uranium-235 aerosols, fissible materials fission products, tritium and various gaseous materials.

The calculated data are displayed by a terminal, read into files and may be read out in tabulated or graphic form.

The engineering model in Pasquill form has been used in safety studies for Russian Fissile Materials Storage Facility.

The final report to be delivered under the Contract will describe the calculations made for Roller Coaster experiments.

2.5. "Prognosis" technique.

Statement of the problem.

"Prognosis" technique is intended for calculations of the ground pollution density for industrial and accidental releases of hazardous materials into the atmosphere. Pollutants transport in the atmosphere is described by the semi-empirical turbulent diffusion equation

$$\frac{\partial n}{\partial t} = \frac{\partial}{\partial x_i} \left[K_{im} \frac{\partial n}{\partial x_m} - v_i n \right] + Q(\vec{x}, r, t), \quad (2.5.1)$$

where recurrent indices imply the addition from 1 to 3, x_i is the Cartesians, r - particle radius, $n(\vec{x}, t)$ - particles of r - radius concentrated at the point $\vec{x}$ at the time t ; $K_{im}(\vec{x}, t)$, $\vec{v}(\vec{x}, t)$ - turbulent diffusion coefficient and macroscopic velocity of particles, respectively; $Q(x, t)$ - source of particles. The problem is solved in a half space $x_3 \geq 0$, i.e. where the underlying surface (US) is regarded as plane $x_3 = 0$. It would be suitable to define the US boundary conditions using a flow of particles j along the axis x_3 , thereby the boundary conditions will be expressed as:

$$j(\vec{x}, t) = K_{33} \frac{\partial n}{\partial x_3} - v_3 n, \quad j(x_1, x_2, 0, t) = \alpha n(x_1, x_2, 0, t), \quad (2.5.2)$$

where α - has velocity dimensions and represents the surface absorbtivity. Note, that v_3 value includes, in addition to the directed particle transport velocity, the particle sedimentation velocity in the gravity field $w(r)$, which depends on the particle size.

The technique is based on the following assumptions:

- turbulent diffusion tensor $K_{ij} = \delta_{ij} K_i$ is diagonal in the US frame of reference;
- velocity and diffusivity fields, $v_i(x_3, t)$ and $K_{im}(x_3, t)$, respectively, are specified and independent of the US frame of reference;
- transport velocities v_1, v_2 and turbulent diffusion coefficients K_i are independent of the particle size.

Atmospheric transport description.

Atmospheric boundary layer (ABL) model [1] is what we use to define velocities $v_i(x_3, t)$ and diffusion coefficient $K_3(x_3, t)$. With this model, the profilers $v_i(x_3, t)$ and $K_3(x_3, t)$ can be reproduced based on the integrated ground data and dimensionless relationships derived from the Obninsk weather mast observations. The technique requires that the following quantities should be specified to describe the profile $v_i(x_3, t)$ and $K_3(x_3, t)$: atmospheric stability level, season of the year, surface roughness, typical velocity 10 m above the ground, and the location latitude. The profile of v_3 velocity

component is defined as sedimentation velocity $w(r)$ [2] added to the source ascent velocity $v_s(x_3, t)$. Generally, horizontal diffusion coefficient can be neither measured directly nor calculated by ABL model. The technique uses the approximation equation formulated in [3] to determine these values.

Source characterization.

The source intensity Q being specified, this should provide a description of the spatial and time behavior of the source of release and also particles size distribution (gases and weightless impurities are taken as a particular case where particles have zero size). The simplest case is point momentary release $Q = q \delta(t) \delta(x_1) \delta(x_2) \delta(x_3 - h)$.

The impulse release cloud represents a hot air mass carrying the released particles along. Accordingly, the technique assumes that following the release impulse all the source particles have the following vertical velocity v_z component:

$$v_z(x_3, t) = \frac{dx_z}{dt} \Phi(x_3 / x_n), \quad \frac{dx_z}{dt} = v_0 \exp(-t / t_0), \quad (2.5.3)$$

where v_0 is the initial ascent velocity and t_0 - typical ascent time of the cloud, $\Phi(y)$ - universal function of the variable $y = x_n / x_3$, which accounts for the velocity field existing during the cloud ascent.

The source may be characterised along each axis by one of the following particle distribution:

1. delta-distribution: $F(x) = \delta(x - x_0)$, x_0 is the source coordinate;
2. Gaussian distribution: $F(x) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(x-x_0)^2}{2\sigma^2}}$, x_0 is source coordinate, σ - variance;
3. uniform distribution over the length $[x_0 - \Delta x, x_0 + \Delta x]$, x_0 - source coordinate, Δx - distribution half-width.

Also, spacial particle distribution can be specified in the forms such as sphere, ellipsoid, or cylinder.

The ways the technique can specify the particle size distributions are:

1. Delta-shaped distribution, or a sum of these, $f(r) = \sum_{i=1}^N f_i \delta(r - r_i)$;
2. Lognormal distribution $f(r) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{\ln^2(\frac{r}{\xi})}{2\sigma^2}}$, where ξ and σ are distribution parameters;
3. Uniform distribution over the length $[r_1, r_2]$;
4. Histogram-based nonstandard distribution.

Underlying surface absorption of impurities.

The absorption factor α in eq. (2.5.2) is an important characteristic to describe surface and at the same time many physical and chemical properties of particles.

Generally, it is the following α values that are only evident: for absolute reflection and absolute absorption surface, $\alpha = 0$ and $\alpha = \infty$, respectively. Of the earliest α measurements for radioactive iodine vapor are those made by Chamberlane [4], where the experimental α values are 0,01 - 0,02 m/s.

Simulation method

An effective scheme of Monte-Carlo method has been developed for numerical solution of eq. (2.5.1) having boundary condition of eq. (2.5.2). This scheme is based on the integral representation of the problem solution [5], which factorizes the solution as related to the coordinates x_1, x_2 . With this factorization, the solution can be calculated through modeling the diffusion trajectories one-dimensional in $x_3(t)$ coordinate. The trajectories $x_3(t)$ are modeled by steps Δt . Prior to the calculation, the region $x_3 \geq 0$ is broken down into cells, so that the coefficients of eq. (2.5.1) inside them would be constant. When these coefficients are constant, there is a possibility to find the

distribution density for the time the particle initially escapes from the cell. This density is approximated by simple enough equations and used for Δt stepping. The particle position at the end of any step is determined by the probability of this particle reaching the definite cell boundary. Each time the particle gets to US, all of the particle conditions required to evaluate the pollution density S in time t using Monte-Carlo method are stored:

$$S(x_1, x_2, t) = \int_0^t j(x_1, x_2, 0, \tau) d\tau \quad (2.5.4)$$

The calculations of trajectories as required are followed by those for pollution density S , while the integral representation [5] allows doing this at any arbitrary US point. Spatial pollutants concentration in the ground air layer $N(x_1, x_2, t)$ for the time t is to be found using the quantity $j(x_1, x_2, 0, t)$ and the boundary condition (2.5.2):

$$N(x_1, x_2, t) = j(x_1, x_2, 0, t) / \alpha \text{ cex}$$

Verification calculations.

The technique has been verified using problems having analytical solutions.

Problem 1. There is a point momentary source of unit power at the height $H = 1$. The velocity components are $v_1 = 0.1$ and $v_{2,3} = 0$. Diffusion coefficients are $K_{1,2,3} = 0.0035$. The underlying surface has absolute absorption, i.e. $\alpha = \infty$. Analytically, this problem has the following solution:

$$S(x_1, x_2) = \frac{1 + 2d/\rho_1}{4\pi H^2 \rho_1^2 d} e^{-\frac{x_1 - \rho_1}{2d}},$$

where x_i have H dimensions; $\rho_1 = \sqrt{x_1^2 + x_2^2 + 1}$, $d = D/(v_1 H) = 0.035$. Sedimentation density for $x_2 = 0$ is given in Table 2.5.1, where S_a indicates the analytical solution, S_{mc} - Monte-Carlo calculation, and Σ - its statistical error.

Table 2.5.1. Sedimentation density for Problem 1.

x_1	Sa	Smc	Σ
0	$1.520 \cdot 10^{-6}$	$7.710 \cdot 10^{-7}$	$1.395 \cdot 10^{-7}$
1	$3.212 \cdot 10^{-3}$	$3.242 \cdot 10^{-3}$	$2.623 \cdot 10^{-4}$
2	$1.609 \cdot 10^{-2}$	$1.675 \cdot 10^{-2}$	$5.051 \cdot 10^{-4}$
3	$2.288 \cdot 10^{-2}$	$2.332 \cdot 10^{-2}$	$4.911 \cdot 10^{-4}$
4	$2.343 \cdot 10^{-2}$	$2.351 \cdot 10^{-2}$	$4.235 \cdot 10^{-4}$
5	$2.154 \cdot 10^{-2}$	$2.159 \cdot 10^{-2}$	$3.623 \cdot 10^{-4}$
7	$1.664 \cdot 10^{-2}$	$1.632 \cdot 10^{-2}$	$2.635 \cdot 10^{-4}$
10	$1.112 \cdot 10^{-2}$	$1.105 \cdot 10^{-2}$	$1.827 \cdot 10^{-4}$
20	$3.982 \cdot 10^{-3}$	$3.935 \cdot 10^{-3}$	$7.754 \cdot 10^{-5}$
50	$7.892 \cdot 10^{-4}$	$7.921 \cdot 10^{-4}$	$2.223 \cdot 10^{-5}$

The further problems have only one of the basic parameters varying and the other taken unchanged.

Problem 2. The coefficient K_3 has a discontinuity at the point $x_3 = 1$, i.e. $K_{31} = 0.0035$ for $x_3 < 1$ and $K_{32} = 0.006$ for $x_3 \geq 1$. Analytically, the solution is given as:

$$S(x_1, x_2) = (4\pi H^2 2d(1+a))^{-1} \sum_{k=0}^{\infty} \frac{(2k+1)b^k}{\rho_k^2} [1 + 2d/\rho_k] e^{\frac{x_1 - \rho_k}{2d}},$$

where $a = \sqrt{K_{31}/K_{32}}$; $b = (a-1)/(a+1)$; $\rho_k = \sqrt{x_1 + x_2 + (2k+1)^2}$. The resulting data are summarised in Table 2.5.2.

Table 2.5.2. Sedimentation density for Problem 2.

x_1	Sa	Smc	Σ
0	$1.317 \cdot 10^{-6}$	$9.708 \cdot 10^{-7}$	$2.553 \cdot 10^{-7}$
1	$2.782 \cdot 10^{-3}$	$2.526 \cdot 10^{-3}$	$2.337 \cdot 10^{-4}$
2	$1.393 \cdot 10^{-2}$	$1.405 \cdot 10^{-2}$	$4.644 \cdot 10^{-4}$
3	$1.981 \cdot 10^{-2}$	$2.009 \cdot 10^{-2}$	$4.560 \cdot 10^{-4}$
4	$2.029 \cdot 10^{-2}$	$2.093 \cdot 10^{-2}$	$4.031 \cdot 10^{-4}$
5	$1.866 \cdot 10^{-2}$	$1.890 \cdot 10^{-2}$	$3.414 \cdot 10^{-4}$
7	$1.441 \cdot 10^{-2}$	$1.441 \cdot 10^{-2}$	$2.514 \cdot 10^{-4}$
10	$9.641 \cdot 10^{-3}$	$9.770 \cdot 10^{-3}$	$1.729 \cdot 10^{-4}$
20	$3.528 \cdot 10^{-3}$	$3.490 \cdot 10^{-3}$	$7.321 \cdot 10^{-5}$
50	$7.729 \cdot 10^{-4}$	$7.615 \cdot 10^{-4}$	$2.205 \cdot 10^{-5}$

Problem 3. There is a particles cloud considered which moves as a whole vertically at a constant velocity v_3 (either ascending or sedimenting in a gravitation field). The analytical solution is expressed as:

$$S(x_1, x_2) = \frac{\sqrt{1+g^2}}{4\pi H^2 \rho_1^2 d} \left[1 + \frac{2d}{\rho_1 \sqrt{1+g^2}} \right] e^{\frac{x_1 - g - \rho_1 \sqrt{1+g^2}}{2d}},$$

where $g = v_3/v_1$. The comparison data for $H = 0.01$ and $v_3 = 0.01$ are shown in Table 2.5.3.

Table 2.5.3. Sedimentation density for Problem 3.

x_1	Sa	Smc	Σ
0	$1.554 \cdot 10^3$	$1.554 \cdot 10^3$	7.089
$2.0 \cdot 10^{-2}$	$1.790 \cdot 10^2$	$1.793 \cdot 10^2$	$4.407 \cdot 10^{-1}$
$4.0 \cdot 10^{-2}$	$3.491 \cdot 10^1$	$3.493 \cdot 10^1$	$1.359 \cdot 10^{-1}$
$7.0 \cdot 10^{-2}$	8.808	8.859	$5.046 \cdot 10^{-2}$
$1.0 \cdot 10^{-1}$	3.722	3.748	$2.684 \cdot 10^{-2}$
$2.0 \cdot 10^{-1}$	$7.437 \cdot 10^{-1}$	$7.424 \cdot 10^{-1}$	$8.129 \cdot 10^{-3}$
$4.0 \cdot 10^{-1}$	$1.603 \cdot 10^{-1}$	$1.579 \cdot 10^{-1}$	$2.575 \cdot 10^{-3}$
$7.0 \cdot 10^{-1}$	$4.803 \cdot 10^{-2}$	$4.759 \cdot 10^{-2}$	$1.063 \cdot 10^{-3}$
1	$2.242 \cdot 10^{-2}$	$2.226 \cdot 10^{-2}$	$6.050 \cdot 10^{-4}$
100	$1.112 \cdot 10^{-4}$	$1.238 \cdot 10^{-4}$	$1.568 \cdot 10^{-5}$

The calculations were all carried out in PC-AT environment using a standard pseudorandom-number generator. The number of trajectories calculated for problems 1 and 2 is 50.000, and 300.000 trajectories have been calculated for problem 3.

Updating the technique.

As shown by experience in solving practical problems, diffusion in x_3 coordinate can be neglected for sufficiently large particles. Moreover, a randomly selected modeling step

At makes it difficult to evaluate particles concentration n at points above US using Monte-Carlo method. Given this considerations, the modeling scheme has the following modifications introduced:

1. possible neglect of diffusion in x_3 coordinate;
2. possible trajectory modelling by steps Δt without breaking the region $x_3 \geq 0$ into cells.

As previously, the modified technique has the source represented by spatial and time characteristics, particle size distribution of the release and particle absorption level of the underlying surface. Moreover, it accounts for the cloud (or jet) climbing by formulating the law of motion for particles belonging to the source.

The source time history is defined by the function of release intensity $P(t)$ where P has mass dimensions per unit time. There may be one of the following ways to specify the form of $P(t)$ function:

1. impulse source: $P(t) = \sum_i M_i \delta(t - t_i)$, where M_i is a release mass in an impulse, t_i - impulse time;

$$2. \text{ uniform source: } P(t) = \begin{cases} 1/(t_2 - t_1), & t \in [t_1, t_2] \\ 0, & t \notin [t_1, t_2] \end{cases}$$

3. $P(t)$ as histogram;

4. $P(t)$ as linear plot;

5. Exponential source: $P(t) = \lambda e^{-\lambda(t-t_0)}$, where t_0 is the source initiation time, $1/\lambda$ - source average life span.

Within its lifetime which depends on the intensity spectrum, the source conditions may be time dependent. These time dependent source conditions include: the release particle size distribution, density, absorbtivity by underlying surface, and spacial characteristics.

The same way as previously, particle size distribution is defined based on the set of standard and user-selected spectra: delta-shaped, uniform, lognormal, and based on a histogram or a linear plot.

The quantities defining the particles absorbtivity by the underlying surface have been now included into the source description. The purpose of doing this is to offer the user an opportunity to use a variety of independent or multicomponent (in release particles' properties) sources in a single problem. Now, it is only the type number of absorption layer that can be specified on the underlying surface, while α (see. 2.5.2) value is taken for the source the release particle has actually escaped from.

By their spacial behaviors, the sources are categorized into three groups:

1. release having spacial parameters as specified by the user;
2. explosion cloud-like release;
3. jet-like release.

The previous version of the of the technique allowed only the use of the first source type.

Consider distributed sources such as jets and explosion clouds. These sources have release particles getting into atmospheric flows not just immediately, but being entrapped before by directed and turbulent motions of the source gases. To account for these, the calculation techniques for jet and explosion cloud dynamics described in Section 2.1 are to be used. Based on the source parameters (jet or explosion cloud cases), calculations include the trajectory of the cloud center or jet axis, and also typical cloud or cross-sectional jet sizes. Average lifetime of the source particle can be defined by the expression:

$$\frac{1}{\tau} = \frac{w}{R} + \frac{4K}{R^2}, \quad (2.5.5)$$

where R is the typical turbulence zone size in the source, K - turbulent diffusion coefficient within the source, w - sedimentation velocity. The probability for the particle escape from the source by the time t can be given as

$$F(t) = \int_0^t \frac{1}{\tau(x)} e^{-\int_0^x \frac{dx}{\tau(y)}} dx. \quad (2.5.6)$$

Eq. (2.5.6) is used to define the initial time for the particle to move independent of the source. This is also the time the initial particle coordinates are specified for.

The technique allows one to consider several isolated or multicomponent (in pollutants) sources. While the result is linearly dependent on the total released mass and additive by sources, the release mass of each source can be normalised to a unity, with calculated sedimentation density data stored separately for each source or source group. This would make it possible to vary the release mass without reconsidering the whole of the problem as a whole.

2.6. INM RAS - VNIIEF technique.

2.6.1 Description of the methods.

With this procedure [1 - 4], the dynamics of atmospheric flows and turbulent diffusion can be described taking into account complex terrain features, heat- and mass transfer in the near-Earth layer, formation and evolution kinetics for various pollution components.

The atmospheric hydrothermodynamics model has been implemented in two versions, such as hydrostatic approximation - to define the general pattern of mesoscaled atmospheric flows, and nonhydrostatic approximation - to describe the dynamics for clouding and atmospheric flows with considerable vertical velocities. Atmospheric turbulence characteristics are determined using Reynolds' viscous (stress) tensor and

equation for turbulent energy balance. The Earth's surface temperature is found from thermal balance in terms of heat and moisture exchanges in soil.

Pollutant transports are to be described by solving hydrodynamics equations in combination with the turbulent diffusion, condensation kinetics and coagulation equations for aerosols, as well as the equations for chemical and photochemical reaction kinetics.

The numerical model of pollutant transport in the atmospheric boundary layer is based on the semi-empirical equation of turbulent diffusion. This model is realized jointly with hydrodynamical numerical models. This is explained by the fact that the process of pollutant transport in the lower layers of the atmosphere depends essentially upon the stratification, wind velocity, and other characteristics of the ground air layer. Hence, the interaction between pollutants and underlying surface is parameterized using the model of boundary layer. The characteristic feature of the equation of turbulent diffusion is that, in the general case, its coefficients are tensors. If the assumption is made that the flow field model grid-values depend only on height and the pollutant concentration is of space structure, then the second momentum equations can be obtained. As a consequence, the diffusion coefficients depend upon the mean characteristics of the atmospheric boundary layer: wind shift, stratification, etc. In so doing, it is vital to develop numerical schemes for the solution of transport and diffusion problems which account for orographical and thermal nonuniformities of the underlying surface.

In numerical simulation of pollutant transport, some additional requirements are imposed upon finite-difference schemes. One of them is the "monotonicity" condition which is necessary to provide the non-negativity of the pollutant concentration values.

For discrete approximation of the equation of transport, a splitting-up method is used which is applied to different physical processes. As a result, three stage numerical scheme is obtained for each time step. The stages are as follows:

1. Pollutant transport over the trajectories,
2. Turbulent diffusion,
3. Pollutant local transformations.

The first stage is the principal in the process of transport and most complicated for numerical realization. Our scheme is a modification of the second-order scheme of Van Leer which provides both monotonicity and conservation properties. The monotonicity is achieved by introducing a non-linear operator of "monotonization" which holds the order of approximation. At the second stage, implicit splitting-up method over variables are used. If the operator includes non-diagonal elements, then an improvement of iteration is performed. This numerical model provides new features which allows to perform a complex approach for the solution of problems of pollutant transport in the atmosphere.

The techniques are intended for PC applications, and the code language is Fortran-77.

With the range of theoretical and numerical models as described above, these methods can be applied to a very wide variety of problems dealing with mesoscaled pollutants transport in the atmosphere. Applications of these methods in practice require specification of meteorological quantity fields at initial time over some spatial region. The further behaviors of these fields are predicted by these techniques up until the times specified by the spatial region scale. For $L \sim 500\text{km}$ scale reliable prediction time is $T \sim 24$ hours. When sources of release are specified, the pollutants propagation and composition variation in the atmosphere should be calculated. This procedure both imposes rather stringent requirements for the completeness of experimental data, and needs careful tentative analysis of the problem as a whole, so that a package of suitable models for calculations will be developed.

2.6.2 Adaptation of methods and illustrative calculations.

Modeling local atmospheric phenomena.

The methods as described in [1-4] are intended for application to mesoscale transport problems. A part of works on the contract topics, a model of local atmospheric phenomena has been developed to describe uprising behavior of thermal non-uniformities (explosion cloud, hot release jet). While there is a substantial medium density change in the vicinity of the source, basic equations included an equation of continuity with the term $\partial \rho / \partial t$. This model was verified by solving Problem 1 for explosion cloud uprise as stated in paragraph 2.2.5. Mesh space was $h = 5\text{m}$ up to the altitude $H = 50\text{m}$, and for $H > 50\text{m}$ the vertical space was increased to 10m . Generally, there is a good agreement with the data of paragraph 2.2.5. Thus, for $t = 10\text{s}$ the cloud center is at 10m height. However, there are substantial flow velocities observed up to 400m , and this is what disagrees with EGAK calculations. Quite possibly, this disagreement arises from large space h due to 3D character of the method.

Reconstruction of atmospheric flow fields, and aerosol pollutants, transport.

For the purpose of verifying the accuracy of meteorological quantity field calculations, a sea breeze problem was considered. Numerical solution used the observation data of 2 Aug. 1958 described in [5] that were acquired through pilot balloon and aircraft sounding. Earth's surface temperature was taken from observation data, while U and V behaviors with time were established by interpolating immediate observations. The time 09 hours was taken as initial. This is the time when gradual change from land to sea breeze is observed. For times $t = 13\text{ h.}$ and $t = 17\text{ h.}$, there results a good agreement between the calculated and actual wind, and not only in strength and direction, but also in the time for peak velocity occurrence. The calculation has been also made for the decrease of land temperature (cold advection) with sea breeze.

In addition, the models described were used as a basis for numerical experiments to provide microclimate modeling of quarries having complex-type relief, and studies on the quarry airing behaviors as related to different meteorological parameters. To account for orography, the following formulae were used to go from Cartesian coordinates (x, y, z) over to generalized coordinates $(\bar{x}, \bar{y}, \sigma)$:

$$x = \bar{x}, \quad y = \bar{y}, \quad \sigma = \frac{z - \tilde{\delta}(\bar{x}, \bar{y})}{H - \tilde{\delta}(\bar{x}, \bar{y})} \hat{H}, \quad (2.6.1)$$

where H and $\hat{H}$ represent the upper boundary height in σ and z systems, respectively, $\tilde{\delta}(\bar{x}, \bar{y})$ - function accounting for relief. With a heat source existing on the bottom of the quarry, there forms a strong upflow resulting from the surface heating, while air going down the slopes is observed, and thus a circulation develops as rotating torus. For similar cases with the thermic rising where the surface is uniform, numerical experiments by Lilli [6] and laboratory experiments by Skorer [7] indicated generation of a pair of symmetric vortices having horizontal axes.

The models meant in these methods to describe the variation in aerosol particle size distribution due to condensation and coagulation, and aerosol transports in the atmosphere are included in [3, 4, 8]. Also included are the data from illustrative calculations for the area of the Lake of Baikal. Thus, for example, for a continuous source of sulfuric acid vapor having intensity $I = 10^{11} \text{ mol/cm}^3 \text{ s}$, there are liquid particles of about $1\mu\text{m}$ size formed by condensation near the source; with longer distance from the source they decreased in size due to lower vapor concentration and particles evaporation [3,4]. However, coagulation, in turn, would result in the particles growing with the distance from the source [8].

3. ANALYSIS OF SPECIFIC EXPERIMENTAL DATA TO CALIBRATE THE SOURCE TERM PARAMETERS AND OF THESE PARAMETERS ON THE CALCULATED DISPERSION AND DEPOSITION OF CONTAMINATION

3.1. Particle size distribution in a source of release.

For the purpose of predicting the ground concentration and fissile materials dispersal in the atmosphere resulting from accidents, the data on RM particle size distribution are of great importance. The particle size distribution was studied by fields experiments (in non-nuclear explosions and fires varying in combustion conditions) and laboratory investigations involving uranium and plutonium [1 - 4].

The field experiments Roller Coaster [1,2] provided the data on plutonium dispersal from non-nuclear explosions simulating NW accidents both on the ground and in underground storage facilities. The experiments Double Tracks and Clean Slate-1 were conducted on the open ground, while Clean Slate-2 and Clean Slate-3 experiments were performed in soil covered bunkers. Distribution of explosion cloud particles ranging within 12 μm size was studied using cascade impactors, thus providing the distribution obtained in terms of equivalent aerodynamic diameter of aerosols having unit density. Distribution of particles actually larger than 2 μm was studied by autoradiography, microscopy and radiochemical analysis. While there was some unknown fraction of larger particles that could be analysed by the techniques mentioned, the complete aerosol distribution in size was obtained through normalization to radiochemical analysis data for particles measured using cascade impactors. The average density of larger particles required for normalization, was determined indirectly, assuming that the volume measured partly contains an oxide, its density known, and the rest of it is a material of 2.6 g/cm³ density. The normalization procedure also included regression analysis used to obtain the relationship between the particle size and the activity of plutonium fraction contributing to these particles. The mass distribution of particles having larger than 2 μm diameter as a function of equivalent unit-density diameter was near-lognormal. Further, with specific renormalization procedure based on impactor measurements, complete mass distribution of particles in equivalent diameter was obtained, which is shown by table 3.1.1 [1]. The aerosol particles distribution in the cloud was measured at 750 m distance from the explosion point, i.e. where the largest particles have fallen out and agglomeration (coagulation) effects no longer existed.

Table 3.1.1 Cumulative plutonium mass (F, %) versus unit-density particles equivalent diameter (μm).

F(%)	1	5	20	50	70	95	99,8
Double Tracks	0,5	3	13,0	44,2	70	200	
Clean Slate-1	0,5	2	10	40	65	134	300

The resulting particle distributions are substantially different from lognormal. They may be approximately represented as made up of two or three portions having lognormal form within limited diameter range. Table 3.1.2 gives the parameters of these distributions for the experiments Double Tracks and Clean Slate-2 [2].

Table 3.1.2 Subscale particle distributions in the experiments.

Parameter	Double Tracks			Clean Slate-2	
	0.1-4	4-60	60-1000	0.1-42	42-1000
Diameter range (μm)					
Average geometric diameter (μm)	9000	38	48	39	41
Geometric square deviation	90	3.8	1.8	7.8	2.3

The respirable fraction, i.e. particles having aerodynamic diameter smaller than 10 μm , accounts for 16 to 26 % in Roller Coaster experiments.

As shown by the field experiments, for rather high-yield non-nuclear explosions, where the HE equivalent mass (M_{HE}) much exceeds that of the inert material (M_{IN}), the explosion energy variation by an order of magnitude or more has small effects on the mass distribution of particles in size. Here, almost all plutonium mass goes to aerosols. For accidents involving low HE energies, Steindler and Seefeldt [3] have suggested a model to calculate the resulting aerosol mass and mass median diameter. The particle average geometric diameter as a function of explosion energy shows a power-law form, with this diameter significantly decreasing with the explosion energy growth for $Q = M_{\text{HE}}/M_{\text{IN}} > Q_{\text{cr}} = 0.2$. According to this model, for an accident where $Q = Q_{\text{cr}}$ there is complete dispersal of materials subjected to explosive loading. We believe, $Q_{\text{cr}} = 0.2$ should be better considered as critical value to predict the assured safety level of accidents involving aerosol releases. The fractional dispersed material (D) as a function of Q ratio, as taken by the model [3] can be expressed for the range $Q < Q_{\text{cr}}$ as

$$D = 2.783 \cdot Q^{0.683} \quad (3.1.1)$$

The extent Pu and U disperse in combustion of metal samples by artificially maintained flame, was investigated by a set of field experiments [4]. The combustion chamber temperature was 800 - 1000 $^{\circ}\text{C}$, temperature growth rate 10 - 86 $^{\circ}\text{C}/\text{min}$, and each experiment lasted for about 30 min. For two experiments for Pu samples of 200 g mass, the dispersed material fraction accounted for 1% and 3%, respectively. In the experiments on U samples of 2 kg mass (the chamber temperature was 1050 $^{\circ}\text{C}$) the dispersed fraction accounted for 1% and 5%. The authors [4] consider ~1% for Pu and ~6% for U as more correct estimate for RM release in fire.

Tables 3.1.3 and 3.1.4 summarise particle distributions of the remaining PuO_2 and UO_2 collected from the bottom of the oil burner in two experiments [4].

Table 3.1.3 Particle distribution of the residual PuO_2

Diameter, μm	20	100	150	600	1000	2000	3000
Mass fraction, %	1	5	10	50	73	95	99

Table 3.1.4 Particle distribution of the residual UO_2

Diameter, μm	50	75	200	400	750	2100	3000
Mass fraction, %	2	10	32	50	70	95	98

The dispersed uranium distributions as measured in a jet at distances 100 to 10000 m were near lognormal, having the respirable fraction accounting for 70 - 80% (the

attempt to obtain dispersed fraction value for Pu was not successful). Naturally, for farther distances from the fire location the median particle diameter in the samples is decreasing (at distances $R = 200$ m the aerosols have average geometric diameter $d = 4 \mu\text{m}$, for $R = 2000$ m $d = 1 \mu\text{m}$).

How large is the respirable fraction in combustion of RM depends on the combustion physics. Table 3.1.5 gives overall material fractions released as respirable aerosols for various experimental conditions (reported by [5,6]). The following Pu and U oxidation and combustion behaviours were studied in [5,6]: 1 - static oxidation and combustion with no dense sample motion observed; 2 - static combustion of melting dense samples; 3 - combustion of liquid drops falling from 0.75 m height, and 4 - combustion of metal drops falling from large height sufficient for their complete destruction.

Table 3.1.5. RM average geometric mass fraction versus combustion conditions.

Experimental conditions	Fraction	
	Pu	U
1	$7 \cdot 10^{-6}$	$1.1 \cdot 10^{-4}$
2	$7 \cdot 10^{-6}$	-
3	$3.5 \cdot 10^{-3}$	$1.9 \cdot 10^{-3}$
4	0.1-0.4	0.2-0.6

Table 3.1.6 shows distributions of aerosol particles obtained using cascade impactors for Pu static and dynamic combustion [5].

Table 3.1.6. Particle distributions of PuO_2 measured using cascade impactors for various experimental conditions.

Experimental conditions							
1	Diameter	0.4	1	2.3	10	23	35
	Fraction	5	10	20	50	80	95
3	Diameter	0.35	0.45	0.7	1.3	5.5	
	Fraction	20	50	80	95	99	
4	Diameter	0.4	0.53	0.9	2.2	9	
	Fraction	20	50	80	95	99	

Note, that for dynamic combustions the aerosol particle distributions are close, the major particle fraction being within submicrons.

Ref.[6] summarises the data from field experiments (PAGE program) for explosive fracturing of cylindrical uranium samples of about 1 kg mass. The experiments did not measure uranium aerosols but did measure particles distribution in the cloud. This was near lognormal distribution having average geometric diameter within $0.5 - 2 \mu\text{m}$ and wide diameter distribution (geometric standard deviation is about 5). As part of PAGE program, the experiments were also conducted to study particle size distribution of aerosols produced by plutonium drops combustion [7]. In this case high-dispersioned aerosols formed as constituted by ultra fine size components (having geometric diameter less than $0.1 \mu\text{m}$). The aerosol spectrum is characterised by active median aerodynamic diameter $1 - 2 \mu\text{m}$ with geometric standard deviation about 1.5.

Some laboratory experiments were made to study the contributions of gaseous medium composition and sample shapes to aerosol formation at high temperature [8]. Table 3.1.7 shows experimental data on the contribution of gaseous medium composition to fractional Pu transforming to gas-suspended aerosols.

Table 3.1.7. Medium composition contribution to aerosol fraction.

Gas composition (volume fractions)	Aerosol fractions
3% H ₂ + Ar	5.2 10 ⁻⁴
Air plus residual 3% H ₂ + Ar	4.4 10 ⁻⁴
3% H ₂ + Ar + 5% N	6.6 10 ⁻⁵
Average for 14 experiments	2.1 10 ⁻⁴
Worst case	4.6 10 ⁻³

The fraction of aerosols produced by heating samples of 1 g mass (such as pellet or foil) proves significantly larger than for experiments for 10 g samples (the aerosol fraction for the latter accounts for $1.5 \cdot 10^{-5}$). The effects of the sample shape in this case are insignificant. The aerosols have aerodynamic diameters within 4 - 10 μm . The particle sizes of the powder remainder range widely from 4 to 400 μm , with the medium diameter being 50 - 350 μm with large statistic spread [8].

3.2. Data on explosion cloud uprise dynamics.

Comprehensive experimental data on the cloud uprise dynamics from explosion resulting from detonation of high explosives, are summarised in [1]. There were 23 experiments involving effective HE mass (see paragraph 2.1) ranging from 53.5 to 1270 kg performed on the ground mostly at nights (within 2.5 hours after the sunrise).

Cloud top height was measured with artificial backlight during 5 minutes both photographically and using theodolites. H.W.Church who analysed the experimental data concluded that the height measurements had accuracy from 15 to 20 %.

Virtually all experiments included measurements of the surrounding air temperature and wind velocity profiles in altitude. It should be noted that the data are represented as graphs, moreover referring to times different from test times, thus of course making weather data less accurate given the necessity to interpolate the graphic information.

Table 3.2.1 gives the data we used in the cloud dynamics calculations.

Table 3.2.1. Weather data for the experiments (H - m, T - °C, V - m/s)

Test No.1 $M_{HE} = 63.5 \text{ kg}$			Test No.3 $M_{HE} = 63.5 \text{ kg}$		
H	T	V	H	T	V
0	17.85	7	0	17.25	7.5
50	17.1	11	50	16.6	10.5
100	16.4	9	100	16.1	10.5
200	15.15	9.5	200	14.9	11.5
300	13.8	10.5	300	13.8	10.5
400	12.4	11.5	400	12.7	12.5
500	11.3	10.5	500	11.8	10.5
600	10.5	11	600	10.95	11
Test No.2 $M_{HE} = 63.5 \text{ kg}$			Test No.4 $M_{HE} = 725.8 \text{ kg}$		
H	T	V	H	T	V
0	17.5	7	0	11.45	3
50	16.85	12	50	13.85	4
100	16.2	10	100	-	4

200	15	9.5	200	-	4.7
300	13.8	10	300	-	5
400	12.6	10	400	-	6
500	11.55	10	500	10.77	6
600	10.75	10			
Test No.5 $M_{HE} = 63.5 \text{ kg}$			Test No.9 $M_{HE} = 63.5 \text{ kg}$		
H	T	V	H	T	V
0	11.3	3	0	10.2	2
50	13.3	4	50	10.7	2.5
100	13.7	4	100	11.3	-
150	13.5	3	120	11.3	2.5
200	12.9	3	150	11.6	3
300	12.1	4	250	11.6	-
400	11.2	5	300	11.3	3
500	10.4	5	Test No.10 $M_{HE} = 190.5 \text{ kg}$		
Test No.6 $M_{HE} = 254 \text{ kg}$			H	T	V
H	T	V	0	10.3	1
0	11.2	1.8	50	10.5	1
50	13.1	-	100	10.8	1.5
100	13.5	-	150	-	3
150	13.35	-	250	10.6	-
200	12.9	-	300	10.3	3
250	12.5	-	400	9.7	2
300	12.1	1.8	Test No.11 $M_{HE} = 63.5 \text{ kg}$		
400	11.2	3.5	H	T	V
500	10.4	4.5	0	10.4	4.2
Test No.7 $M_{HE} = 63.5 \text{ kg}$			100	10.4	-
H	T	V	200	10	4.2
0	11.1	2.5	250	9.8	7
50	12.8	1	300	9.5	-
100	13.3	-	400	8.8	-
150	13.3	-	500	8.1	7
200	12.9	1	Test No.12 $M_{HE} = 63.5 \text{ kg}$		
250	12.6	2	H	T	V
300	12.15	-	0	10.6	5
400	11.3	2	50	9.8	6
Test No.8 $M_{HE} = 725.8 \text{ kg}$			100	9.6	7
H	T	V	120	9.2	-
0	10	1	150	8.9	-
50	10.9	2	200	8.5	7.5
100	11.9	2.2	250	8	-
120	12.3	-	300	7.8	8.5
150	12.45	2.2	400	7	8.5
200	12.65	1	500	6.25	8

250	12.7	0.5	600	5.7	7.5
300	12.4	1	Test No.17 M _{HE} =1017kg	Clean Slate-3	
400	11.9	1	H	T	V
500	11.2	2.5	0	6.7	2
600	10.3	2.5	100	9	4.2
Test No.13 M _{HE} =254 kg			140	10	5
H	T	V	200	10.5	6
0	10.7	2.7	300	10.8	2
50	9.5	5.5	370	11	-
100	9.0	6.5	400	10.5	-
120	8.4	-	500	9.3	-
150	8.0	-	600	8.7	2
200	7.5	7.2	Test No.18 M _{HE} =63.5 kg	P3	
250	6.8	-	H	T	V
300	6.6	8.0	0	-12	-
400	5.7	8.0	30	-7.5	-
500	5.1	7.5	60	-7	-
600	4.5	7.0	94	-7.7	-
Test No.14 M _{HE} =53.5 kg			300	-7	-
Double Tracks					
H	T	V	Test No.19 M _{HE} =63.5 kg	P4	
0	7	5.2	H	T	V
100	7.2	7	0	-9	-
200	7.5	7.8	60	-7	-
300	7.5	8.5	300	-7.1	-
Test No.15 M _{HE} =481.7 kg			Test No.20 M _{HE} =63.5 kg	P5	
Clean Slate-1			H	T	V
H	T	V	0	-6	-
0	5.6	1	30	-6.5	-
50	-	5.2	60	-6	-
120	6.8	6	87	-7	-
200	-	7.2	300	-7.7	-
300	-	8			
400	-	8.2	Test No.21 M _{HE} =63.5 kg	P6	
500	-	7	H	T	V
600	5.4	-	0	-4	-
700	-	7	30	-4	-
Test No.16 M _{HE} =1017 kg			87	-5.5	-
Clean Slate-2					
H	T	V	133	-5.5	-
0	13.3	1.5	300	-7.6	-
40	14.7	-	Test No.22 M _{HE} =635 kg	P7	
50	-	3.2	H	T	V
125	-	4.2	0	-1	1
175	-	7.2	30	4	-

225	-	5	60	5.2	-
275	-	3	120	6	-
325	-	2	150	6	-
600	14.0	2	180	5.4	-
Test No.23 $M_{HE} = 1270 \text{ kg}$			P8	300	4.6
H	T	V	565	4.3	5
0	-3.2	1			
35	-1	-			
95	-3	-			
190	-3	-			
240	-2	-			
300	-1.5	-			
536	-0.15	5			
240	-2	-			
300	-1.5	-			
536	-0.15	5			

Table 3.2.2 shows calculated data for cloud dynamics with the initial data as given in paragraph 2.1 ("Cloud" technique) and the input weather information taken from table 3.2.1.

Table 3.2.2. Cloud top height (m) versus time (s).

Time	No.1		No.2		No.3	
	Calculated	Test	Calculated	Test	Calculated	Test
30	117	126-127	117	87-111	117	111-123
60	173	225-263	173	143-152	173	193-204
120	260	397	259	208-232	259	333-345
180	333	557	327	270	325	343
240	404	678	390	266	385	488
300	486	-	460	-	444	592
t_1	735	(261)	697	(261)	623	(261)
t_2	-	-	-	-	-	-

Time	No.4		No.5		No.6		No.7	
	Calculated	Test	Calculated	Test	Calculated	Test	Calculated	Test
30	217	293	117	120	160	147	115	-
60	307	385	166	175	235	225	166	197
120	443	498	238	257	342	377	232	271
180	538	584	292	320	422	458	273	327
240	602	-	334	-	480	-	300	-
300	624	598	368	419	525	667	317	369
t_1	602	(481)	371	(261)	534	(370)	318	(261)
t_2	656	-	427	-	591	-	324	-

Time	No.8		No.9		No.10		No.11	
	Calculated	Test	Calculated	Test	Calculated	Test	Calculated	Test
30	212	212	115	122	149	152	115	135

60	296	316	165	189	217	219	167	179
120	415	450	220	193	302	286	232	283
180	487	562	236	189	350	319	278	374
240	530	-	-	-	370	-	296	-
300	547	580	-	205	377	324	298	-
t ₁	450	(481)	200	(261)	328	(344)	260	(261)
t ₂	547	-	236	-	283	-	298	-

Time	No.12		No.13		No.14		No.15	
	Calculated	Test	Calculated	Test	Calculated	Test	Calculated	Test
30	117	155	163	186	107	118	185	249
60	173	237	243	291	160	164	267	378
120	254	392	361	382	215	210	382	558
180	313	476	438	461	232	216	444	643
240	355	524	508	557	-	-	464	-
300	374	583	555	615	-	-	-	-
t ₁	338	(261)	519	(370)	200	(250)	420	(434)
t ₂	380	-	574	-	232	-	464	-

Time	No.16		No.17		No.18		No.19	
	Calculated	Test	Calculated	Test	Calculated	Test	Calculated	Test
30	220	242	218	262	112	47	113	84
60	327	298	318	377	166	84	167	142
120	453	415	423	494	229	76	229	186
180	518	440	457	520	-	-	254	-
240	-	426	-	510	-	-	-	-
300	-	412	-	-	-	-	-	-
t ₁	470	(523)	400	(523)	215	(261)	226	(261)
t ₂	526	-	460	-	243	-	256	-

Time	No.20		No.21		No.22		No.23	
	Calculated	Test	Calculated	Test	Calculated	Test	Calculated	Test
30	113	88	115	105	200	251	230	358
60	173	142	174	168	293	389	340	432
120	245	207	255	280	423	565	440	536
180	285	271	325	-	493	668	-	645
240	297	-	393	-	507	759	-	695
300	-	-	463	-	-	832	-	740
t ₁	262	(261)	-	(261)	490	(465)	417	(553)
t ₂	297	-	-	-	507	-	458	-

Here, t_1 is the time when material density in the cloud becomes equal to that of the surrounding air; t_2 - time when the cloud has its velocity changed in direction.

Note, that tests Nos. 1 through 3 used two techniques to measure the cloud top height. Others involved measurements either using photography techniques or theodolites (two or three pairs). Tests Nos. 18 through 23 did not measure wind velocity, and tests Nos. 22 and 23 had no temperature measurements at altitudes above 300 m. Brackets are used in the table to indicate the stabilization altitude, which as the author [1] suggests, should be assumed based on the analysis of the experimental data of table 3.2.2:

$$H, m = 92.5(M_{HE})^{0.25},$$

(see paragraph 2.1). According to H.W.Church, the cloud would become no longer buoyant two minutes after the explosion, though it is not obvious; clearly, the cloud should stabilise in stable atmosphere later than in unstable one. This fact has been supported by calculations.

Ref. [2] describes experimental studies of the earlier vortex ring development phase. The source term was generated by detonating methan-air mixture in a tank of 10 m diameter. Test No.3 had energy output 3 GJ and No.4 - 2.72 GJ.

Table 3.2.3 gives dimensions of the vortex ring generated: $t_{34,s}$ - array of times, identical for tests Nos.3 and 4; $R_{34,m}$ - maximum cloud horizontal radius in both tests; $h_{3,m}$ - cloud uprise in test No.3, and $h_{4,m}$ - uprise height in test No.4.

Table 3.2.3. Cloud dimensions versus altitude.

t_{34}	0.1	1.1	2.1	3.1	4.1	5.1	6.1	7.1	8.1	9.1	10.1
R_{34}	13.5	13	15.8	17	18	19.5	22	22.5	23.8	24.5	26
h_3	0	2.79	16.3	24.4	34.9	43.7	51.2	61.6	69.8	79.1	84.9
h_4	0	2.79	16.3	24.4	34.9	41.9	48.8	58.1	65.1	69.8	75.6

As results from the calculations, the cloud top rises up to about 81 m height in 10 s.

Generally, there is a rather good agreement between the calculated and experimental data [1,2]. One can make use of the cloud dynamics calculations to characterise the source in Roller Coaster test.

3.3 Data of release jet formation.

1) Ref. [1] uses the horizontal wire heated at a constant rate as a source of buoyancy in air. This problem may be considered plane given the relation $L \gg H$, where L is the thread length, and H - maximum distance from the thread as referred in the problem.

The number Re ($Re = U_{max}D/V$, with D - characteristic velocity profile width, V - kinematic molecular viscosity factor) goes as high as 100, the flow behavior being laminar; this has been confirmed by comparison with the relevant theoretical solution.

Ref. [2] analyses experimental data for turbulent gravitational convection from point and line sources of buoyancy. In this case, Re number is significantly higher than Re_c . What is suggested is that average velocity and buoyancy values be described semi-empirically.

Unlike [2], ref. [3] also includes measurements of fluctuation values for axisymmetric problem with $Re = 87$ and Froude number $F = 1.4$. Moreover, average profile measurements of the vertical velocity component w in [3] have the results noticeably different from those given in [2].

Ref. [4] addresses buoyant turbulent jet problems. It concludes that there exist flow conditions, i.e. one for a jet developing at a short distance from the source, where Richardson number $R \ll 1$, and the other related to the constant number $R = 0.63$.

The turbulence structure in a buoyant plane turbulent jet is considered in ref. [5].

Refs. [6,7] address basic mechanisms of buoyant plumes propagating in a steadily stratified atmosphere. The observations are shown to be consistent with the predictions of theory referring mostly to the highest buoyancy altitude.

2) The experimental data of ref. [3] are given by table 3.3.1 through 3.3.5. These tables include the following quantities related to $\eta \cong r/z$ for these different altitudes (the bar indicates averaging, and " ' " designates fluctuation component):

- average buoyancy profile: $F1 = \frac{\bar{g}\Delta\rho}{\rho_\infty} \cdot \left(\frac{z^5}{F_0} \right)^{1/5}$, where $F_0 \cong 10^6 \text{ cm}^4/\text{s}^3$ is the buoyancy source parameter;

- average vertical velocity profile $\bar{W}$: $F2 = \bar{W} \cdot \left(\frac{z}{F_0} \right)^{1/5}$;

- relative rms temperature fluctuations profile: $F3 = \frac{(\overline{T'^2})^{1/2}}{\Delta T}$;

- rms velocity fluctuations: $F4 = \frac{(\overline{w'^2})^{1/2}}{\bar{W}}$;

- correlation function for temperature and velocity fluctuations: $F5 = \overline{T'w'} \cdot [\overline{T'^2} \cdot \overline{w'^2}]^{-1/2}$.

Table 3.3.1. Average buoyancy profile F_1

z/D					
16	η	0.000e+00	2.406e-02	2.406e-02	7.252e-02
16	F1	8.780e+00	8.699e+00	8.910e+00	6.585e+00
12	η	0.000e+00	4.945e-02	9.890e-02	1.005e-01
12	F1	8.536e+00	7.967e+00	4.878e+00	4.227e+00
8	η	2.538e-02	7.450e-02	7.450e-02	9.890e-02
8	F1	7.609e+00	6.097e+00	6.292e+00	4.308e+00
16	η	7.483e-02	1.252e-01	1.269e-01	1.500e-01
16	F1	6.422e+00	4.146e+00	3.333e+00	2.113e+00
12	η	1.500e-01	1.523e-01		
12	F1	1.951e+00	2.032e+00		
8	η	1.252e-01	1.252e-01	1.747e-01	
8	F1	3.333e+00	3.983e+00	1.544e+00	

Table 3.3.2. Average vertical velocity profile F_2

z/D					
16	η	0.000e+0	2.413e-2	2.478e-2	7.336e-2
16	F2	3.252e+0	3.284e+0	3.219e+0	2.556e+0
12	η	0.000e+0	4.891e-2	9.847e-2	1.010e-1
12	F2	3.577e+0	3.024e+0	2.048e+0	2.016e+0
8	η	2.510e-2	7.500e-2	7.500e-2	9.945e-2
8	F2	3.349e+0	2.666e+0	2.764e+0	2.081e+0
16	η	7.663e-2	1.239e-1	1.239e-1	1.467e-1
16	F2	2.634e+0	1.691e+0	2.634e+0	1.255e+0
12	η	1.483e-1	1.483e-1		
12	F2	1.203e+0	1.333e+0		
8	η	9.978e-2	1.239e-1	1.239e-1	1.728e-1
8	F2	1.821e+0	1.821e+0	1.951e+0	1.040e+0

Table 3.3.3. Root-mean-square temperature fluctuation profile F_3

z/D					
16	η	0.000e+0	2.445e-2	2.445e-2	7.500e-2
16	F3	3.934e-1	3.770e-1	3.901e-1	3.606e-1
12	η	0.000e+0	4.891e-2	9.782e-2	9.880e-2
12	F3	3.436e-1	3.508e-1	3.016e-1	2.636e-1
8	η	2.445e-2	7.500e-2	7.500e-2	9.945e-2
8	F3	2.786e-1	2.963e-1	3.081e-1	2.754e-1
16	η	7.500e-2	1.239e-1	1.239e-1	1.500e-001
16	F3	3.770e-1	3.081e-1	3.167e-1	2.150e-001
12	η	1.490e-1	1.490e-1		
12	F3	1.868e-1	1.934e-1		
8	η	1.239e-1	1.239e-1	1.744e-1	
8	F3	2.459e-1	2.622e-1	1.481e-1	

Table 3.3.4. Root-mean-square velocity fluctuation profile F_4

z/D					
16	η	0.000e+0	2.608e-2	2.771e-2	7.500e-2
16	F4	2.640e-1	2.556e-1	2.569e-1	2.666e-1
12	η	0.000e+0	4.891e-2	9.945e-2	1.010e-1
12	F4	2.373e-1	2.504e-1	2.276e-1	2.406e-1
8	η	2.543e-2	7.500e-2	7.532e-2	1.004e-1
8	F4	2.874e-1	2.744e-1	2.796e-1	2.406e-1
16	η	7.695e-2	1.239e-1	1.239e-1	1.500e-1
16	F4	2.634e-1	2.341e-1	2.484e-1	1.853e-1
12	η	1.486e-1			
12	F4	1.723e-1			
8	η	1.239e-1	1.239e-1	1.744e-1	
8	F4	2.211e-1	2.276e-1	1.430e-1	

Table 3.3.5. Correlation function for temperature and velocity fluctuations F_5

z/D						
16	η	0.000e+0	2.678e-2	7.738e-2	1.250e-1	1.250e-1
16	F5	6.666e-1	6.666e-1	6.857e-1	6.666e-1	7.142e-1
12	η	0.000e+0	5.238e-2	5.238e-2	8.630e-2	1.011e-1
12	F5	6.380e-1	6.476e-1	6.952e-1	7.047e-1	6.704e-1
8	η	2.678e-2	2.678e-2	7.738e-2	1.011e-1	1.261e-1
8	F5	6.285e-1	6.476e-1	6.761e-1	7.238e-1	7.085e-1
16	η	1.517e-1				
16	F5	6.857e-1				
12	η	1.011e-1	1.517e-1	1.517e-1	1.994e-1	1.994e-1
12	F5	6.952e-1	6.476e-1	6.952e-1	2.666e-1	6.666e-1
8	η	1.755e-1	2.261e-1			
8	F5	6.380e-1	6.000e-1			

3) The data of ref. [3] given by tables 3.3.1 - 3.3.5 will be used for calibration.

3.4 Data on ground and ground air pollutions resulting from accidental and industrial releases.

Experimental data on ground contaminations by plutonium from dummy nuclear weapon explosion obtained in Roller Coaster operation are given in [1]. Roller Coaster operation was performed since 15 May through June 1963. Two explosions of this series - Double Tracks (DT) and Clean Slate 1 (CS-1) were performed on an open ground, DT - on a steel plate and CS-1 - on a concrete pad. HE masses used were 53.5 kg in DT and 481.7 kg in CS-1. Plutonium was used as tracer material to consider how much dispersed radioactive materials fall out on the ground.

The experiments were conducted early in the morning to have wind direction, air turbulence and wind velocity all well predictable. The experimental measurements included: 1 - weather conditions, 2 - surface-air aerosol concentrations, 3 - plutonium fall-out density on the underlying surface, 4 - particle size distribution at different altitudes, 5 - the explosion cloud shape and activity distribution.

Specifically, it follows from Roller Coaster test results, that

- 1 - larger portion of plutonium mass resulting from the dummy nuclear weapon explosion is aerosols,
- 2 - the particle size distribution indicates that respirable fraction (i.e. the fractional activity associated with particles of less than 10 μm aerodynamic diameter) accounts for 20% for plutonium, and
- 3 - respirable fraction has median aerodynamic diameter $\sim 5 \mu\text{m}$ with standard geometric deviation about 2.5.

Experimental data are given below for plutonium fall-out and surface-air concentration for the two Roller Coaster tests mentioned above, together with the weather conditions at test times. Data on particle size distribution in the source of release are included in paragraph 3.1 above.

A. Double Track test.

The explosion cloud uprise was observed in the test by filming and reached 220 m altitude [2].

The weather conditions during the test are included in table 3.4.1. [2].

Table 3.4.1. Weather conditions for Double Track test.

Altitude (m)	Wind direction	Wind velocity (m/s)
2	350	5.2
20	370	5.6
50	350	6.4
100	345	7.0
200	340	7.8

Fig. 3.4.1 gives surface air concentrations of aerosols in the trace axis for various distances. Plutonium fall-out densities in the trace axis are shown for various distances in fig. 3.4.2.

Fig. 3.4.1 Peak airborne dosage - Double Tracks.

Fig. 3.4.2 Peak deposited dosage - Double Tracks.

B. Clean Slate 1 test

The explosion cloud climb altitude was 710 meters [2].
The weather conditions of the test are given in table 3.4.2 [2].

Table 3.4.2. Weather conditions for Clean Slate 1 test.

Altitude (m)	Wind direction	Wind velocity (m/s)
2	55	1.2
25	350	2.8
50	315	5.2
100	325	5.5
200	325	7.2
300	325	8.0
400	325	8.2
500	325	7.0
600	325	7.0
700	325	7.0

Fig. 3.4.3 gives surface air concentrations of aerosols in the trace axis for various distances.

Fig. 3.4.3 Peak airborne dosage - Clean Slate 1.

Plutonium fall-out densities in the trace axis are shown for various distances in fig. 3.4.4.

Fig. 3.4.4 Peak deposited dosage - Clean Slate 1.

As part of this project, the cited initial and experimental data are to be used to demonstrate the capabilities of the engineering technique and "Prognosis" technique to calculate the aerosol fall-out and surface-air concentrations.

In 1959, the experiments were conducted under Vixen A program in Australia to study the combustions of plutonium, uranium and beryllium in the controlled flame of an oil burner at temperatures up to 1100°C [3]. The experiments had the smoke jets stabilizing at the height about 60m and about 150m distance from the source.

Tables 3.4.3 and 3.4.4 summarize the processed Vixen A data on surface contaminations in the trace axis for plutonium and uranium experiments (tables 3.4.3 and 3.4.4 respectively).

Table 3.4.3 Ground contamination by plutonium in the trace axis.

Distance, m	9.1	35	92	210	521	649	914	3200
Contamination $\mu\text{G}/\text{m}^2$	847	139	18	1.4	1	0.14	0.02	0.0014

Average wind velocity in the surface-air layer is ~ 11 km/hour.

Table 3.4.4 Ground contamination by uranium in the trace axis.

Distance, m.	9.1	18.3	46	91	138	220	366	550
Contamination $\mu\text{G}/\text{m}^2$	8000	4000	1000	250	35	80	116	120

Distance, m.	732	914	1100	1280	1370	1830	2000
Contamination $\mu\text{G}/\text{m}^2$	116	100	70	30	9	2	1

Average wind velocity in surface air is ~ 14 km/hour.

There are rather well detailed experimental data on the atmosphere and surface air pollutions by industrial releases described in ref. [4], that includes the monitoring data for area around Navajo thermal power station which is a coal-burning facility. This power station is located at the bottom of a canyon near Page, Arizona. Within about 10 km distance south-east of the station and about 20 km in other directions there is a flat underlying surface.

The power station includes three power units with the rate $W = 750$ MW each. It has a smoke stack of 240 m height, 6.2 m diameter, with gas effluence at 30 m/s, and gas temperature $\sim 160^\circ\text{C}$. Measurements were conducted during the period from 1 Oct 1974 to 17 Feb 1975. The surface-air concentrations of SO_2 were measured by 26 measurement stations located in the area surrounding the site. Additionally, SO_2 concentration was measured for a smoke plume during the airplane flight. In most cases, the smoke uprising height was 400 or 500 meters.

Totally, there were 204 non-zero measurements over 80 days. For each measurement, ref. [4] indicates the rate of a source of release Q , the highest SO_2 surface-air concentrations at measuring locations, the day's maximum SO_2 concentrations averaged over three-hours' observations, wind velocity at 612 m altitude and the quantity $\bar{\chi}/Q$, where $\chi = Q/\pi u \sigma_y \sigma_z$ is the short-term meteorological dilution factor, Q - rate of the source of release, averaged over three-hours' observation.

For the purposes of this project, more important are three series of measurements showing high concentrations for stations 105, 106, 107 and 119 located near Vermilion Cliffs (~20 km west of the power station, at the canyon end) and the three series for station 110 located near Leche-e-Rock (~8 km south-east of the facility, up on a hill). High-concentration measurements were done for Vermilion Cliffs on 16 Oct 1974, 24 Nov 1974 and 2 Dec 1974, and for Leche-e-Rock - on 10 Dec 1974, 5 Jan 1974 and 25 Jan 1975. For this series of measurements, ref. [4] describes detailed data on wind direction and velocity at 612 m altitude, temperature profile in altitude and smoke plume characteristics, and surface-air SO_2 concentration, and also the plume concentrations obtained by airborne measurements. On the above-mentioned dates, there was either isothermal layer or temperature inversion existing in the atmosphere, thereby impeding SO_2 dilution there. Thus, according to airborne measurements on 16 Oct 1974, SO_2 concentration in the smoke plume was $917 \mu\text{g}/\text{m}^3$ at 10 km from the power station, $996 \mu\text{g}/\text{m}^3$ and $891 \mu\text{g}/\text{m}^3$ at 20 km distance (in the station 105 area). Then, the rate of the source of SO_2 release was about 2000 kg/hour.

Under the task order, the data from the above measurements will be used to calibrate the calculations of the source of jet release forming above flat surface, and also to proof-test the IMN RAS VNIIEF techniques as applied to the calculations of pollutants build-up in stagnant areas (measuring stations of Vermilion Cliffs were located at the canyon end).

Appendix B to ref. [5] describes numerical simulation data for releases of tracer gas SF_6 in two experiments (by day and by night) at Tooele location 60 km south-west of Salt-Lake City, Utah. There is a section in ref. [5] which includes the description of this experiment. For each experiment, the tracer was released into the atmosphere near the ground at the rate 50 g/s during 1 hour.

For night experiments (3 Aug 1987), comparatively high concentrations 700-9000 ppt were measured during 7 hours. In daytime (7 Aug 1987) SF_6 concentration was measured at 80-350 ppt during 3 hours.

The experimental data and numerical simulation results described in [5] offer valuable information for testing the calculation techniques for atmospheric flows over complex-terrains and pollutants transport.

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