STUDIES IN MATHEMATICS AND ITS APPLICATIONS

16

MATHEMATICAL MODELS IN ENVIRONMENTAL PROBLEMS

G.I. Marchuk

NORTH-HOLLAND

Mathematical Models
in Environmental Problems

STUDIES IN MATHEMATICS AND ITS APPLICATIONS

VOLUME 16

NORTH-HOLLAND – AMSTERDAM • NEW YORK • OXFORD • TOKYO

MATHEMATICAL MODELS IN ENVIRONMENTAL PROBLEMS

G. I. MARCHUK
Academician
Head of the
Computer Mathematics Department
of the U.S.S.R. Academy of Science
Moscow, U.S.S.R.

1986

NORTH-HOLLAND – AMSTERDAM • NEW YORK • OXFORD • TOKYO

ISBN: 0 444 87965 x

Translation of:

Matematicheskoye Modelirovanye
v Problyem'e Okrazhayouschchey Sredy
© Nauka, Moscow, 1982

Publishers:

ELSEVIER SCIENCE PUBLISHERS B.V.
P.O. BOX 1991
1000 BZ AMSTERDAM
THE NETHERLANDS

Sole distributors for the U.S.A. and Canada:

ELSEVIER SCIENCE PUBLISHING COMPANY, INC.
52 VANDERBILT AVENUE
NEW YORK, N.Y. 10017
U.S.A.

Library of Congress Cataloging-in-Publication Data

Marchuk, G. I. (Guriĭ Ivanovich), 1925-
Mathematical models in environmental problems.
(Studies in mathematics and its applications ; v. 16)
Translation of: Matematicheskoe modelirovanie v probleme okruzhaiushcheĭ sredy.
Bibliography: p.
1. Environmental protection--Mathematical models.
I. Title. II. Series.
TD170.2.M3713 1986 363.7'00724 85-31160
ISBN 0-444-87965-X

PRINTED IN THE NETHERLANDS

LIST OF CONTENTS

PREFACE

In the past few years, environmental protection has become a challenging scientific task whose importance is highlighted by ever-increasing pace of technological progress throughout the world. The swift industrial development resulting in increased level of industrial pollution of the environment has already begun disturbing the ecological equilibrium in many regions of the globe. Meanwhile industry continues to develop at unprecedented rates, giving a powerful impetus to research associated with the location of new industrial plants and complexes exerting minimum impacts on the environment. The problem of environmental contamination by industrial plants whose maximum permissible level of safe pollution is still inconsistent with current requirements has become even more pressing. All this refers equally to the processes occurring on land and in the ocean.

Environmental protection problems have been taken up in a series of investigations carried out in the Soviet Union, specifically at the Chief Geophysical Observatory of the State Hydrometeorological Committee, as well as abroad. Selective information on such investigations can be gained from the references at the end of this book. In the present monograph, special attention is paid to mathematical modelling of optimization problems associated with environmental protection. These problems were first posed by the author in 1970 at the International Environmental Protection Symposium, which was held in Czechoslovakia (Rudohoři). The author's talk at this Symposium served a starting point for his further research in the field, which was reported subsequently at international symposia in Italy (Rome, 1973), France (Nice, 1975), and FRG (Würzburg, 1977). These findings provided the basis for the monograph. A substantial amount of research along these lines has been accomplished by staff of the Computer Center of the Siberian Division of the USSR Academy of Sciences. An active role in these efforts belongs to V.V.Penenko, N.N.Obraztsov, V.I.Kuzin, A.E.Aloyan, E.A.Tsvetova, and some other scientists. Much work has been done by the research probationer A.Yu.Sokolov, who computed examples illustrating the opportunities provided by the methods. Besides, the monograph draws on the calculations conducted by A.E.Aloyan, A.A.Kordzadze, V.I.Kuzin, N.N.Obraztsov, and V.A.Sukhorukov, to whom the author expresses his deep gratitude.

In the present book, the author restricts himself to the study of direct environmental impact, leaving aside the problem of climatic fluctuations caused by man-made factors, which seems to be of interest in its own right. This latter issue is expected to be treated in a specific monograph which is being prepared at the Computer Center of the Siberian Division of the USSR Academy of Sciences.

Much of the monograph's text was edited by N.N.Obraztsov to whom the author pays special tribute.

The book was primarily written by the author during his staying on vacation in the Turkmen Soviet Socialist Republic, where the environmental protection problems are being intensely studied in connection with major industrialization and irrigation projects for desert and arid regions of the republic. The author is grateful to M.G.Gaporov, Ch.S.Karriyev, and A.G.Babayev for many helpful discussions of these issues.

G.I.MARCHUK

INTRODUCTION

The rapid industrial development all over the world has posed an acute problem before the mankind striving to preserve the ecological systems that have formed historically in various regions of the globe. Local pollution caused by industrial emissions in many cities of the world have long surpassed the maximum permissible values of safe standards. The gigantic scale of work associated with the mining of coal, ferrous ores, non-ferrous metals and other mineral resources has resulted in erosion and contamination of vast expanses of land. Freon discharges from industrial and domestic refrigerators exert adverse effect on ozone layers of the atmosphere. Increased concentration of carbon dioxide as a result of burning a great amount of hydrocarbons needed for large-scale power generation has begun to tell on the heat balance of the globe. Volcanic eruptions change the optic and radiation properties of the atmosphere. All this has led to the global disturbance of the existing ecological systems. Therefore, an important task of contemporary science is to forecast changes in the ecological systems under the impact of natural and anthropogenic factors. First we should investigate the process of environmental pollution with industrial emissions and wastes and then assess the impact of noxious contaminations on the biological environment.

The present monograph deals with an estimation of atmospheric pollution and contamination of the underlying surface with passive and active pollutants. A passive pollutant is taken to mean here the pollutant which underwent no changes up to its fall on the earth surface. Conversely, a pollutant will be called active if in the course of its spreading in the air it enters into chemical reactions with water vapors or other atmospheric components or passes from one chemical state to another.

Industrial emissions spread in the air due to their advective transfer by air masses and diffusion caused by turbulent gusts of the air. If one watches a torch of smoke over a chimney, one may notice, firstly, that the smoke is being carried away by air and, secondly, that it grows larger and larger due to minor turbulences as the distance from the chimney is increasing. As a result the torch of smoke acquires the shape of an elongated cone expanding toward the direction of the air mass movement. Then under the effect of major turbulent fluctuations, the torch starts disintegrating into spaced whirl formations which are carried away far from its source.

If pollutants in the atmospheric emissions consist of large particles, they in the course of their spreading in the air begin to fall down by gravity with a constant velocity in compliance with Stock's law. Naturally, practically all the pollutants sooner or later settle on the earth surface, heavy particles fall down mainly due to the gravitation field, whereas light ones are precipitated by diffusion. Gravitation flow of heavy particles by far surpasses that of diffusion, whereas for light pollutants it is vertually insignificant. Since gaseous pollutants of oxide type pose a greater danger to the environment, it is the light compounds that the author treats at length in the monograph.

Apart from minor diffusions dispersing torch pollutants much attention in the pollution dissipation theory is given to fluctuations of velocity and direction of wind over a long period of time, generally about one year. Over this period, the air masses carrying pollutants away from the source repeatedly change their direction and velocity. Statistically such many-year observations are generally described by a special diagram called the wind rose in which the size of the vector is proportional to the number of recurrent events connected with the movement of air masses toward a given direction. This means that the longer the vectors in the wind rose diagram the more often the air masses change their movement in a given direction. Thus, maxima in the wind rose diagram correspond to winds predominant in the given region. This information is used as a starting point for planning new industrial projects, but it proves insufficient in drafting plans for the location of industrial plants among a great number of ecologically important zones (human settlements, recriation zones, agricultural and forest lands, etc.) since each of them has a maximum permissible dose of pollution of its own. Maximum permissible doses should, of course, take into account pollution from already existing industrial plants in the given region, therefore, while planning the establishment of a new industrial unit, limitations by safe standards should be laid down with reference to actual pollution from operating plants.

The monograph describes a method for preliminary calculations of regions for a possible location of industrial plants meeting safe pollution requirements for all ecologically important zones. To this end adjoint equations of substance transfer and diffusion have been introduced as a basis for solving the problem in question. The physical solution of adjoint problems is a function of impacts or a function of sensitivity with regard to the main functional of the problem. Specifically such a functional may be represented by the number of pollutants settled down in an ecological zone during one year or permissible hazardness of pollutants in both settled and suspended states. These problems are considered in chapter 4 in which findings are summed up for cases when there is a wider set of functionals.

Much attention in the book is given to problems of estimating expenditures for environment restoration, the gist of which lies in the following. If it is necessary to establish a new industrial plant with a specified level of noxious aerosols emission, the first thing to do is to assess consequencies of environmental pollution: the state of agricultural lands, forest areas, water bodies, animals, birds, insects, soil, etc. To do this, it is convenient to use statistical estimates of detriment to the environment and a nature restoration programme the cost of which should be included in the cost of products being manufactured and be allocated directly for nature restoration purposes. All this has makes it possible to solve, in the final analysis, the optimization problem with several limitations of a sanitary, ecological and economic nature.

Apart from the importance of the planned building of new industrial projects it is practically equally important to elucidate requirements for industrial emissions from already operating plants so as to ensure a minimum dose of environmental pollution of ecologically important zones. This problem is treated in chapter 6. To solve it, the author chose as the basic criterion economic expenditures for technological changes in the industrial plant in question so that total outlays at a specified decrease in the pollution level would be minimal for all the enterprises in the region. As a result, the problem may be reduced to a linear programming problem with the use of solutions of main and adjoint equations for the transfer and diffusion of aerosol pollutants.

Chapter 7 is primarily concerned with emissions of active aerosols which in the course of their interaction with water vapor and other air components are transferring from one compound to another with simultaneous change in the nature of its toxicity with respect to the environment. This problem may be boiled down to consideration of the optimization problems which have been considered earlier on the basis of pertinent adjoint equations.

The last chapter deals with problems of modelling, locating pollution sources in water bodies and coastal seas, and studying the processes involved in pollutants transfer and diffusion with reference to mesometeorological and mesooceanic processes.

Chapter 1. BASIC EQUATIONS OF TRANSPORT AND DIFFUSION

Polluting substances are transported in atmosphere by wind air streams which contain some short-range fluctuations. The averaged flux of the substances carried by air flows has, in general, advective and convective components, and their averaged fluctuational motions can be considered as diffusion against the background of the main stream. The purpose of the present chapter is to consider various models for substance transport and diffusion, the basic equations describing these processes, and the domains of definition and properties of the solutions.

1.1. Equation Describing Pollutant Transport in Atmosphere. Uniqueness of the Solution

Let ϕ (x, y, z, t) be the concentration of an aerosol substance transported with an air flow in the atmosphere. We will state the problem for a cylindrical domain G with the surface S consisting of the lateral surface of the cylinder $\sum$, the base $\sum_0$ (at z = 0), and other cover $\sum_H$ (at z = H). We write the velocity vector of air particles, which is a function of x, y, z, and t, as $\underline{u} = u\underline{i} + v\underline{j} + w\underline{k}$ (where $\underline{i}$, $\underline{j}$, $\underline{k}$ are unit vectors along the axes x, y, z, respectively). *Substance transport* along the trajectories of air particles, when the particle concentration is conserved, is described in the simplest way, namely,

$$d\phi/dt = 0$$

The explicit form of this equation is

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} + v\frac{\partial \phi}{\partial y} + w\frac{\partial \phi}{\partial z} = 0. \qquad (1.1)$$

Since the continuity equation

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0, \qquad (1.2)$$

holds with a reasonable accuracy in the lower atmosphere, we have the equation

$$\frac{\partial \phi}{\partial t} + \text{div}\,\underline{u}\phi = 0 \qquad (1.3)$$

In the following we shall suppose that div $\underline{u}$ = 0, unless it is stated otherwise. Besides, we shall assume that

$$w = 0, \text{ at } z = 0,\ z = H \qquad (1.4)$$

In the derivation of Eq.(1.3) we have used the identity

$$u\frac{\partial \phi}{\partial x} + v\frac{\partial \phi}{\partial y} + w\frac{\partial \phi}{\partial z} = \text{div}\,\underline{u}\phi - \phi\text{div}\,\underline{u} \qquad (1.5)$$

which is valid if the functions ϕ and $\underline{u}$ are differentiable. The second term on the right-hand side vanishes by virtue of Eq.(1.2), and Eq.(1.5) becomes

$$u \frac{\partial \phi}{\partial x} + v \frac{\partial \phi}{\partial y} + w \frac{\partial \phi}{\partial z} = \operatorname{div} \underline{u}\phi \tag{1.5'}$$

This is an important relation which will frequently be used in the sequel.

Equation (1.3) should be supplemented with the initial data

$$\phi = \phi_o \quad \text{at} \quad t = 0, \tag{1.6}$$

and the boundary conditions on the surface S of the domain G

$$\phi = \phi_S \quad \text{on} \quad S \quad \text{for } u_n < 0, \tag{1.7}$$

where ϕ_o and ϕ_S are given functions and u_n is the projection of the vector $\underline{u}$ onto the outward normal to the surface S. Condition (1.7) defines the solution in the region of S where the air bulk containing the substance in question is "injected" into the domain G. The exact solution of the problem given by Eq.(1.3) is possible if the functions u, v, and w are known throughout the space and for every time moment. If information on the components of the velocity vector is insufficient, one has to resort to an approximation; some of these relevant methods are discussed below.

Equation (1.3) can be generalized. For instance, if a fraction of the substance participates in a chemical reaction with the external medium, or is decaying during transport, the process can be treated as absorption of the substance. In this case, the equation includes an extra term

$$\frac{\partial \phi}{\partial t} + \operatorname{div} \underline{u}\phi + \sigma\phi = 0, \tag{1.8}$$

where $\sigma \geqq 0$ is a quantity having the inverse time dimension. The meaning of this quantity is especially clear if we put $u = v = w = 0$ in Eq.(1.8). Now the equation is just $\partial\phi/\partial t + \sigma\phi = 0$, and its solution is $\phi = \phi_o \exp(-\sigma t)$. Hence, we see that σ is the reciprocal time period during which the substance concentration falls by a factor of e as compared with the initial concentration ϕ_o.

If the domain of the solution contains sources of the polluting substance described by a distribution function $f(x, y, z, t)$, Eq.(1.8) becomes inhomogeneous,

$$\frac{\partial \phi}{\partial t} + \operatorname{div} \underline{u}\phi + \sigma\phi = f. \tag{1.9}$$

Now we turn to investigating the problem statement and conditions relevant to Eq.(1.9). Let us multiply the equation by ϕ and integrate it with respect to time t from 0 to T, and over the space domain G. The result is the identity

$$\int_G \frac{\phi^2}{2}\, dG \Big|_{t=T} - \int_G \frac{\phi^2}{2}\, dG \Big|_{t=0} + \int_0^T dt \int_G \operatorname{div} \frac{\underline{u}\phi^2}{2}\, dG + \sigma \int_0^T dt \int_G \phi^2 dG =$$

$$= \int_0^T dt \int_G f\, \phi\, dG. \tag{1.10}$$

Applying the Ostrogradsky-Gauss formula, one gets

$$\int_G \operatorname{div} \frac{\underline{u}\phi^2}{2}\, dG = \int_S \frac{u_n \phi^2}{2}\, dS. \tag{1.11}$$

By virtue of Eq.(1.4) u_n vanishes for $z = 0$, $z = H$, so that integration over S in Eq.(1.11) can be replaced by the integration over the lateral cylindrical surface Σ. For the sake of generality, however, we retain here the symbol S, having in mind condition (1.4). Taking into account the initial and boundary conditions,

$$\begin{aligned} \phi &= \phi_o \quad \text{at } t = 0, \\ \phi &= \phi_S \quad \text{on } S \text{ for } u_n < 0 \end{aligned} \tag{1.12}$$

where ϕ_o and ϕ_S are given, we obtain from Eq.(1.10)

$$\int_G \frac{\phi_T^2}{2}\, dG + \int_0^T dt \int_S \frac{u_n^+ \phi_S^2}{2}\, dS + \sigma \int_0^T dt \int_G \phi^2\, dG = \int_G \frac{\phi_o^2}{2}\, dG - \int_0^T dt \int_S \frac{u_n^- \phi_S^2}{2}\, dS +$$

$$+ \int_0^T dt \int_G f\phi\, dG, \tag{1.13}$$

where $u_n^+ = \{u_n, \text{ if } u_n > 0, \text{ or } 0, \text{ if } u_n < 0\}$; $u_n^- = u_n - u_n^+$.

Identity (1.13) is fundamental in investigating the uniqueness of the solutions to the problem stated in Eqs.(1.9) and (1.12). Indeed, suppose we have two different solutions, say, ϕ_1 and ϕ_2, satisfying Eq.(1.9) and the conditions (1.12). The problem for the difference $\omega = \phi_1 - \phi_2$, is

$$\frac{\partial \omega}{\partial t} + \operatorname{div} \underline{u}\omega + \sigma\omega = 0, \tag{1.14}$$

$$\begin{aligned} \omega &= 0 \quad \text{at} \quad t = 0, \\ \omega &= 0 \quad \text{on } S, \text{ if } u_n < 0 \end{aligned} \tag{1.15}$$

Eq.(1.13) for the function ω takes the form

$$\int_G \frac{\omega_T^2}{2}\, dG + \int_0^T dt \int_S \frac{u_n^+ \omega^2}{2}\, dS + \sigma \int_0^T dt \int_G \omega^2\, dG = 0 \qquad (1.16)$$

If $\omega \neq 0$, all the terms on the left-hand side are positive, so that this expression vanishes only if $\omega = 0$, i.e. $\phi_1 = \phi_2$. Thus, we have proved the uniqueness of the solution.

It goes without saying that our deduction is true, provided all the procedures and transformations used in the proof are correct. It is not difficult to see that this is the case if the solution ϕ and the velocity components u, v, w are differentiable functions, and the integrals appearing in Eq.(1.13) do exist. We will assume in the sequel that all the smoothness conditions ensuring the uniqueness of the solutions are valid.

So we have proved that the problem

$$\frac{\partial \phi}{\partial t} + \operatorname{div} \underline{u}\phi + \sigma\phi = f, \qquad (1.17)$$

$$\phi = \phi_0 \quad \text{at} \quad t = 0,$$
$$\phi = \phi_S \quad \text{on } S, \text{ if } u_n < 0 \qquad (1.18)$$

has a unique solution.

1.2. Stationary Equation for Substance Propagation

We now describe a stationary process of substance propagation. If input data u, v, w, f, ϕ_S are time-independent, the stationary problem corresponding to Eqs.(1.17) and (1.18) becomes quite simple

$$\operatorname{div} \underline{u}\phi + \sigma\phi = f, \qquad (2.1)$$

$$\phi = \phi_S \text{ on } S \text{ for } u_n < 0 \qquad (2.2)$$

Evidently, the identity corresponding to Eq.(1.13) is

$$\int_S \frac{u_n^+ \phi^2}{2}\, dS + \sigma \int_G \phi^2\, dG = -\int_S \frac{u_n^- \phi_S^2}{2}\, dS + \int_G f\phi\, dG. \qquad (2.3)$$

The method described in the preceding section can be used to show that the problem given by Eqs.(2.1), (2.2) has a unique solution.

Thus the problem in view, Eqs.(2.1), (2.2), is a particular case where substance transport proceeds with invariable input data. However, the set of such particular solutions corresponding to various stationary input functions $\underline{u}$, f, ϕ_S, is also useful in treating more complicated physical situations, which take place in practice. To demonstrate this fact, we suppose that in a region under study the motions of air masses are stationary during certain time periods specific for the existence of any particular configuration of atmospheric flows. Every such steady-state period ends in the rearrangement of the air motion, and a new stationary configuration is established. Since the rearrangement time is much less than the time of the existence of any particular configuration, it can be assumed that the states are changed instantly. Suppose we have a sequence of n stationary configurations; this leads to a set of n independent equations,

$$\operatorname{div} \underline{u}_i \phi_i + \sigma\phi_i = f \tag{2.4}$$

$$\phi_i = \phi_{iS} \quad \text{on } S \quad \text{for } u_{in} < 0, \; i = \overline{1,n} \tag{2.5}$$

The problem stated in Eqs.(2.4), (2.5), where ϕ_{iS} is the boundary value of the function ϕ_i on the surface S and u_{in} is the projection of the i-type wind stream upon the outward normal to the boundary surface, corresponds to the time intervals $t_i < t < t_{i+1}$, the interval lengths being $\Delta t_i = t_{i+1} - t_i$.

Suppose Eqs.(2.4), (2.5) are solved for every i. Then the impurity distribution function averaged over the whole time interval $T = \sum_{i=1}^{n} \Delta t_i$ is the linear combination of the solutions

$$\tilde{\phi} = \frac{1}{T} \sum_{i=1}^{n} \phi_i \, \Delta t_i . \tag{2.6}$$

The approach presented in Eqs.(2.4), (2.5), (2.6) may be called the *statistical model.*

The solution of stationary problems (2.1), (2.2) and (2.4), (2.5) is similar to determining a time averaged, over a period T, of the substance distribution, proceeding from specially formulated nonstationary problems. Actually, we can consider the following problem:

$$\frac{\partial\phi}{\partial t} + \operatorname{div} \underline{u}\phi + \sigma\phi = f, \tag{2.7}$$

$$\begin{gathered} \phi = \phi_S \quad \text{on } S \quad \text{for } u_n < 0, \\ \phi(\underline{r},T) = \phi(\underline{r},0), \; \underline{r} = (x,y,z) \in G. \end{gathered} \tag{2.8}$$

As in Eqs.(2.1), (2.2), we assume that the functions $\underline{u}$ and ϕ_S are time-independent.

The same method as that of section 1.1 is used to prove that the problem stated in Eqs.(2.7), (2.8) has a unique solution under some proper assumptions on the smoothness of the functions involved.

Integrating Eq.(2.7) over the interval [0,T], we obtain the equation

$$\operatorname{div} \overline{\underline{u}\phi} + \sigma\overline{\phi} = f, \quad \overline{\phi} = \frac{1}{T}\int_0^T \phi \, dt. \tag{2.9}$$

As the problem stated in Eqs.(2.1) and (2.2) has a unique solution, we see from Eq.(2.9) that the solution of Eqs.(2.7), (2.8) averaged over the period T, coincides with the solution of Eqs.(2.1), (2.2).

Let us consider a more complicated case. Suppose we have a function $\underline{u}$ which is sufficiently smooth for $t \in [0,T]$, does not depend on time for every interval $t_i + \tau \leq t \leq t_{i+1}$ $(i = \overline{0, n-1})$, and coincides on these intervals with $\underline{u}_i$ in Eq. (2.4). The rearrangement time for the stream circulations, τ, is by assumption much less than the time intervals Δt_i, i.e.

$$\tau \ll \Delta t_i. \tag{2.10}$$

We now deal with the non-stationary problem (2.7), (2.8), corresponding to the vector function $\underline{u}$ defined above

$$\frac{\partial\phi}{\partial t} + \operatorname{div} \underline{u}\phi + \sigma\phi = f, \tag{2.11}$$

$$\begin{aligned} &\operatorname{div} \underline{u} = 0, \\ &\phi = \phi_S \quad \text{on} \quad S \quad \text{for } u_n < 0 \end{aligned} \tag{2.12}$$

where ϕ_S is related to ϕ_{iS} in Eq.(2.5) in the same fashion as $\underline{u}$ is related to $\underline{u}_i$ in Eq.(2.4). Furthermore, suppose that $\underline{u}$ and ϕ_S are periodic functions of a period T equal to one year. The boundary-value problem (2.11), (2.12) should be considered for the set of time-periodic functions, that is to say

$$\phi(\underline{r},T) = \phi(\underline{r},o), \quad \underline{r} = \underline{r}(x,y,z) \tag{2.13}$$

Thus, solving the problem (2.11)-(2.13), we obtain the annual average for the substance distribution

$$\overline{\phi} = \frac{1}{T}\int_0^T \phi \, dt. \tag{2.14}$$

It is not difficult to see that there is an intimate relation between the non-stationary problem (2.11)-(2.13) and the problem (2.4), (2.5) treated above.

Consider Eq.(2.11)

$$\frac{\partial\phi}{\partial t} + \operatorname{div} \underline{u}_i\phi + \sigma\phi = f \tag{2.15}$$

with boundary condition (2.12),

$$\phi = \phi_S \quad \text{on} \quad S \quad \text{for } u_{in} < 0, \tag{2.16}$$

for the time interval $[t_i + \tau, t_{i+1}]$. Let at the moment $t = t_i + \tau$ the function ϕ take the value

$$\phi(t_i + \tau) = \phi^0. \tag{2.17}$$

Introduce the function

$$\omega_i = \phi - \phi_i, \tag{2.18}$$

where ϕ_i is the solution for the problem (2.4), (2.5). This is the solution of the boundary-value problem

$$\frac{\partial\omega_i}{\partial t} + \operatorname{div} \underline{u}_i\omega_i + \sigma\omega_i = 0, \tag{2.19}$$

$$\omega_i = 0 \quad \text{on} \quad S \quad \text{for } u_{i\,n} < 0,$$

$$\omega_i(t_i + \tau) = \phi^0 - \phi_i$$

for the interval $t \in [t_i + \tau, t_{i+1}]$.

The next step is to multiply differential Eq.(2.19) by ω_i and integrate over the domain G. The result is

$$\|\omega_i\| \left(2\frac{d}{dt}\|\omega_i\| + \sigma\|\omega_i\|\right) + \int_S \frac{\omega_i^2 u_{in}^+}{2}\, dS = 0, \tag{2.20}$$

where $\|\omega\| = \left(\int_G \omega^2 dG\right)^{1/2}$. Hence, we get the inequality

$$\|\omega_i\| \leq \exp\{-\frac{\tau}{2}(t - t_i - \tau)\}\|\phi^0 - \phi_i\|. \tag{2.21}$$

Thus, the solution of the problem (2.11)-(2.13) for every time interval $t_i \leq t \leq t_{i+1}$, starting from a certain time moment, may deviate only slightly from the solution of the corresponding problem stated in Eqs.(2.4), (2.5). In general, the extent of the difference between the solutions depends essentially on the time intervals Δt_i. It is natural for the class of the problems considered here that the lengths of the time intervals Δt_i $(i = \overline{1,n})$ are so chosen that the interval where the functions ϕ and ϕ_i have a negligible difference is substantially greater than its complement to Δt_i. With this in mind, we introduce a quantity ε and regard two concentrations of the polluting substance ϕ^1 and ϕ^2 as coinciding, if

$$\|\phi^1 - \phi^2\| \leq \varepsilon \tag{2.22}$$

Let τ_i denote the time necessary for stabilization, in the sense of the definition (2.22), of a steady-state propagation of the substance, given by the function ϕ, during the time period $t_i + \tau \leq t \leq t_{i+1}$. Then we have

$$\tau_i = \frac{2}{\sigma} \ln \frac{\|\phi^0 - \phi_i\|}{\varepsilon} \leq \Delta t_i . \tag{2.23}$$

Proceeding along the same line, as it was shown above, we get by means of inequality (2.21) an estimate for the function ϕ in the time interval $t_i \leq t \leq t_i + \tau$,

$$\|\phi\| \leq e^{-\sigma(t-t_i)} (\|\phi_{i-1}\| + \varepsilon) + \frac{\|f\|}{\sigma}(1-e^{-\sigma(t-t_i)}). \tag{2.24}$$

The annual average of the impurity concentration ϕ is

$$\bar{\phi} = \frac{1}{T}\int_0^T \phi dt = \frac{1}{T}\sum_{i=1}^{n} \phi_i \Delta t_i + \frac{1}{T}\sum_{i=1}^{n-1} \int_{t_i+\tau+\tau_i}^{t_{i+1}} \omega_i dt - \frac{1}{T}\sum_{i=1}^{n} \phi_i(\tau+\tau_i) + $$
$$+ \frac{1}{T}\sum_{i=0}^{n-1} \int_{t_i}^{t_i+\tau+\tau_i} \phi \, dt. \tag{2.25}$$

Hence, using relations (2.21)-(2.24), we get the inequality for the difference between the solutions of the boundary-value problems (2.4), (2.5) and (2.11)-(2.13) averaged over the time interval [0,T]: $\|\bar{\phi} - \tilde{\phi}\| \leq \varepsilon + (\varepsilon + 3\|f\|/\sigma)r/\Delta t$, where $r = \max(\tau + \tau_i)$, $\Delta t = T/n$. Taking into account condition (2.10) and choosing the interval lengths Δt, τ_i according to the requirement $r/\Delta t \leq \varepsilon$, we obtain

$$\|\bar{\phi} - \tilde{\phi}\| \leq (1 - 3\|f\|/\sigma)\varepsilon + \varepsilon^2. \tag{2.26}$$

Thus, under the assumptions adopted, the solution of the boundary-value problem for the substance distribution averaged over the time period T, as obtained by means of the statistical model, is sufficiently close to the solution of the non-stationary problem (2.11)-(2.13).

Note in conclusion that solving problem (2.4), (2.5) or (2.11)-(2.13) and averaging the results by means of Eqs.(2.6) or (2.14), respectively, we do take into account substance diffusion induced by fluctuations of the input data.

1.3. Diffusion Approximation. Uniqueness of the Solution

The models for impurity propagation in the atmosphere from the air pollution sources considered in the preceding section describe the process in the essence; but they idealize, to a certain extent, the real processes, which have a more complicated and varied physical contents. Take, for instance, the case where the atmosphere is free from advective and convective motions, that is to say, $u = v = w = 0$. Then, according to the models considered above, the non-stationary problem for substance transport is

$$\frac{\partial \phi}{\partial t} + \sigma\phi = f, \tag{3.1}$$

$$\phi = \phi_o \quad \text{at } t = 0$$

If f does not depend on t, the solution is

$$\phi = \phi_o e^{-\sigma t} + \frac{f}{\sigma}(1 - e^{-\sigma t}) \tag{3.2}$$

and it approaches the solution of the corresponding stationary problem, $\sigma\phi = f$, i.e. $\phi = f/\sigma$, as t goes to infinity.

It is known that the simplest model of this type does not describe the main properties of substance transport from a source f. Actually, we do know that in the atmosphere any impurity is as if dispersing, thereby forming a rather complicated aerosol distribution in a considerable neighbourhood of the exhaust source. No wonder, because even though the weather is calm there always exists turbulence in the atmosphere, where spontaneous short-range fluctuations (mostly, vortices) are permanently dissipated thereby giving rise to new short-range phenomena.

The spectrum of such fluctuations has been investigated thoroughly enough, and we know that precisely these fluctuations are responsible for the dispersion of exhaust sources in the atmosphere. Since the effect in view is purely statistical, it is impossible to pre-calculate the fluctuations, or even detect them, in the real situation. If there were such a possibility, one could calculate the dispersion of an aerosol source and substance propagation, using the model of Eqs. (2.4), (2.5), or the more accurate model of Eqs.(2.7), (2.12), (2.13). This is inconceivable, however, so we should modify the models in such a way that they be appropriate to account for continuously generated atmospheric fluctuations.

The physical nature of the fluctuational phenomena has been comprehended well enough, but until now their mathematical description has been based, for the most part, upon semi-empirical relations. The simplest approach is briefly considered below.

Suppose we deal with a function a which is represented as the sum of its averaged value $\bar{a}$ and the fluctuational component a', i.e. $a = \bar{a} + a'$, where

$$a' << \bar{a} \tag{3.3}$$

in other words, the fluctuations of the quantity a are small. Suppose further that the quantity a is averaged over a sufficiently large time interval T

$$\bar{a} = \frac{1}{T} \int_t^{t+T} a dt, \tag{3.4}$$

and on this interval

$$\bar{a}' = \frac{1}{T} \int_t^{t+T} a' dt = 0. \tag{3.5}$$

If the process in view satisfies conditions (3.3)-(3.5), we can apply the following method of constructing the equations describing substance propagations in various cases.

Calculate the integral of Eq.(1.8) over the interval $t \leq \tau \leq t + T$,

$$\frac{\phi\ (t+T) - \phi(t)}{T} + \operatorname{div} \int_t^{t+T} \underline{u}\phi dt + \sigma \int_t^{t+T} \phi dt = 0 \tag{3.6}$$

Assuming $\phi = \bar{\phi} + \phi'$ and $\underline{u} = \bar{\underline{u}} + \underline{u}'$, as in Eq.(3.4), we get from Eq.(3.6).

$$\frac{\phi(t+T) - \phi(t)}{T} + \operatorname{div} \bar{\underline{u}}\bar{\phi} + \operatorname{div} \overline{\underline{u}'\phi'} + \sigma\bar{\phi} = 0, \tag{3.7}$$

or equivalently

$$\frac{\bar{\phi}(t + T) - \bar{\phi}(t)}{T} + \operatorname{div} \bar{\underline{u}}\bar{\phi} + \operatorname{div} \overline{\underline{u}'\phi'} + \sigma\bar{\phi} = - \frac{\phi'(t + T) - \phi'(t)}{T} \tag{3.8}$$

Next, we do a rescaling of the functions involved. We write $\bar{\phi} = A\bar{\Phi}$, $\phi' = a\Phi'$, where $\bar{\Phi}$ and Φ' have the same order of magnitude. By the assumption, $\phi' \leq \bar{\phi}$, so $a << A$ and we have $a/A = \varepsilon << 1$. Then Eq.(3.8) is reduced to

$$\frac{\bar{\Phi}(t + T) - \bar{\Phi}(t)}{T} + \operatorname{div} \bar{\underline{u}}\bar{\Phi} + \sigma\bar{\Phi} + \varepsilon \operatorname{div} \overline{\underline{u}'\Phi'} = \frac{\varepsilon}{T} O\ (1), \tag{3.9}$$

where $O(1)$ stands for a quantity of the order of Φ'. Thus, the right-hand side of (3.9) is small because of the parameter ε/T, and can be neglected. The resulting equation is

$$\frac{\bar{\phi}(t + T) - \bar{\phi}(t)}{T} + \operatorname{div} \bar{\underline{u}}\bar{\phi} + \operatorname{div} \overline{\underline{u}'\phi'} + \sigma\bar{\phi} = 0 \tag{3.10}$$

If the function $\bar{\phi}(t)$ has a small variation on the time interval T, we can replace $(\bar{\phi}(t+T) - \bar{\phi}(t))/T$ by the time derivative $\partial\bar{\phi}/\partial t$ to obtain the equation for the averaged component

$$\frac{\partial \bar{\phi}}{\partial t} + \operatorname{div} \overline{\underline{u}}\bar{\phi} + \operatorname{div} \overline{\underline{u}'\varphi'} + \sigma\bar{\varphi} = 0, \tag{3.11}$$

which differs from Eq.(1.8) by the presence of the fluctuational moment div $\overline{\underline{u}'\varphi'}$. It is this new term which is responsible for the dispersion of air streams carrying particles of polluting substances.

It has been found that in the case of atmospheric processes the components of the vector $\overline{\underline{u}'\phi'}$ can be expressed semi-empirically in terms of the averaged substance fields

$$\overline{u'\phi'} = -\mu\frac{\partial\bar{\phi}}{\partial x}, \quad \overline{v'\phi'} = -\mu\frac{\partial\bar{\phi}}{\partial y}, \quad \overline{w'\phi'} = -\nu\frac{\partial\bar{\phi}}{\partial z} \tag{3.12}$$

Here $\mu \geqq 0$ and $\nu \geqq 0$ are the horizontal and vertical diffusion coefficients, respectively; they are to be determined experimentally.

If we substitute relations (3.12) into Eq.(3.11), we get the diffusion approximation for the equation of substance propagation in the atmosphere

$$\frac{\partial\bar{\phi}}{\partial t} + \operatorname{div} \bar{\underline{u}}\bar{\phi} + \sigma\bar{\phi} = D\bar{\phi}, \tag{3.13}$$

where

$$D\bar{\phi} = \frac{\partial}{\partial x}\mu\frac{\partial\bar{\phi}}{\partial x} + \frac{\partial}{\partial y}\mu\frac{\partial\bar{\varphi}}{\partial y} + \frac{\partial}{\partial z}\nu\frac{\partial\bar{\phi}}{\partial z} . \tag{3.14}$$

Of course, Eq.(3.13) should be completed with the continuity equation

$$\operatorname{div} \bar{\underline{u}} = 0 \tag{3.15}$$

and the initial data

$$\bar{\phi} = \bar{\phi}_o \quad \text{at} \quad t = 0. \tag{3.16}$$

As regards the boundary conditions, they are derived in the investigation of the solution uniqueness for the problem.

In the following we shall omit the bar over the function, assuming that we deal with the averaged quantity. Again, we multiply Eq.(3.13) by ϕ and integrate the result over the time interval $0 \leqq t \leqq T$ and the space domain:

$$\int_G \frac{\phi_T^2}{2}\,dG - \int_G \frac{\phi_0^2}{2}\,dG + \int_0^T dt \int_S \frac{u_n\phi^2}{2}\,dS + \sigma\int_0^T dt \int_G \phi^2 dG =$$

$$= -\int_0^T dt \int_G \left(\mu \left[\left(\frac{\partial\phi}{\partial x}\right)^2 + \left(\frac{\partial\phi}{\partial y}\right)^2\right] + \nu\left(\frac{\partial\phi}{\partial z}\right)^2\right) dG + \tag{3.17}$$

$$+ \int_0^T dt \left[\mu \int_\Sigma \phi\frac{\partial\phi}{\partial n}\, d\Sigma + \nu\left(\int_{\Sigma_H} \phi\, \frac{\partial\phi}{\partial z}\, d\Sigma - \int_{\Sigma_0} \phi\, \frac{\partial\phi}{\partial z}\, d\Sigma\right)\right].$$

Here $\phi_T = \phi(T)$, $\phi_o = \phi(0)$, $\partial\phi/\partial n$ is the derivative along the outward normal to the surface Σ. Recall that S is the total surface of the domain G, Σ is the lateral cylindrical surface, Σ_H is the horizontal cross-section of the cylinder at the height $z = H$, Σ_o is the cross-section at $z = 0$. Eq.(3.17) is further reduced to

$$\int_G \frac{\phi_T^2}{2}\, dG + \int_0^T dt \int_S \frac{u_n^+\phi^2}{2}\, dS + \int_0^T dt \int_G \left\{\mu \left[\left(\frac{\partial\phi}{\partial x}\right)^2 + \left(\frac{\partial\phi}{\partial y}\right)^2\right] + \right.$$

$$\left. + \nu\left(\frac{\partial\phi}{\partial z}\right)^2\right\} dG + \sigma\int_0^T dt \int_G \phi^2 dG = \int_G \frac{\phi_0^2}{2}\, dG - \int_0^T dt \int_S \frac{u_n^-\phi^2}{2}\, dS + \tag{3.18}$$

$$+ \int_0^T dt \left[\mu \int_\Sigma \phi\, \frac{\partial\phi}{\partial n}\, d\Sigma + \nu\left(\int_{\Sigma_H} \phi\, \frac{\partial\phi}{\partial z}\, d\Sigma - \int_{\Sigma_0} \phi\, \frac{\partial\phi}{\partial z}\, d\Sigma\right)\right].$$

We set the following boundary conditions:

$$\begin{aligned} \phi &= \phi_S \quad \text{on } \Sigma \text{ for } u_n < 0 \\ \partial\phi/\partial n &= 0 \quad \text{on } \Sigma \text{ for } u_n \geqq 0 \\ \partial\phi/\partial z &= \alpha\phi \quad \text{on } \Sigma_o, \\ \partial\phi/\partial z &= 0 \quad \text{on } \Sigma_H. \end{aligned} \tag{3.19}$$

Here $\alpha \geqq 0$ is a function defining the interaction of the impurities with the underlying surface. Besides,

$$w = 0 \quad \text{at} \quad z = 0, \quad z = H. \tag{3.20}$$

Let us show that conditions (3.19), (3.20) together with initial data (3.16) ensure the uniqueness of the solution. Actually, using Eq.(3.19), we obtain the fundamental relation.

$$\int\limits_G \frac{\phi_T^2}{2}\,dG + \int\limits_0^T dt \int\limits_\Sigma \frac{u_n^+\phi^2}{2}\,d\Sigma + \int\limits_0^T dt \int\limits_G \Big\{ \mu \left[\left(\frac{\partial\phi}{\partial x}\right)^2 + \left(\frac{\partial\phi}{\partial y}\right)^2 \right] +$$

$$+ \nu \left(\frac{\partial\phi}{\partial z}\right)^2 \Big\}\,dG + \sigma \int\limits_0^T dt \int\limits_G \phi^2 dG + \nu \int\limits_0^T dt \int\limits_{\Sigma_0} \alpha\phi^2\,d\Sigma = \tag{3.21}$$

$$= \int\limits_G \frac{\phi_0^2}{2}\,dG - \int\limits_0^T dt \int\limits_\Sigma \frac{u_n^-\phi_S^2}{2}\,d\Sigma + \mu \int\limits_0^T dt \int\limits_\Sigma \phi_S \frac{\partial\phi}{\partial n}\,d\Sigma .$$

Here we have replaced S by Σ, in view of Eq.(3.10).

We now prove that the solution is unique. As in section 1.2, we assume that there are two solutions, ϕ_1 and ϕ_2, satisfying differential Eq.(3.13), initial data (3.16), boundary conditions (3.19), and subsidiary conditions (3.15) and (3.20). Then for the difference $\omega = \phi_1 - \phi_2$ we get the differential equation

$$\frac{\partial\omega}{\partial t} + \operatorname{div} \underline{u}\omega + \sigma\omega = D\omega, \tag{3.22}$$

with the initial data

$$\omega = 0 \quad \text{at} \quad t = 0, \tag{3.23}$$

and the boundary conditions

$$\begin{aligned} \omega &= 0 \quad \text{on } \Sigma \quad \text{for} \quad u_n < 0, \\ \partial\omega/\partial n &= 0 \quad \text{on } \Sigma \quad \text{for} \quad u_n \geqq 0 \\ \partial\omega/\partial z &= \alpha\omega \quad \text{on} \quad \Sigma_o, \\ \partial\omega/\partial z &= 0 \quad \text{on} \quad \Sigma_H. \end{aligned} \tag{3.24}$$

For this problem statement, integral relation (3.21) is reduced to

$$\int\limits_G \frac{\omega_T^2}{2}\,dG + \int\limits_0^T dt \int\limits_\Sigma \frac{u_n^+\omega^2}{2}\,d\Sigma + \int\limits_0^T dt \int\limits_G \Big\{ \mu \left[\left(\frac{\partial\omega}{\partial x}\right)^2 + \left(\frac{\partial\omega}{\partial y}\right)^2 \right] +$$

$$+ \nu \left(\frac{\partial\omega}{\partial z}\right)^2 \Big\}\,dG + \sigma \int\limits_0^T dt \int\limits_G \omega^2 dG + \nu \int\limits_0^T dt \int\limits_{\Sigma_0} \alpha\omega^2\,d\Sigma = 0. \tag{3.25}$$

Since the functions u_n^+, μ, ν, σ, α in Eq. (3.25) are non-negative, the relation holds only in the case where $\omega = 0$, i.e. $\phi_1 = \phi_2$. Thus, the solution is unique. For the sake of simplicity we have assumed here that $f = 0$. The effect of a sources can be accounted for as in section 1.1.

If one has to include the sources, the problem to be also considered has a unique solution in the diffusion approximation, provided the input data are smooth. The problem is

$$
\begin{aligned}
&\frac{\partial\phi}{\partial t} + \operatorname{div} \underline{u}\phi + \sigma\phi = D\,\phi + f, \\
&\phi = \phi_o \quad \text{at} \quad t = 0, \\
&\phi = \phi_S \quad \text{on} \quad \Sigma \quad \text{for} \quad u_n < 0, \\
&\partial\phi/\partial n = 0 \quad \text{on} \quad \Sigma \ \text{for} \ u_n \geqq 0, \\
&\partial\phi/\partial z = \alpha\phi \quad \text{on} \quad \Sigma_o, \\
&\partial\phi/\partial z = 0 \quad \text{on} \quad \Sigma_H.
\end{aligned}
\tag{3.26}
$$

We also assume here that

$$\operatorname{div} \underline{u} = 0, \quad w = 0 \quad \text{at} \ z = 0, \ z = H.$$

Note that there is another problem, beside that of Eq.(3.26), which is sometimes used in calculations and has a unique solution.

$$
\begin{aligned}
&\frac{\partial\phi}{\partial t} + \operatorname{div} \underline{u}\phi + \sigma\phi = D\phi + f, \\
&\phi = \phi_o \quad \text{at} \quad t = 0, \\
&\phi = \phi_S \quad \text{on} \quad \Sigma, \\
&\partial\phi/\partial z = \alpha\phi \quad \text{on} \cdot \Sigma_o, \\
&\partial\phi/\partial z = 0 \quad \text{on} \quad \Sigma_H.
\end{aligned}
\tag{3.27}
$$

It goes without saying that there are other statements of the problem ensuring a unique solution.

To proceed further, we represent the operator D defined by Eq.(3.14) as the sum of two operators

$$D = \mu\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{\partial}{\partial z}\,\nu\,\frac{\partial}{\partial z} = \mu\Delta + \frac{\partial}{\partial z}\,\nu\,\frac{\partial}{\partial z}.$$

To facilitate the following analysis, we assume that the diffusion coefficient μ does not depend on the space coordinates and time.

Until now we have considered the general three-dimensional problems, but there are many cases where two-dimensional (x,y)-approximations are adequate, to be stated on the basis of Eqs.(3.26) or (3.27). Take, for instance, Eqs.(3.27). Integrating the diffusion equation over the altitude, we get

$$\frac{\partial}{\partial t}\int_0^H \phi\,dz + \int_0^H \operatorname{div}\underline{u}\phi dz + \sigma\int_0^H \phi\,dz = \int_0^H \frac{\partial}{\partial z}\nu\frac{\partial\phi}{\partial z}dz + \mu\Lambda\int_0^H \phi\,dz + \int_0^H f\,dz. \tag{3.28}$$

Let us transform the second term on the left-hand side and the first term on the right-hand side to a more explicit form. Assuming that the horizontal components u and v of the velocity vector do not depend on the altitude in the active layer of substance transport and diffusion, we obtain

$$\int_0^H \operatorname{div}\underline{u}\,\phi dz = \frac{\partial}{\partial x}\left(u\int_0^H \phi\,dz\right) + \frac{\partial}{\partial y}\left(v\int_0^H \phi\,dz\right) + w\phi\Big|_{z=0}^{z=H} \tag{3.29}$$

The last term vanishes, since $w = 0$ for $z = 0$ and $z = H$, so that

$$\int_0^H \operatorname{div}\underline{u}\phi\,dz = \frac{\partial}{\partial x}\left(u\int_0^H \phi dz\right) + \frac{\partial}{\partial y}\left(v\int_0^H \phi\,dz\right) \tag{3.30}$$

We now turn to the relation

$$\int_0^H \frac{\partial}{\partial z}\nu\frac{\partial\phi}{\partial z}dz = \nu\frac{\partial\phi}{\partial z}\Big|_{z=0}^{z=H} = -\nu\frac{\partial\phi}{\partial z}\Big|_{z=0}. \tag{3.31}$$

It can be simplified by virtue of the boundary conditon $\partial\phi/\partial z = \alpha\phi$ at $z = 0$ as follows:

$$\int_0^H \frac{\partial}{\partial z}\nu\frac{\partial\phi}{\partial z}dz = -\alpha\nu\phi\Big|_{z=0}.$$

Assuming the approximate relation

$$\phi\Big|_{z=0} = \frac{1}{H}\int_0^H \phi\,dz,$$

one finally gets

$$\int_0^H \frac{\partial}{\partial z}\nu\frac{\partial\phi}{\partial z}dz = -\frac{\alpha\nu}{H}\int_0^H \phi\,dz. \tag{3.32}$$

Introduce the integral intensities for the aerosol distribution and the source

$$\bar{\phi} = \int_0^H \phi \, dz, \quad \bar{f} = \int_0^H f \, dz.$$

Putting them into Eq.(3.28), we obtain

$$\frac{\partial \bar{\phi}}{\partial t} + \frac{\partial \overline{u\phi}}{\partial x} + \frac{\partial \overline{v\phi}}{\partial y} + \bar{\sigma}\bar{\phi} = \mu\Delta\bar{\phi} + \bar{f}, \tag{3.33}$$

where $\bar{\sigma} = \sigma + \alpha\nu/H$. Note that $\sigma\bar{\phi}$ is the amount of the aerosol decaying in the process of its propagation in the atmosphere, integrated over the altitude, while $(\alpha\nu/H)\ \bar{\phi}$ is the amount of the aerosol deposited at the earth's surface. Omitting the bar over the symbols ϕ, f, and σ, we arrive at the two-dimensional problem statement

$$\begin{aligned} &\frac{\partial \phi}{\partial t} + \frac{\partial u\phi}{\partial x} + \frac{\partial v\phi}{\partial y} + \sigma\phi = \mu\Delta\phi + f, \\ &\phi = \phi_o \quad \text{at} \quad t = 0 \\ &\phi = \phi_S \quad \text{on} \ \Sigma \ \text{for} \quad u_n < 0, \\ &\partial\phi/\partial n = 0 \quad \text{on} \ \Sigma \ \text{for} \quad u_n \geqq 0. \end{aligned} \tag{3.34}$$

Another statement of the problem is also possible,

$$\begin{aligned} &\frac{\partial \phi}{\partial t} + \frac{\partial u\phi}{\partial x} + \frac{\partial v\phi}{\partial y} + \sigma\phi = \mu\Delta\phi + f, \\ &\phi = \phi_o \quad \text{at} \quad t = 0, \\ &\phi = \phi_S \quad \text{on} \quad \Sigma. \end{aligned} \tag{3.35}$$

It is worth noting that all the arguments presented in section 1.2 are valid for the diffusion approximation as well. This is also true for the stationary problem where the solution of the basic problem is obtained, to within the transient processes, by averaging over the ensemble of particular stationary problems of the following form:

$$\operatorname{div} \underline{u}_i\phi_i + \sigma\phi_i = D\phi_i + f, \qquad \operatorname{div} \underline{u}_i = 0 \tag{3.36}$$

with the boundary conditions

$$\begin{aligned} &\phi_i = \phi_{iS} \quad \text{on} \ \Sigma \ \text{for} \quad u_{in} < 0, \\ &\partial\phi_i/\partial n = 0 \quad \text{on} \ \Sigma \ \text{for} \quad u_{in} \geqq 0, \end{aligned} \tag{3.37}$$

$$\partial\phi_i/\partial z = \alpha_i\phi_i \quad \text{on} \quad \Sigma_o,$$

$$\partial\phi_i/\partial z = 0 \quad \text{on} \quad \Sigma_H.$$

The substance distribution averaged over the time period T is

$$\phi = \frac{1}{T} \sum_{i=1}^{n} \phi_i \, \Delta t_i, \tag{3.38}$$

where $T = \sum_{i=1}^{n} \Delta t_i$, and Δt_i is the time during which there exists a steady-state configuration of the air streams.

1.4. Simple Diffusion Equation

It is reasonable to begin an analysis of substance transport and diffusion with the simplest examples of one-dimensional problems, gradually complicating the mathematical problem statement. So, we are going to start with the pure diffusion in an infinite one-dimensional medium

$$\sigma\phi = \mu \frac{d^2\phi}{dx^2} + Q\delta\ (x - x_0) \tag{4.1}$$

where $-\infty < x < \infty$, Q is the capacity of the source exhausting the aerosol into the atmosphere. The boundary conditions in this case are reduced to the requirement that the solution should be finite throughout the domain of definition. Note that the source function f in Eq.(4.1) is taken in a particular form characteristic of the problems of the class considered here. It is convenient to state the problem in an equivalent form without the δ function. To this end, we integrate Eq.(4.1) in the vicinity of the point $x = x_o$; the result is

$$\sigma \int_{x_o-\varepsilon/2}^{x_o+\varepsilon/2} \phi\, dx = \mu \frac{\partial\phi}{\partial x}\Big|_{x_o+\varepsilon/2} - \mu \frac{d\phi}{dx}\Big|_{x_o-\varepsilon/2} + Q.$$

As ε tends to zero, we obtain the important relation

$$\mu \frac{d\phi}{dx}\Big|_{x_o+} - \mu \frac{d\Phi}{dx}\Big|_{x_o-} + Q = 0. \tag{4.2}$$

Let us consider two regions, $-\infty < x \leq x_o$ and $x_o \leq x < \infty$; the corresponding solutions will be denoted by ϕ_- and ϕ_+, and the problems to be solved are

$$\mu \frac{d^2\phi_+}{dx^2} - \sigma\phi_+ = 0, \qquad \phi_+ = 0 \quad \text{for } x \to \infty; \tag{4.3}$$

$$\mu \frac{d^2\phi_-}{dx^2} - \sigma\phi_- = 0,$$
$$\phi_- = 0 \quad \text{for } x \to -\infty. \tag{4.4}$$

The coupling between the solutions of the problems is given by the boundary condition at $x = x_o$

$$\mu \frac{d\phi_+}{dx} - \mu \frac{d\phi_-}{dx} + Q = 0 \quad \text{at} \quad x = x_o \tag{4.5}$$

The second condition follows from the requirement that the solution must be continuous everywhere, including the point $x = x_o$,

$$\phi_+ = \phi_- \quad \text{at} \quad x = x_o. \tag{4.6}$$

It is easy to see that the solutions for problems (4.3) and (4.4) are of the form

$$\phi_+ = C_+ \quad \exp \quad \{-\sqrt{\sigma/\mu}(x-x_o)\},$$
$$\phi_- = C_- \quad \exp \quad \{-\sqrt{\sigma/\mu}(x_o-x)\} \tag{4.7}$$

Substitution of these expressions into Eqs.(4.5) and (4.6) yields a set of linear equations for the coefficients C_+ and C_-; the solution is

$$C_+ = C_- = \frac{Q}{2\sqrt{\mu\sigma}}.$$

Thus, the solution of problem (4.1) is of the form

$$\phi(x) = \frac{Q}{2\sqrt{\sigma\mu}} \begin{cases} \exp \quad \{-\sqrt{\sigma/\mu}(x-x_o)\} & \text{for } x \geq x_o \\ \exp \quad \{-\sqrt{\sigma/\mu}(x_o-x)\} & \text{for } x \leq x_o \end{cases} \tag{4.8}$$

The graph of the function $\phi(x)$ is given in figure 1.1. It shows that the diffusion

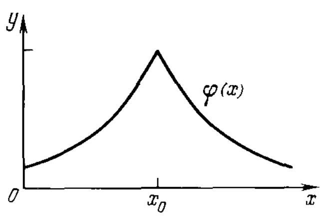


FIGURE 1.1.

process results in the distribution which falls exponentially and symmetrically in both directions from the source at $x = x_o$. It is a simple matter to verify that

$$\int_{-\infty}^{\infty} \phi\ (x)\ dx = \frac{Q}{\sigma}.$$

We now turn to a more interesting case where the air stream velocity is non-zero. Suppose that it is constant and positive. Then we have the differential equation

$$u \frac{d\phi}{dx} + \sigma\phi = \mu \frac{d^2\phi}{dx^2} + Q\delta\ (x - x_o) \tag{4.9}$$

for all x, $-\infty < x < \infty$. Just like the preceding case, Eq.(4.9) with the appropriate condition at infinity is reduced to a pair of problems

$$\begin{aligned} &\mu \frac{d^2\phi_+}{dx^2} - u \frac{d\phi_+}{dx} - \sigma\phi_+ = 0, \\ &\phi_+ = 0 \quad \text{for} \quad x \to \infty; \end{aligned} \tag{4.10}$$

$$\begin{aligned} &\mu \frac{d^2\phi_-}{dx^2} - u \frac{d\phi_-}{dx} - \sigma\phi_- = 0, \\ &\phi_- = 0 \quad \text{for} \quad x \to -\infty. \end{aligned} \tag{4.11}$$

The solutions of these problems are coupled, as before, by the boundary condition at $x = x_o$,

$$\mu \frac{d\phi_+}{dx} - \mu \frac{d\phi_-}{dx} + Q = 0, \quad \phi_+ = \phi_- \quad \text{at} \quad x = x_o \tag{4.12}$$

The solutions of problems (4.10) and (4.11) are represented as

$$\begin{aligned} \phi_+ &= C_+ \exp\left\{-\left(\sqrt{\frac{\sigma}{\mu} + \frac{u^2}{4\mu^2}} - \frac{u}{2\mu}\right)(x-x_o)\right\}, \quad x \geq x_o, \\ \phi_- &= C_- \exp\left\{-\left(\sqrt{\frac{\sigma}{\mu} + \frac{u^2}{4\mu^2}} + \frac{u}{2\mu}\right)(x_o-x)\right\}, \quad x \leq x_o. \end{aligned} \tag{4.13}$$

Substituting these expressions into Eq.(4.12), we get $C_+ = C_- = C$, and

$$C_+ = C_- = C = \frac{Q}{\sqrt{4\sigma\mu+u^2}}.$$

The resulting solution is of the form

$$\phi(x) = \frac{Q}{\sqrt{4\sigma\mu+u^2}} \begin{cases} \exp\left\{-\left(\sqrt{\frac{\sigma}{\mu} + \frac{u^2}{4\mu^2}} - \frac{u}{2\mu}\right)(x-x_o)\right\}, \\ \qquad x \geq x_o, \\ \exp\left\{-\left(\sqrt{\frac{\sigma}{\mu} + \frac{u^2}{4\mu^2}} + \frac{u}{2\mu}\right)(x_o-x)\right\}, \\ \qquad x \leq x_o. \end{cases} \tag{4.14}$$

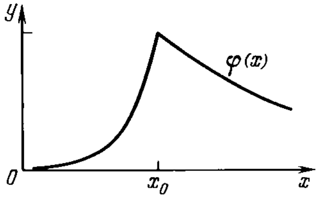


FIGURE 1.2

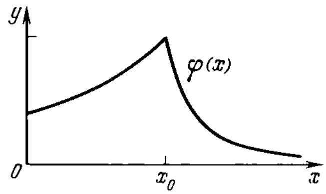


FIGURE 1.3

The graph of the solution is given in figure 1.2. It is clearly seen that for $u > 0$ the left-hand part of the exponent (with respect to the point $x = x_o$) gets nearer to the source, while the right-hand part is pulled from the source and spreading; the effect is evidently caused by substance drift due to the wind with simultaneous diffusion.

A more complicated situation takes place when the wind is blowing for a long time towards positive values of x ($u_1 > 0$) and then changes the direction and is blowing towards negative values ($u_2 < 0$). In this case, we have two solutions

$$\phi_1 = \frac{Q}{\sqrt{4\sigma\mu+u_1^2}} \begin{cases} \exp\left\{-\left(\sqrt{\frac{\sigma}{\mu}+\frac{u_1^2}{4\mu^2}} - \frac{|u_1|}{2\mu}\right)(x - x_o)\right\}, & x \geq x_o, \\ \exp\left\{-\left(\sqrt{\frac{\sigma}{\mu}+\frac{u_1^2}{4\mu^2}} + \frac{|u_1|}{2\mu}\right)(x_o - x)\right\}, & x \leq x_o; \end{cases} \tag{4.15}$$

$$\phi_2 = \frac{Q}{\sqrt{4\sigma\mu+u_2^2}} \begin{cases} \exp\left\{-\left(\sqrt{\frac{\sigma}{\mu}+\frac{u_2^2}{4\mu^2}} + \frac{|u_2|}{2\mu}\right)(x - x_o)\right\}, & x \geq x_o, \\ \exp\left\{-\left(\sqrt{\frac{\sigma}{\mu}+\frac{u_2^2}{4\mu^2}} - \frac{|u_2|}{2\mu}\right)(x_o - x)\right\}, & x \leq x_o. \end{cases} \tag{4.16}$$

If the first period endures for Δt_1 days and the second period ($u_2 < 0$), for Δt_2 days, the average density of the substance is given by the formula

$$\phi(x) = \frac{\Delta t_1}{\Delta t_1+\Delta t_2}\,\phi_1(x) + \frac{\Delta t_2}{\Delta t_1+\Delta t_2}\,\phi_2(x). \tag{4.17}$$

Solution (4.17) is shown schematically in figure 1.3. Note that we have used the direct simulation method when the transient processes are not taken into account.

Finally, let us consider the statistical model where the wind is also described statistically. Let the wind velocity be

$$u(\xi) = \bar{u} p(\xi), \tag{4.18}$$

where ξ is a random quantity in the unit interval, $0 \leq \xi \leq 1$, and $p(\xi)$ is the probability density normalized to unity, i.e. $\int_0^1 p(\xi)\, d\xi = 1$. If the air streams follow the wind immediately, then by analogy with the preceding case we can write the solution of problem (4.9), under condition (4.18), in the form of the integral with respect to the random variable

$$\phi(x) = \frac{Q}{2\mu} \int_0^1 \frac{w(x-x_o,\ u(\xi))}{\sqrt{\frac{\sigma}{\mu} + \frac{u^2(\xi)}{4\mu^2}}}\, d\xi; \tag{4.19}$$

where

$$w(x - x_o,\ u(\xi)) = \begin{cases} \exp\left\{-\left(\sqrt{\frac{\sigma}{\mu} + \frac{u^2(\xi)}{4\mu^2}} - \frac{u(\xi)}{2\mu}\right)(x - x_o)\right\}, & x \geq x_o, \\ \exp\left\{-\left(\sqrt{\frac{\sigma}{\mu} + \frac{u^2(\xi)}{4\mu^2}} + \frac{u(\xi)}{2\mu}\right)(x_o - x)\right\}, & x \leq x_o. \end{cases} \tag{4.20}$$

For each fixed value of x, the integral in Eq.(4.19) is calculated by the Monte Carlo method.

1.5. Transport and Diffusion of Heavy Aerosols

Heavy aerosols are of special interest for problems relevant to the local environmental pollution. Propagating in the atmosphere, heavy aerosols are diffusing and sinking to the soil under the action of gravity. The sinking velocity is calculated from the Stokes problem; it is a constant vector directed downwards. So, if we denote by $\bar{w}_g$ the absolute value of the particle velocity due to gravity, the new term, $w_g\, \partial\phi/\partial z$, appears in the aerosol transport equations, and the transport and diffusion problem of Eq.(3.27) takes the form

$$\begin{gathered} \frac{\partial\phi}{\partial t} + \frac{\partial u\phi}{\partial x} + \frac{\partial v\phi}{\partial y} + \frac{\partial(w-\bar{w}_g)\phi}{\partial z} + \sigma\phi = \frac{\partial}{\partial z}\nu\frac{\partial\phi}{\partial z} + \mu\,\Delta\phi + f, \\ \phi = \phi_o \quad \text{at} \quad t = 0, \\ \phi = 0 \quad \text{on} \quad \textstyle\sum, \\ \partial\phi/\partial z = \alpha\phi \quad \text{on} \quad \textstyle\sum_o, \\ \phi = 0 \quad \text{on} \quad \textstyle\sum_H. \end{gathered} \tag{5.1}$$

Let us determine the amount of aerosol deposited during the time interval $0 \leqq t \leqq T$ upon an area $\sum_i \subset \sum_o$ on the plane $z = 0$. For this purpose, we integrate Eq.(5.1) with respect to z over the interval $0 \leqq z \leq H$. Using the notation

$$\int_0^H \phi \, dz = \overline{\phi}, \qquad \int_0^H f dz = F,$$

and assuming that u and v do not depend on z in the "active" zone, we get the equation

$$\frac{\partial \overline{\phi}}{\partial t} + \frac{\partial u\overline{\phi}}{\partial x} + \frac{\partial v\overline{\phi}}{\partial y} + \sigma\overline{\phi} = \mu\Delta\overline{\phi} - (\overline{w}_g + \nu\alpha)\, \phi_g + F, \tag{5.2}$$

where $\phi_g = \phi|_{z=0}$. In the derivation of Eq.(5.2) we have used the conditions

$$w = 0 \quad \text{at} \quad z = 0 \quad \text{and} \quad z = H,$$

$$\partial\phi/\partial z = \alpha\phi \quad \text{at} \quad z = 0,$$

as well as another condition, natural for the case in view,

$$\phi \to 0, \quad \text{as} \quad z \to H.$$

It is seen from Eq.(5.2) that the amount of aerosol in the atmosphere above the point (x, y) decreases by $(\overline{w}_g + \nu\alpha)\, \phi_g$ per unit time period. Here $\overline{w}_g \phi_g$ is the fraction of the aerosol deposit due to the particle free fall under the action of gravity, and $\nu\alpha\, \phi_g$ is the deposit due to the turbulent exchange motion in the layer adjacent to the earth's surface. If $\overline{w}_g \ll \nu\alpha$, one can neglect the term containing $\overline{w}_g$ in Eq.(5.1). If, however, $\overline{w}_g$ is comparable with or exceeds $\nu\alpha$, one should consider problem (5.1), instead of problem given by Eq.(3.27).

Two functionals are, as a rule, used in the problems considered. First, the total amount of aerosol in a given domain G_i,

$$J_i = \frac{1}{T} \int_0^T dt \int_{G_i} \phi \, dG, \tag{5.3}$$

Second, the total amount of aerosol deposited onto the area $\sum_i$ at the bottom of a cylindrical domain G,

$$J_i = a \int_0^T dt \int_{\Sigma_i} \phi_g \, d\sum. \tag{5.4}$$

The constant a is related to the gravitational and diffusion mechanism of aerosol deposition. In view of the above discussion we have

$$a = \overline{w}_g + \nu\alpha . \tag{5.5}$$

Thus, we have defined the main functionals.

In the sequel we will not draw special attention to the case of heavy aerosols; one should, however, bear in mind that if the gravitational fall is appreciable the problem should be modified to include the results presented in this section. This topic hardly deserves special consideration, for the necessary modification is trivial.

1.6. The Structure and Simulation of Turbulent Motions in the Atmosphere

It is quite important to reconcile the advective and convective transport processes with substance diffusion processes, when investigating the propagation of passive impurities in the atmosphere. A correct combined model taking into account both phenomena would, probably, provide us with an adequate description of the physical processes underlying impurity propagation in the atmosphere. An incorrect or, to be more precise, an incompatible account for both types of the processes may lead to large errors. Now we are going to concentrate on a consisten combination of the advective-convective transport and diffusion.

Suppose we deal with short-range transport processes of specific times of a few hours. In this case,one can neglect the variability of the meteorological conditions, regarding them as stable, in the first approximation; this means that u, v, and w are constant. If the problem of substance propagation from a source is solved with no account for diffusion, we obtain a single trajectory along which the impurity is transferred. This approach is, of course, in contradiction with the essence of the physical process. As the substance experiences spreading all the way from its source along the trajectory, we do not deal, in fact, with a single trajectory, but with a whole region where the concentration of the polluting aerosol is non-zero. What are the factors governing the smearing of the distribution? First, it is short-range fluctuations of the wind velocity inherent in the stochastic nature of the atmospheric motions. Measuring the divergence cone and using the solutions of model problems, one can determine the diffusion coefficients pertaining to the motions of the space-time scale considered. To make this point clear, we shall analyse the following example.

Suppose substance transport is a two-dimensional process described by the equation

$$u \frac{\partial \phi}{\partial x} + v \frac{\partial \phi}{\partial y} - \mu \Delta \phi = Q\delta\ (\underline{r} - \underline{r}_o), \tag{6.1}$$

where u and v are the velocity components regarded, for simplicity, constant, and μ is the diffusion coefficient to be determined. For an infinite domain the solution of Eq.(6.1) is

$$\phi = \frac{Q}{2\pi\mu} \exp\left\{\frac{u(x-x_o) + v(y-y_o)}{2\mu}\right\} K_o\left(\frac{\sqrt{u^2+v^2}}{2\mu}\,|\underline{r} - \underline{r}_o|\right), \qquad (6.2)$$

where $K_o(x)$ is the McDonald function

$$K_o(x) = \int_0^\infty e^{-x \operatorname{ch} y}\, dy, \qquad x > 0$$

Perform the coordinate transformation, so that the origin is put at the source, $\underline{r}_o$, and the x-axis is directed along the velocity vector $\underline{u}$. Then the solution takes the form,

$$\phi = \frac{Q}{2\pi\mu} \exp\left\{\frac{\tilde{u}x}{2\mu}\right\} K_o\left(\frac{\tilde{u}}{2\mu}\,|\underline{r}|\right), \qquad (6.3)$$

where $\tilde{u} = (u^2 + v^2)^{\frac{1}{2}}$.

Now, let the divergence cone of the substance distribution have the width $2y_1$ at a distance x_1 from the exhaust point (figure 1.4). Assuming that the

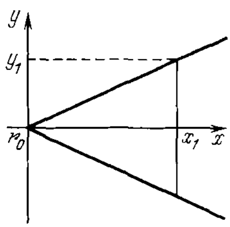


FIGURE 1.4

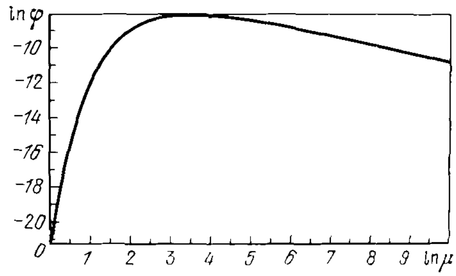


FIGURE 1.5

distance x_1 is large enough to use the asymptotics of the function $K_o(x)$ and that the accuracy of measuring the impurity density in the divergence cone is about ε, we obtain the equation for determining the coefficient μ

$$\phi\,(x_1,\, y_1,\, \mu) = \varepsilon, \qquad (6.4)$$

or, explicitly,

$$\frac{Q}{2\sqrt{\pi\mu(x_1^2+y_1^2)}} \exp\left\{\frac{\tilde{u}}{2\mu}\left(x_1 - \sqrt{x_1^2 + y_1^2}\right)\right\} = \varepsilon. \qquad (6.5)$$

The graphical solution of problem (6.5) is presented in figure 1.5.

Next, we shall consider a transport process with a time scale of several days (an intermediate-range process). Using a similar procedure, averaging the weather factors, with due regard to their type, over the given time scale, and neglecting the diffusion processes, we obtain an averaged trajectory. Evidently, this solution does not describe the physical nature of impurity propagation, as the given mean interval consists of a set of ensembles of transport mesoprocesses with specific time periods of several hours, within which they can be considered as weakly variable. Meanwhile, the set of such mesoprocesses does determine their variations during several days.

If we know the types of mesoprocesses and wind variations during several days, we can solve the corresponding mesoscale transport problems, determine the divergence cones for the polluting substance, and perform statistical averaging over the ensemble of mesoprocesses. As a result, we obtain the substance distribution in the transport process with specific time scales of several days. The solution of this combined problem can be compared with the actual cloud shape, as observed experimentally. Performing the analysis, one gets an impression on how adequate is the description based on the set of typical mesoprocesses for understanding the physical nature of the phenomenon simulated.

Clearly, in this case there is no need to introduce the macro-diffusion coefficient; it is sufficient to have information on the statistical nature of the mesoprocesses which constitute the overall transport process. The macro-diffusion approximation is, nevertheless, useful in some cases. Let us formally apply the diffusion equation to describe impurity propagation,

$$\frac{\partial \phi}{\partial t} + \operatorname{div} \underline{u}\, \phi + \sigma\phi - \mu\Delta\phi = f. \tag{6.6}$$

Assuming that the vector $\underline{u}$ is the result of averaging over several days and considering the coefficient μ as unknown, we can use the methods of perturbation theory to find the value of μ which would lead to the best value, in a certain sense, of some functional. It is possible, however, that even though the functional is obtained correctly with the chosen value of μ, the differential field of solutions for the direct problem (6.6) may differ considerably from the actual one (or from the model field calculated using the set of the meso-problems). Hence, if we are interested in a single fixed functional, the model for substance transport with the chosen diffusion coefficient will be a suitable tool for the investigation.

If we are interested in more subtle characteristics of the pollution field or in various functionals, it would be better to simulate the process by a set of small-scale models. Therefore, while solving optimization problems analysed in the present book we shall proceed from the assumption that the model can be used in the macro-diffusion process approximation. Meanwhile, to handle the subject in greater detail and test the reliability of the results obtained it is required to find solutions for a set of problems corresponding to short-range fluctuations.

The mathematical presentation of the formalism is as follows. We describe substance transport by the elementary diffusion equation

$$\frac{\partial\phi}{\partial t} + u\frac{\partial\phi}{\partial x} + v\frac{\partial\phi}{\partial y} + w\frac{\partial\phi}{\partial z} = \mu'\Delta\phi + \nu'\frac{\partial^2\phi}{\partial z^2} + Q\delta(\underline{r} - \underline{r}_o). \qquad (6.7)$$

We assume here that u, v, and w are functions given by

$$u = \bar{u} + u', \quad v = \bar{v} + v', \quad w = \bar{w} + w'; \qquad (6.8)$$

where u', v', w' are the components of the velocity vector varying during specific times of a few hours; these components are deviations from the main stream $\bar{u}$, $\bar{v}$, $\bar{w}$ at a rate known a priori; μ' and ν' are the diffusion coefficients corresponding to the meso-processes. The problem is treated as periodic with a period T typical of the process characteristic scale. The boundary conditions are

$$\begin{aligned} \partial\phi/\partial z &= 0 \quad \text{at} \quad z = H, \\ \partial\phi/\partial z &= \alpha\phi \quad \text{at} \quad z = 0, \\ \phi &\to 0 \quad \text{as} \quad x, y \to \pm\infty \end{aligned} \qquad (6.9)$$

All statistical features of the meso-processes are taken into account by solving the set of problems stated in this way. Thus, we need to simulate the behaviour of the functions u', v', and w'.

Since the process is linear, in the simulation of these quantities care should be taken of their recurrence corresponding to their action during time intervals which are longer than T. The final result must be averaged over the time interval $[0, T]$.

Thus, all the models considered in the book can naturally be generalized to account more accurately for the stochastic structure of the input data.

This reasoning can be illustrated by a simple example. Let substance transport be described by Eq.(6.1), as it was discussed above, and the solution is (6.2). Write the functions u and v as

$$u = \bar{u} + u'(\alpha), \quad v = \bar{v} + v'(\alpha), \qquad (6.10)$$

where the deviations u' and v' from the main stream, given by the components $\bar{u}$ and $\bar{v}$, depend on the parameter α and are treated as random fluctuations of a quantity restricted a priori. Substituting expressions (6.10) into Eq.(6.2) we have

$$\phi\ (x,\ y,\ \alpha) = \frac{Q}{2\pi\mu} \exp\left\{\frac{\bar{u}(x - x_o) + \bar{v}(y - y_o)}{2\mu}\right\} \cdot$$

$$\cdot \exp\left\{\frac{u'(\alpha)(x - x_o) + v'(\alpha)(y - y_o)}{2\mu}\right\} \cdot \tag{6.11}$$

$$\cdot\ K_o\left(\frac{\sqrt{(\bar{u} + u'(\alpha))^2 + (\bar{v} + v'(\alpha))^2}}{2\mu}\ |\underline{r} - \underline{r}_o|\right).$$

The function $\phi(x,\ y,\ \alpha)$ is a family of possible realizations of the aerosol cloud, depending on the statistical structure of the fluctuations. The isolines for the function ϕ, averaged over the parameter α under the assumption that the fluctuation distribution is normal, are presented in figure 1.6 (dashed lines). For comparison, the figure also shows isolines of the function ϕ for $u' = v' = 0$ (solid lines).

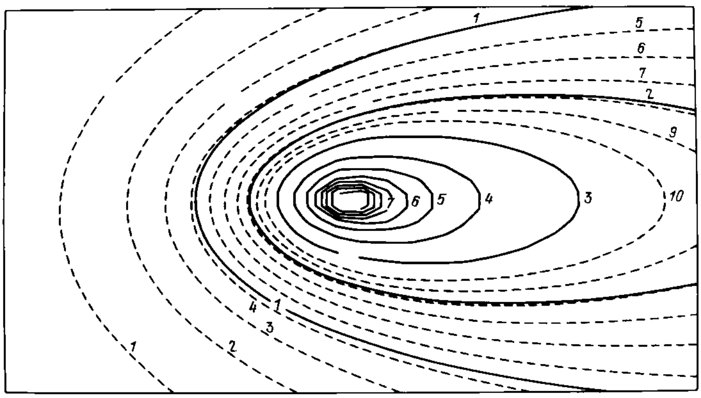


FIGURE 1.6

In the investigation of global processes with characteristic time scales of several weeks or even months the methods suggested above enable the construction of a hierarchy of the models which can be identified, say, by means of pictures made from a spacecraft.

Chapter 2. ADJOINT EQUATIONS OF TRANSPORT AND DIFFUSION

The interest in adjoint equations, as applied to particular functionals of problems in mathematical physics, arose long ago. But only on rare occasions adjoint equations have been instrumental in solving these problems. The construction of adjoint problems was highly stimulated by perturbation theory, since its correct formulation involves both basic and adjoint problems. As regards problems on searching for one linear functional or another, the adjoint formulation, reflecting the duality principle, also provides algorithms which prove to be optimal, under specific conditions, both for analysis of problems and for their implementation. Such applications of adjoint equations will be exemplified in this and subsequent chapters.

2.1. An Adjoint Equation for a Simple Diffusion Equation

Consider a simple diffusion equation

$$\frac{\partial \phi}{\partial t} + \sigma\phi - \mu \frac{\partial^2 \phi}{\partial x^2} = Q\delta\ (x - x_o) \tag{1.1}$$

with the condition

$$\phi = \phi_o \quad \text{for } t = 0, \tag{1.2}$$

(ϕ_o is a given function of x) and under the assumption that the solution ϕ is finite in the entire range of x ($-\infty < x < \infty$).

First, we define the space of functions ϕ, on which a solution for the problem will be sought. Suppose it is the space of functions which are t- and x-differentiable and have a generalized second derivative with respect to x. We shall assume these functions to be finite in the entire range $-\infty < x < \infty$ and rapidly decreasing when $x \to \pm\infty$, thereby ensuring a quadratic summation, i.e.

$$\int_0^T dt \int_{-\infty}^{\infty} \phi^2 dx < \infty.$$

Let us write Eq.(1.1) formally as

$$L\phi = f, \tag{1.3}$$

where $$L = \frac{\partial}{\partial t} + \sigma - \mu \frac{\partial^2}{\partial x^2}, \quad f = Q\delta\ (x - x_o).$$

We will consider that ϕ is a Gilbert space with the scalar product

$$(g, h) = \int_0^T dt \int_{-\infty}^{\infty} gh\ dx.$$

We now proceed to constructing an adjoint problem. To this end, we multiply (1.1) by some function ϕ^*, whose properties will be clarified later on, and integrate the result over time and space

$$\int_0^T dt \int_{-\infty}^{\infty} \phi^* \left(\frac{\partial \phi}{\partial t} + \sigma\phi - \mu \frac{\partial^2 \phi}{\partial x^2} \right) dx = Q \int_0^T dt \int_{-\infty}^{\infty} \phi^* \delta(x-x_o)\ dx. \tag{1.4}$$

Let us transform the left-hand side so that the function ϕ appears under the integral out of the parenthesis, whereas the differential relation containing ϕ^* appears in the parenthesis. For this purpose, we integrate by parts to obtain

$$\int_0^T dt \int_{-\infty}^{\infty} \phi^* \frac{\partial \phi}{\partial t}\, dx = \int_{-\infty}^{\infty} \phi\phi^*\, dx \Bigg|_{t=0}^{t=T} - \int_0^T dt \int_{-\infty}^{\infty} \phi \frac{\partial \phi^*}{\partial t}\, dx, \tag{1.5}$$

$$\begin{aligned}\int_0^T dt \int_{-\infty}^{\infty} \phi^* \frac{\partial^2 \phi}{\partial x^2}\, dx &= \int_0^T \left(\phi^* \frac{\partial \phi}{\partial x} - \phi \frac{\partial \phi^*}{\partial x}\right) dt \Bigg|_{x=-\infty}^{x=\infty} + \\ &+ \int_0^T dt \int_{-\infty}^{\infty} \phi \frac{\partial^2 \phi^*}{\partial x^2}\, dx.\end{aligned} \tag{1.6}$$

Substitution of (1.5) and (1.6) into (1.4) yields

$$\begin{aligned}&\int_0^T dt \int_{-\infty}^{\infty} \phi \left(-\frac{\partial \phi^*}{\partial t} + \sigma\phi^* - \mu \frac{\partial^2 \phi^*}{\partial x^2}\right) dx + \int_{-\infty}^{\infty} \phi\phi^*\, dx \Bigg|_{t=0}^{t=T} - \\ &- \mu \int_0^T \left(\phi^* \frac{\partial \phi}{\partial x} - \phi \frac{\partial \phi^*}{\partial x}\right) dt \Bigg|_{x=-\infty}^{x=\infty} = Q \int_0^T \phi^* (x_o, t)\, dt.\end{aligned} \tag{1.7}$$

Assume that

$$\phi^* = 0 \quad \text{for} \quad x \to \pm\infty \tag{1.8}$$

Then relation (1.7) is simplified as follows

$$\begin{aligned}&\int_0^T dt \int_{-\infty}^{\infty} \phi \left(-\frac{\partial \phi^*}{\partial t} + \sigma\phi^* - \mu \frac{\partial^2 \phi^*}{\partial x^2}\right) dx + \int_{-\infty}^{\infty} (\phi_T\phi_T^* - \phi_o\phi_o^*)\, dx = \\ &= Q \int_0^T \phi^* (x_o, t)\, dt.\end{aligned} \tag{1.9}$$

We now assume that ϕ^* satisfies the equation

$$-\frac{\partial \phi^*}{\partial t} + \sigma\phi^* - \mu \frac{\partial^2 \phi^*}{\partial x^2} = p \tag{1.10}$$

with the initial data

$$\phi^* = 0 \quad \text{for} \quad t = T \tag{1.11}$$

and boundary conditions (1.8). Here p is a function of x and t to be determined. This problem will be referred to as an *adjoint problem*. With due account for (1.10), we reduce (1.9) to the form

$$\int_0^T dt \int_{-\infty}^{\infty} p\phi\, dx = Q \int_0^T \phi^*(x_o, t)\, dt + \int_{-\infty}^{\infty} \phi(x, 0)\, \phi^*(x, 0)\, dx. \tag{1.12}$$

Let

$$J = \int_0^T dt \int_{-\infty}^{\infty} p\phi\, dx \tag{1.13}$$

be a linear functional of ϕ which is to be calculated from the solution of basic problem (1.1), (1.2). It follows from (1.12) that this functional can also be evaluated by solving adjoint problem (1.10), (1.11), so that

$$J = Q \int_0^T \phi^*(x_o, t)\, dt + \int_{-\infty}^{\infty} \phi(x, 0)\, \phi^*(x, 0)\, dx. \tag{1.14}$$

This is precisely the *duality principle.*

Consider the problem of functionals. Functional (1.13) admits a variety of physical meanings. Let

$$p(x, t) = \delta(x - \xi)\, \delta(t - \tau). \tag{1.15}$$

Substituting (1.15) into (1.13), we derive the functional

$$J = \phi(\xi, \tau), \tag{1.16}$$

i.e. the value of the solution at the point $x = \xi$, $t = \tau$. It should be noted that the same value will be obtained by (1.14) if p in adjoint problem (1.10), (1.11) is given by expression (1.15).

Consider another case, where it is necessary to find the total amount of substance in the interval $a \leqq x \leqq b$. In this case, the function $p(x,t)$ will be taken in the form

$$p(x, t) = \begin{cases} 1, & x \in [a, b], \\ 0, & x \notin [a, b]. \end{cases} \tag{1.17}$$

Substituting (1.17) into (1.13), we obtain

$$J = \int_0^T dt \int_a^b \phi\, dx. \tag{1.18}$$

The same functional can be derived using (1.14).

Next, suppose that we measure the total amount of substance ϕ on [a, b] during the time interval $[\tau_1, \tau_2]$. Suppose also that the resolution of the instrument depends on x and y, i.e. the instrumental characteristic is fitted by the function $x = V(t)\,\chi(x)$. It is necessary to compare the measured and calculated functionals. Then, choosing the function p(x, t) in the form

$$p(x, t) = \begin{cases} V(x)\,\chi(x), & x \in [a,b] \text{ and } t \in [\tau_1, \tau_2], \\ 0, & x \notin [a, b] \text{ or } t \notin [\tau_1, \tau_2], \end{cases} \tag{1.19}$$

we arrive at the functional

$$J = \int_{\tau_1}^{\tau_2} dt \int_a^b \chi(x)\, V(x)\, \phi dx. \tag{1.20}$$

The set of possible functionals could be extended. It is important to note that in this way we can represent any linear functional of a solution and, hence, construct its own adjoint problem.

Thus, if we consider some functionals of a solution rather than the solution itself,we can formulate a particular adjoint problem for each of them. It seems at first glance that the most natural way is to solve the basic problem and, using (1.13), calculate any functional. Sometimes, this approach is most favourable, indeed. Yet, adjoint equations are quite indispensable when we plan aerosol-emitting plants, or estimate the functional sensitivity to the ambient parameter variations or solve other similar problems. Consider, for example, the following problem.

Let the process of pollutant propagation in the region $G = (-\infty, \infty)$ be described by (1.1). It is necessary to find such a region ω G that the functional of the form (1.16) - the amount of pollutant at the point $x = \xi_1$ at the moment $t = \tau_1$ - does not exceed a given constant C (the pollution source of capacity Q is assumed to be located at the point $x_o \in \omega$). In this problem the initial value of the function ϕ can be taken zero

$$\phi = 0 \quad \text{for} \quad t = 0 \tag{1.21}$$

The problem can be solved in two ways at least. The first way is to solve repeatedly Eq.(1.1) for different values of $x_o \in G$, to evaluate functional (1.16), and, hence, to determine the region in question ω. This way, however, requires the solution of a great number of problems of the type (1.1) and is not likely to be practicable.

The other approach is based on a dual representation of functional (1.16) and the use of a solution of the adjoint equation. For our problem, this representation is

$$J = Q \int_0^T \phi^*(x_o, t)\, dt, \tag{1.22}$$

where ϕ^* is the solution for the equation

$$-\frac{\partial \phi^*}{\partial t} + \sigma\phi^* - \mu \frac{\partial^2 \phi^*}{\partial x^2} = \delta\,(x - \xi_1)\ \delta(t - \tau_1) \tag{1.23}$$

with the initial data

$$\phi^* = 0 \quad \text{at} \quad t = T. \tag{1.24}$$

Thus, proceeding from dual representation (1.22) of functional (1.16), we can select a permissible pollution-source region $\omega \subset G$ by solving the problem adjoint to (1.1) only once.

Let us find the function ϕ^* which fits (1.23), (1.24). Introducing a new variable

$$t_1 = T - t, \qquad t_1 \in [0, T]. \tag{1.25}$$

we reduce problem (1.23), (1.24) to the problem

$$\begin{gathered} \frac{\partial \phi^*}{\partial t_1} + \sigma\phi^* - \mu \frac{\partial^2 \phi^*}{\partial x^2} = \delta\,(x - \xi_1)\ \delta(T - t_1 - \tau_1), \\ \phi^* = 0 \quad \text{at} \quad t_1 = 0. \end{gathered} \tag{1.26}$$

It is noteworthy that the operator of problem (1.26) coincides formally with the operator of problem (1.1). The solution for problem (1.26) is given by

$$\begin{gathered} \phi^*\,(x, t_1) = \int_0^{t_1} \int_{-\infty}^{\infty} \tilde{\phi}\,(x - \xi, t_1 - \tau)\delta(\xi - \xi_1)\delta(T - \tau - \tau_1)\cdot \\ \cdot\, d\xi\, d\tau, \end{gathered} \tag{1.27}$$

where $\tilde{\phi}\,(x, t)$ is the fundamental solution for the operator of problem (1.26)

$$\tilde{\phi}\,(x, t) = \frac{\theta(t)}{2\sqrt{\mu\pi t}}\ \exp\ \left\{ - \left(\sigma t + \frac{x^2}{4\mu t} \right) \right\};$$

θ is the *Heaviside function*

$$\theta\,(t) = \begin{cases} 0, & t \leqq 0, \\ 1, & t > 0. \end{cases}$$

Referring again to the previous variables we obtain

$$\phi^*(x,\ t) = \begin{cases} \dfrac{1}{2\sqrt{\mu\pi(\tau_1-t)}} \exp\left\{ -\left[\sigma(\tau_1-t) + \dfrac{(x-\xi)^2}{4\mu(\tau_1-t)} \right]\right\} & \text{for } t \in [0,\ \tau_1] \\ 0 & \text{for } t \in [\tau_1,\ T] \end{cases} \tag{1.28}$$

In accordance with (1.27), dual representation (1.22) of functional (1.16) is

$$J = \frac{Q}{2\sqrt{\mu\pi}} \int_0^{\tau_1} \frac{\exp\left\{-\left[\sigma(\tau_1-t) + \dfrac{(x_o-\xi_1)^2}{4\mu(\tau_1-t)} \right]\right\}}{\sqrt{\tau_1 - t}}\, dt \tag{1.29}$$

or

$$J = \frac{Q}{2\sqrt{\mu\pi}} \sum_{j=0}^{K-1} \frac{\exp\left\{ -\left[\sigma(\tau_1-t_j) + \dfrac{(x_o-\xi_1)^2}{4\mu(\tau_1-t_j)} \right]\right\}}{\sqrt{\tau_1-t_j}}\, \Delta t + O(\Delta t), \tag{1.30}$$

where $t_j = j\Delta t$, $\Delta t = \tau_1/K$.

Consider functional (1.29) as a function of $J(x_o)$ for $x_o \in G$ and plot this function. A permissible pollution-source region ω is found from the inequality $J(x) < C$. The above example is solved graphically in figure 2.1, where the region ω is denoted by a double line on the abscissa.

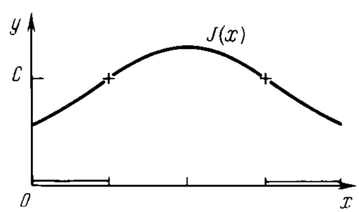


FIGURE 2.1

Pollutant distribution for any particular $x_o \in \omega$ is determined from the solution of problem (1.1), (1.2), which is written, with due reference to the above, as follows

$$\phi(x,t) = \frac{Q}{2\sqrt{\mu\pi}} \sum_{j=0}^{K-1} \frac{\exp\left\{-\left[\sigma\ (t-t_j) + \dfrac{(x-x_o)^2}{4\mu(t-t_j)} \right]\right\}}{\sqrt{t-t_j}}\, \Delta t + O(\Delta t). \tag{1.31}$$

The isolines of the function ϕ (x, t) are shown in figure 2.2.

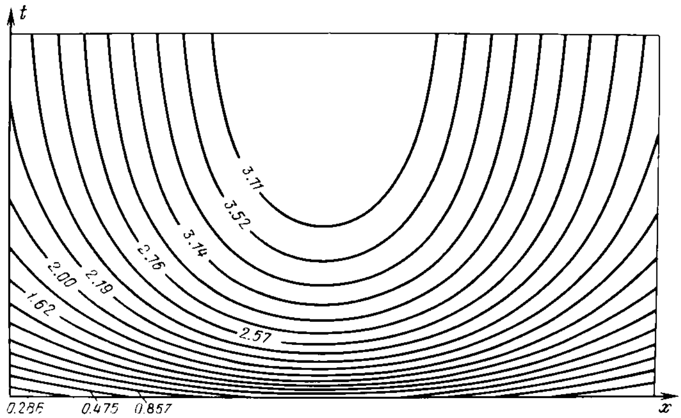


FIGURE 2.2

Thus, we have considered a non-stationary problem. If the basic problem is stationary,

$$\mu \frac{d^2\phi}{dx^2} - \sigma\phi = Q\delta\ (x - x_o), \qquad \phi = 0 \text{ when } x \to \pm\infty \tag{1.32}$$

the adjoint problem is also stationary

$$\mu \frac{d^2\phi^*}{dx^2} - \sigma\phi^* = p(x), \qquad \phi^* = 0 \text{ when } x \to \pm\infty \tag{1.33}$$

Clearly, the linear functional J in this case is of the form

$$J = \int_{-\infty}^{\infty} p\ (x)\phi\ dx \tag{1.34}$$

or

$$J = Q\ \phi^*\ (x_o). \tag{1.35}$$

If the function p(x) is taken as

$$p(x) = \delta\ (x - \xi), \tag{1.36}$$

the solution of adjoint problem (1.22), just as (4.8) of 1.4 is of the form

$$\phi^*(x,\ \xi) = \frac{1}{2\mu\sqrt{\sigma/\mu}} \begin{cases} \exp\ \{-\sqrt{\sigma/\mu}(x-\xi)\}, & x \geqq \xi, \\ \exp\ \{-\sqrt{\sigma/\mu}(\xi-x)\}, & x \leqq \xi. \end{cases} \tag{1.37}$$

If we seek a solution for $p(x)$ other than (1.36), we have

$$\phi^*(x) = \int_{-\infty}^{\infty} p(x)\ \phi^*\ (x,\ \xi)\ d\xi, \tag{1.38}$$

Here $\phi^*\ (x,\ \xi)$ is the fundamental solution (1.37). In particular, if the function $p(x)$ is taken in the form given by (1.17), we obtain

$$\phi^*(x) = \int_a^b \phi^*\ (x,\ \xi)\ d\xi.$$

Substitution of (1.37) into this expression yields

$$\phi^*(x) = \frac{1}{2\sigma}\left(2 - \exp\ \{-\sqrt{\sigma/\mu}(b-x)\} - \exp\ \{-\sqrt{\sigma/\mu}(x-a)\}\right). \tag{1.39}$$

This function is plotted in figure 2.3.

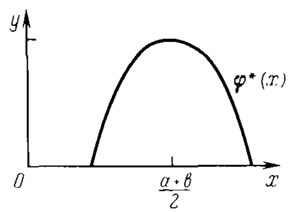


FIGURE 2.3

We now consider substance transport by diffusion with due account for advection. In this case,the basic problem is

$$\begin{gathered} \frac{\partial\phi}{\partial t} + u\,\frac{\partial\phi}{\partial x} + \sigma\phi - \mu\,\frac{\partial^2\phi}{\partial x^2} = Q\delta(x - x_o), \\ \phi = \phi_o \quad \text{at} \quad t = 0 \\ \phi = 0 \quad \text{as} \quad x \to \pm\,\infty \end{gathered} \tag{1.40}$$

Similarly to the foregoing examination, the adjoint problem is of the form

$$\begin{gathered} -\frac{\partial\phi^*}{\partial t} - u\,\frac{\partial\phi^*}{\partial x} + \sigma\phi^* - \mu\,\frac{\partial^2\phi^*}{\partial x^2} = p, \\ \phi^* = 0 \quad \text{for} \quad t = T,\ x \to \pm\,\infty. \end{gathered} \tag{1.41}$$

The basic functional of the problem is

$$J = \int_0^T dx \int_{-\infty}^{\infty} p\phi \; dx, \tag{1.42}$$

and its dual representation is

$$J = Q \int_0^T \phi^* (x_o, t) \; dt + \int_{-\infty}^{\infty} \phi_o \phi^* (x, 0) \; dx. \tag{1.43}$$

Consider another example related to construction planning. Let the propagation to pollutant ϕ in the region G by described by problem (1.40) for $u = \text{const} > 0$ and $\phi_o = 0$. It is necessary to determine a point x_o for locating a pollution source such that

$$\phi(\xi_1, \tau_1) < C, \tag{1.44}$$

$$|x_o - \xi_1| = \min_{x_o \in G}, \tag{1.45}$$

where ξ_1, τ_1, C are given constants.

To solve this problem, we will again employ the dual representation of functional (1.16)

$$J = Q \int_0^T \phi^* (x_o, t) \; dt. \tag{1.46}$$

In this case, ϕ^* is the solution for Eq.(1.41) with the right-hand side of the form given by (1.15). A fundamental solution for the operator of problem (1.41) is obtained by calculating the Fourier transform of the equation

$$\frac{\partial \phi}{\partial t_1} - u \frac{\partial \phi}{\partial x} + \sigma \phi - \mu \frac{\partial^2 \phi}{\partial x^2} = \delta (t_1) \delta(x), \tag{1.47}$$

Here $t_1 = T - t$. Hence, we arrive at

$$\frac{\partial}{\partial t_1} F[\phi] + (iu\xi + \sigma + \mu\xi^2) F[\phi] = \delta(t_1), \tag{1.48}$$

where

$$F[\phi] = \int_{-\infty}^{\infty} \phi(x, t) \; e^{i\xi x} \; dx.$$

The solution of Eq.(1.48) is the function

$$F[\phi]\,(\xi,\ t_1) = \theta(t_1)\ \exp\ \{-(iu\xi + \sigma + \mu\xi^2)\ t_1\}.$$

Performing the inverse Fourier transform we obtain the fundamental solution in question

$$\phi(x,t_1) = \frac{\theta(t_1)}{2\sqrt{\mu\pi t_1}}\ \exp\ \{-\ [\sigma t_1 + \frac{(x+ut_1)^2}{4\mu t_1}\ ]\}. \tag{1.49}$$

Using (1.27) and the above variables, we obtain a solution for the problem, which is adjoint to (1.40), with the right-hand side $p = \delta(x - \xi_1)\delta(t - \tau_1)$

$$\phi^*(x,t) = \begin{cases} \dfrac{1}{2\sqrt{\mu\pi(\tau_1-t)}}\ \exp\ \{-\ [\sigma(\tau_1-t) + \dfrac{(x-\xi_1+u(\tau_1-t))^2}{4\mu(\tau_1-t)}\ ]\}, & t\in [0,\tau_1), \\ 0, \quad t\in [\tau_1,\ T]. \end{cases} \tag{1.50}$$

Substituting (1.50) into (1.46), we derive an expression for the functional studied

$$J = \frac{Q}{2\sqrt{\mu\pi}} \sum_{j=0}^{K-1} \frac{\exp\ \{-\ [\sigma(\tau_1-t_j) + \dfrac{(x_0-\xi_1+u(\tau_1-t_j))^2}{4\mu(\tau_1-t_j)}\ ]\}}{\sqrt{\tau_1-t_j}}\ \Delta t + O(\Delta t), \tag{1.51}$$

Here $t_j = j\Delta t$, $\Delta t = \tau_1/K$.

Similarly to the above procedure, we shall determine the region $\omega\subset G$ in which inequality (1.44) remains valid. The point x_0 is found from condition (1.45). Figure 2.4 is a graphical solution for this problem. Figure 2.5 gives

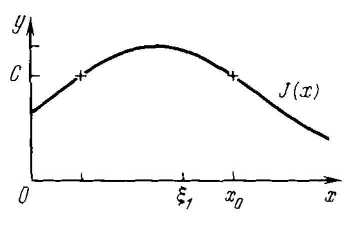


FIGURE 2.4

the isolines of the function $\phi(x,t)$, which are solutions for direct problem (1.40), with x_0 found from the solution of the adjoint problem.

Allowing for the formal coincidence of the operators of problems (1.40) and (1.47), we can express the function $\phi(x,t)$ analytically as

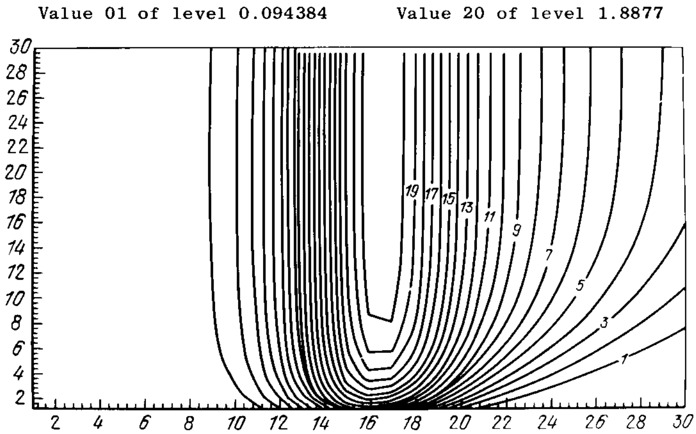


FIGURE 2.5

$$\phi(x,t) = \frac{Q\Delta t}{2\sqrt{\mu\pi}} \sum_{j=0}^{K-1} \frac{\exp\left\{-\left[\sigma(t-t_j) + \frac{(x-x_o-u(t-t_j))^2}{4\mu(t-t_j)}\right]\right\}}{\sqrt{t-t_j}} + O(\Delta t), \tag{1.52}$$

where $K = [t/\Delta t]$.

If problem (1.40) is stationary:

$$u\frac{\partial\phi}{\partial x} + \sigma\phi = \mu\frac{\partial^2\phi}{\partial x^2} + Q\delta(x - x_o), \tag{1.53}$$

$$\phi = 0 \quad \text{when} \quad x \to \pm\infty,$$

it will also generate a stationary adjoint problem

$$-u\frac{\partial\phi^*}{\partial x} + \sigma\phi^* = \mu\frac{\partial^2\phi^*}{\partial x^2} + p(x), \qquad \phi^* = 0 \quad \text{for} \quad x \to \pm\infty. \tag{1.53'}$$

The basic problem (1.53) was solved in 1.4 (see (4.14)).

Let us solve the adjoint problem. To this end, we first find a fundamental solution of (1.53') for $p(x) = \delta(x - \xi)$. Similarly to (4.14), we obtain

$$\phi^*(x,\xi) = \frac{1}{2\mu\sqrt{\frac{\sigma}{\mu} + \frac{u^2}{4\mu^2}}}\begin{cases} \exp\left\{-\left(\sqrt{\frac{\sigma}{\mu} + \frac{u^2}{4\mu^2}} + \frac{u}{2\mu}\right)(x - \xi)\right\}, & x \geq \xi, \\ \exp\left\{-\left(\sqrt{\frac{\sigma}{\mu} + \frac{u^2}{4\mu^2}} - \frac{u}{2\mu}\right)(\xi - x)\right\}, & x \leq \xi. \end{cases} \tag{1.54}$$

Any other solution of (1.53') can be derived from the fundamental solution

$$\phi^* (x) = \int_{-\infty}^{\infty} p(\xi)\, \phi^*(x,\xi)\, d\xi. \tag{1.55}$$

In particular, if p(x) is taken in the form (1.17), then we have

$$\phi^*(x) = \int_a^b \phi^*(x,\xi)\, d\xi. \tag{1.56}$$

Substitution of (1.54) into (1.56) yields

$$\phi^*(x) = \frac{1}{2\mu\sqrt{\frac{\sigma}{\mu} + \frac{u^2}{4\mu^2}}} \left[\frac{1}{\sqrt{\frac{\sigma}{\mu} + \frac{u^2}{4\mu^2}} - \frac{u}{2\mu}} \cdot \right.$$

$$\cdot \left[1 - \exp\left\{- \left(\sqrt{\frac{\sigma}{\mu} + \frac{u^2}{4\mu^2}} - \frac{u}{2\mu} \right) (x - a)\right\}\right] + \tag{1.57}$$

$$\left. + \frac{1}{\sqrt{\frac{\sigma}{\mu} + \frac{u^2}{4\mu^2}} + \frac{u}{2\mu}} \left[1 - \exp\left\{- \left(\sqrt{\frac{\sigma}{\mu} + \frac{u^2}{4\mu^2}} + \frac{u}{2\mu} \right) (b - x)\right\}\right] \right]$$

The function $\phi^*(x)$ is plotted in figure 2.6.

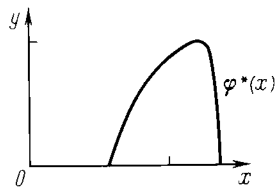


FIGURE 2.6

If we deal with a set of basic stationary problems related to various types of motion at different air stream velocities, we should consider a relevant set of adjoint problems. In this case, the functional in question is obtained either from the basic equations

$$J = \frac{1}{T} \sum_{i=1}^{n} \int_{-\infty}^{\infty} p(x)\, \phi_i(x)\, dx, \tag{1.58}$$

or from the adjoint equations

$$J = \frac{Q}{T} \sum_{i=1}^{n} \phi_i^* (x_o). \tag{1.59}$$

2.2. A General Case of an Adjoint Problem for a Three-Dimensional Region

Consider a general three-dimensional problem

$$\begin{aligned}
&\frac{\partial\phi}{\partial t} + \text{div}\, \underline{u}\phi + \sigma\phi - \frac{\partial}{\partial z}\, \nu\, \frac{\partial\phi}{\partial z} - \mu\Delta\phi = f, \\
&\phi = 0 \quad \text{on } \Sigma \quad \text{for } u_n < 0 \\
&\frac{\partial\phi}{\partial n} = 0 \quad \text{on } \Sigma \quad \text{for } u_n \geq 0 \\
&\frac{\partial\phi}{\partial z} = \alpha\phi \quad \text{on } \Sigma_o \\
&\frac{\partial\phi}{\partial z} = 0 \quad \text{on } \Sigma_H
\end{aligned} \tag{2.1}$$

Let us derive adjoint equations. Assume that the solution for problem (2.1) belongs to the Hilbert space Φ of sufficiently smooth functions, each element of the space being quadratically summable, i.e.

$$\int_0^T dt \int_G \phi^2\, dG < \infty.$$

Multiply Eq.(2.1) by a function ϕ^* and integrate the result over the entire domain of the solution. Then we have

$$\begin{aligned}
&\int_0^T dt \int_G \phi^* \frac{\partial\phi}{\partial t}\, dG + \int_0^T dt \int_G \phi^*\, \text{div}\, \underline{u}\phi dG + \sigma \int_0^T dt \int_G \phi\phi^*\, dG - \\
&- \int_0^T dt \int_G \phi^* \frac{\partial}{\partial z}\, \nu\, \frac{\partial\phi}{\partial z}\, dG - \mu \int_0^T dt \int_G \phi^*\Delta\phi\, dG = \int_0^T dt \int_G \phi^* f\, dG.
\end{aligned} \tag{2.2}$$

Integrating by parts, using the Ostrogradsky-Gauss theorem, and allowing for the relation $\text{div}\, \underline{u} = 0$, we can transform some expressions of (2.2) to the form

$$\int_0^T dt \int_G \phi^* \frac{\partial\phi}{\partial t}\, dG = \int_G \phi^*\phi \quad dG \Big|_{t=0}^{t=T} - \int_0^T dt \int_G \phi\, \frac{\partial\phi^*}{\partial t}\, dG, \tag{2.3}$$

$$\int_0^T dt \int_G \phi^*\, \text{div}\, \underline{u}\phi dG = \int_0^T dt \int_S u_n\, \phi\phi^*\, dS - \int_0^T dt \int_G \phi\, \text{div}\, \underline{u}\phi^*\, dG, \tag{2.4}$$

$$\int_0^T dt \int_G \phi^* \frac{\partial}{\partial z} \nu \frac{\partial \phi}{\partial z} dG = \int_0^T dt \int_{\Sigma_H} \nu\left(\phi^* \frac{\partial \phi}{\partial z} - \phi \frac{\partial \phi^*}{\partial z}\right) d\Sigma -$$
$$- \int_0^T dt \int_{\Sigma_o} \nu\left(\phi^* \frac{\partial \phi}{\partial z} - \phi \frac{\partial \phi^*}{\partial z}\right) d\Sigma + \int_0^T dt \int_G \phi \frac{\partial}{\partial z} \nu \frac{\partial \phi^*}{\partial z} dG, \tag{2.5}$$

$$\mu \int_0^T dt \int_G \phi^* \Delta\phi \, dG = \mu \int_0^T dt \int_\Sigma \left(\phi^* \frac{\partial \phi}{\partial n} - \phi \frac{\partial \phi^*}{\partial n}\right) d\Sigma + \mu \int_0^T dt \cdot$$
$$\cdot \int_G \phi \, \Delta \, \phi^* \, dG. \tag{2.6}$$

Substituting (2.3)-(2.6) into (2.2), we obtain

$$\int_0^T dt \int_G \phi \left(- \frac{\partial \phi^*}{\partial t} - \operatorname{div} \underline{u} \, \phi^* + \sigma\phi^* - \frac{\partial}{\partial z} \nu \frac{\partial \phi^*}{\partial z} - \mu \, \Delta\phi^* \right) dG =$$
$$= \int_0^T dt \int_G \phi^* f \, dt - \int_G \phi_T \phi_T^* \, dG + \int_G \phi_o \phi_o^* \, dG -$$
$$- \int_0^T dt \int_S u_n \phi\phi^* \, dS + \int_0^T dt \int_{\Sigma_H} \nu \left(\phi^* \frac{\partial \phi}{\partial z} - \phi \frac{\partial \phi^*}{\partial z} \right) d\Sigma -$$
$$- \int_0^T dt \int_{\Sigma_o} \nu \left(\phi^* \frac{\partial \phi}{\partial z} - \phi \frac{\partial \phi^*}{\partial z} \right) d\Sigma + \mu \int_0^T dt \int_\Sigma \left(\phi^* \frac{\partial \phi}{\partial n} - \phi \frac{\partial \phi^*}{\partial n} \right) d\Sigma. \tag{2.7}$$

Let us assume that ϕ^* satisfies the equation

$$- \frac{\partial \phi^*}{\partial t} - \operatorname{div} \underline{u} \, \phi^* + \sigma\phi^* - \frac{\partial}{\partial z} \nu \frac{\partial \phi^*}{\partial z} - \mu \, \Delta\phi^* = p, \tag{2.8}$$

and transform the right-hand side of (2.7). For this purpose, we will employ the boundary conditions for the function ϕ as given by (2.1) and the condition that the function ϕ is periodic in time. The function ϕ^* will be also assumed time-periodic with period T. Then we have

$$- \int_G \phi_T \phi_T^* \, dG + \int_G \phi_o \phi_o^* \, dG = 0. \tag{2.9}$$

Since, by the assumption,

$$\phi = 0 \quad \text{on } S, \ \text{if} \ u_n < 0,$$

then

$$\int_0^T dt \int_S u_n \phi\phi^* \, dS = \int_0^T dt \int_\Sigma u_n^+ \phi\phi^* \, d\Sigma . \tag{2.10}$$

Here it is also taken $w = 0$ for $z = 0$, $z = H$. Next, we have

$$\int_0^T dt \int_{\Sigma_H} \nu\left(\phi^* \frac{\partial\phi}{\partial z} - \phi \frac{\partial\phi^*}{\partial z}\right) d\Sigma = - \int_0^T dt \int_{\Sigma_H} \phi \frac{\partial\phi^*}{\partial z} \, d\Sigma , \tag{2.11}$$

$$\int_0^T dt \int_{\Sigma_o} \nu \left(\phi^* \frac{\partial\phi}{\partial z} - \phi \frac{\partial\phi^*}{\partial z}\right) d\Sigma = - \int_0^T dt \int_{\Sigma_o} \nu\phi \left(\frac{\partial\phi^*}{\partial z} - \alpha\phi^*\right) d\Sigma . \tag{2.12}$$

Expressions (2.11) and (2.12) involve the boundary conditions from (2.1) for $z = H$ and $z = 0$, respectively. And finally, assuming $\phi = 0$ Σ for $u_n < 0$ and $\partial\phi/\partial n = 0$ on Σ for $u_n \geqq 0$, we obtain

$$\mu \int_0^T dt \int_\Sigma \left(\phi \frac{\partial\phi^*}{\partial n} - \phi^* \frac{\partial\phi}{\partial n}\right) d\Sigma = \mu \int_0^T dt \int_{\Sigma^+} \phi \frac{\partial\phi^*}{\partial n} \, d\Sigma - \mu \int_0^T dt \int_{\Sigma^-} \phi^* \frac{\partial\phi}{\partial n} \, d\Sigma , \tag{2.13}$$

Here $\Sigma^+ = \{(x, y, z) \in \Sigma \mid u_n \geqq 0\}$, $\Sigma^- = \{(x, y, z) \in \Sigma \mid u_n < 0\}$.

With due regard to (2.8)-(2.13) we have

$$\int_0^T dt \int_G p\phi \, dG = \int_0^T dt \int_G \phi^* f \, dG - \int_0^T dt \int_\Sigma u_n^+ \phi\phi^* \, d\Sigma - \int_0^T dt \int_{\Sigma_H} \nu\phi \frac{\partial\phi^*}{\partial z} \, d\Sigma + \int_0^T dt \int_{\Sigma_o} \nu\phi\left(\frac{\partial\phi^*}{\partial z} - \alpha\phi^*\right) d\Sigma - \mu \int_0^T dt \int_{\Sigma^+} \phi \frac{\partial\phi^*}{\partial n} \, d\Sigma + \mu \int_0^T dt \int_{\Sigma^-} \phi^* \frac{\partial\phi}{\partial n} \, d\Sigma . \tag{2.14}$$

So far, no boundary conditions have been fixed for the adjoint problem solution. Now (in conjunction with (2.8)) we assume that

$$
\begin{gathered}
-\frac{\partial\phi^*}{\partial t} + \operatorname{div}\underline{u}\,\phi^* + \sigma\phi^* - \frac{\partial}{\partial z}\nu\frac{\partial\phi^*}{\partial z} - \mu\Delta\phi^* = p, \\
\mu\frac{\partial\phi^*}{\partial n} + u_n\,\phi^* = 0 \quad \text{on } \textstyle\sum \quad \text{for } u_n \geqq 0 \\
\phi^* = 0 \quad \text{on } \textstyle\sum \ \text{ for } u_n < 0 \\
\frac{\partial\phi^*}{\partial z} = \alpha\phi^* \quad \text{on } \textstyle\sum_o \\
\frac{\partial\phi^*}{\partial z} = 0 \quad \text{on } \textstyle\sum_n \\
\phi^*(\underline{r}, T) = \phi^*(\underline{r}, 0).
\end{gathered}
\tag{2.15}
$$

In this case, the dual relation takes the form

$$\int_0^T dt \int_G p\phi\, dG = \int_0^T dt \int_G \phi^* f\, dG. \tag{2.16}$$

If the basic functional is defined by the equality

$$J = \int_0^T dt \int_G p\phi\, dG, \tag{2.17}$$

its identical dual representation is

$$J = \int_0^T dt \int_G \phi^*\, f\, dG. \tag{2.18}$$

Choosing different p-functions, we can derive different functionals and corresponding adjoint equations.

It is noteworthy that the above method can be used to derive a somewhat different adjoint problem for the basic equations of the form (3.27) in chapter 1, additional conditions for the problem being $\operatorname{div}\underline{u} = 0$ and $w = 0$ at $z = 0$, $z = H$.

$$
\begin{gathered}
-\frac{\partial\phi^*}{\partial t} - \operatorname{div}\underline{u}\,\phi^* + \sigma\phi^* = D\phi^* + p, \\
\phi^* = 0 \quad \text{for } t = T \\
\phi^* = 0 \quad \text{on } \textstyle\sum \\
\frac{\partial\phi^*}{\partial z} = \alpha\phi^* \quad \text{on } \textstyle\sum_o
\end{gathered}
$$

$$\frac{\partial\phi^*}{\partial z} = 0 \quad \text{on } \sum\nolimits_H$$

We note in conclusion that our primary problem was homogeneous with respect to the boundary conditions and initial data. However, the above analysis can easily be extended to inhomogeneous conditions for the basic problem. In the latter case, only the form of functional (2.18) changes to include new terms related to the inhomogeneity.

Some features underlying the statement of two-dimensional problems are also worth mentioning. Since we have already defined two-dimensional basic problems (see Eqs.(3.34) and (3.35) of the previous chapter), we can derive, using the above methods, the corresponding adjoint problems. Thus, the problem adjoint to (3.34) is

$$\begin{gathered}
-\frac{\partial\phi^*}{\partial t} - \frac{\partial u\phi^*}{\partial x} - \frac{\partial v\phi^*}{\partial y} + \sigma\phi^* = \mu\,\Delta\phi^* + p, \\
\phi^* = \phi^*_T \quad \text{for } t = T, \\
\frac{\partial\phi^*}{\partial n} + u_n\phi^* = 0 \quad \text{on } \sum \text{ for } u_n \geq 0, \\
\phi^* = 0 \quad \text{on } \sum \text{ for } u_n < 0
\end{gathered} \tag{2.19}$$

and that to (3.35),

$$\begin{gathered}
-\frac{\partial\phi^*}{\partial t} - \frac{\partial\phi^*}{\partial x} - \frac{\partial\phi^*}{\partial y} + \sigma\phi^* = \mu\,\Delta\phi^* + p, \\
\phi^* = \phi^*_T \quad \text{for } t = T, \\
\phi^* = 0 \quad \text{on } \sum
\end{gathered} \tag{2.20}$$

The corresponding functionals are of the form

$$J = \int_0^T \int_G p\phi \, dG, \tag{2.21}$$

$$J = \int_0^T \int_G f\phi^* \, dG. \tag{2.22}$$

Let us consider the problem of determining the amount of the pollutant which is expected to fall down on the underlying surface. As was shown in chapter 1, this problem can be solved in terms of a two-dimensional model under the assumption

$$\phi \cong \frac{1}{H}\int_0^H \phi\, dz, \tag{2.23}$$

(H is the height of a cylindrical region).

The problem will be formulated as follows. Let an amount Q of the pollutant ϕ be discharged at a moment $\tau_o \in [0, T]$ at a point $\underline{r}_o \in G$. It is necessary to determine the total amount of the pollutant that will fall down at the point $\underline{r}_1 \in \phi$ of the surface at the moment $\tau_1 \in [\tau_j\ T]$. Basing on the results of the preceding chapter and according to the formulation of the problem, we can write the basic functional (2.21) in the form

$$J = \frac{\overline{w}_g + \alpha\nu}{H}\ \phi\ (\underline{r}_1,\ \tau_1). \tag{2.24}$$

where $\overline{w}_g$ is the absolute velocity of the particle falldown due to gravity. The identical dual representation of the functional is

$$J = Q\phi^*\ (\underline{r}_o,\ \tau_o). \tag{2.25}$$

Suppose the boundary of the region G is sufficiently far away from the points $\underline{r}_o$, $\underline{r}_1$ and the discharge effect near the boundary is negligible. Then we can employ the following model:

$$\begin{gathered}\frac{\partial\phi}{\partial t} + \frac{\partial u\phi}{\partial x} + \frac{\partial v\phi}{\partial y} + (\sigma+\overline{\sigma})\ \phi - \mu\Delta\phi = Q\delta(\underline{r}-\underline{r}_o)\delta(t-\tau_o),\\ \phi = 0 \quad \text{for} \quad t = 0\\ \phi \to 0 \quad \text{for} \quad |\underline{r}| \to \infty\\ \overline{\sigma} = \frac{\overline{w}_g + \alpha\nu}{H}\ .\end{gathered} \tag{2.26}$$

The corresponding adjoint problem is written as

$$\begin{gathered}-\frac{\partial\phi^*}{\partial t} - \frac{\partial u\phi^*}{\partial x} - \frac{\partial v\phi^*}{\partial y} + (\sigma+\overline{\sigma})\phi^* - \mu\Delta\phi^* = \overline{\sigma}\delta(\underline{r}-\underline{r}_1)(t-\tau_1),\\ \phi^* = 0 \quad \text{for} \quad t = T,\\ \phi^* \to 0 \quad \text{for} \quad |\underline{r}| \to \infty\end{gathered} \tag{2.27}$$

Solutions of problems (2.26) and (2.27) are obtained from the fundamental solutions of the corresponding operators. The fundamental solutions for one-dimensional diffusion equations including the advective terms were derived in 2.1 of this chapter. The fundamental solutions $\tilde{\phi}$, $\tilde{\phi}^*$ for the operators of problems (2.26), (2.27) can be found in a similar way:

$$\tilde{\phi}(x, y, t) = \frac{\theta(t)}{4\mu\pi t} \exp \{- [(\sigma + \bar{\sigma})t + \frac{(x - ut)^2 + (y - vt)^2}{4\mu t}]\}, \tag{2.28}$$

$$\tilde{\phi}^*(x,y,t_1) = \frac{\theta(t_1)}{4\mu\pi t_1} \exp \{- [(\sigma + \bar{\sigma})t_1 + \frac{(x + ut_1)^2 + (y + vt_1)^2}{4\mu t_1}]\}, \tag{2.29}$$

where $t_1 = T - t$. Formulas (2.28), (2.29) were derived assuming that $u = \text{const} > 0$, $v = \text{const} > 0$.

With the latter relations in mind, we arrive at the following solutions for the direct and adjoint problems:

$$\phi(x, y,t) = \begin{cases} \dfrac{Q}{4\pi\mu(t-\tau_o)} \exp \{- \alpha(\underline{r} - \underline{r}_o, t - \tau_o)\}, \\ \qquad t \in (\tau_o, T], \\ 0, \qquad t \in [0, \tau_o]; \end{cases} \tag{2.30}$$

$$\phi^*(x, y, t) = \begin{cases} \dfrac{\bar{\sigma}}{4\pi\mu(\tau_1-t)} \exp \{- \beta(\underline{r} - \underline{r}_1, \tau_1 - t)\}, \\ \qquad t \in [0, \tau_1], \\ 0, \qquad t \in [\tau_1, T]; \end{cases} \tag{2.31}$$

where

$$\alpha(\underline{r}, t) = (\sigma + \bar{\sigma})t + \frac{(x - ut)^2 + (y - ut)^2}{4\mu t},$$

$$\beta(\underline{r}, t) = (\sigma + \bar{\sigma})t + \frac{(x + ut)^2 + (y + ut)^2}{4\mu t}.$$

Figures 2.7 and 2.8 show the isolines for the functions $\phi(x, y, \tau_1)$ and ϕ (x, y, τ_o), respectively.

Thus, the amount of the pollutant falling out at a given point can be determined by substituting either (2.30) into (2.24) or (2.31) into (2.25).

It should be stressed here that although the final result does not depend on whether the basic functional or its dual representation has been used, solutions for the direct and adjoint problems yield qualitatively different data. For example, solving the direct problem, we gain information on the spatial and temporal distributions of the pollutant for aerosol discharge at a fixed point and at a given moment. On the other hand, solution of the adjoint problem gives information on how much of the pollutant emitted by a pollution source at an arbitrary moment will fall down at a fixed point and at a given moment. This implies, for instance, that if we do not know a priori the time and the coordinates of a single emission, the problem for the point (r_1, τ_1) should be solved using dual representation (2.25) of the functional.

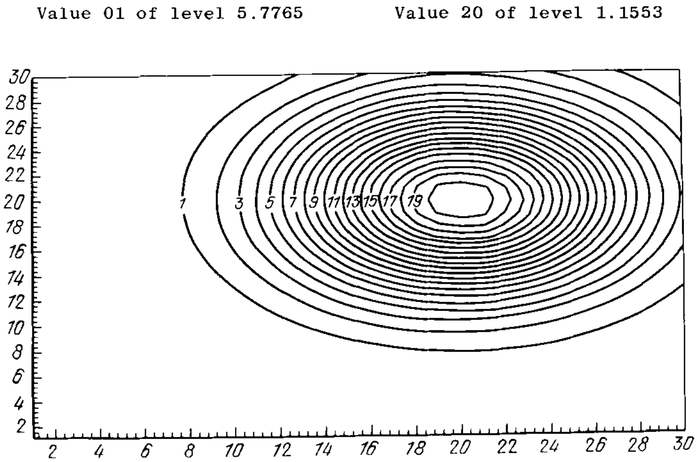


FIGURE 2.7

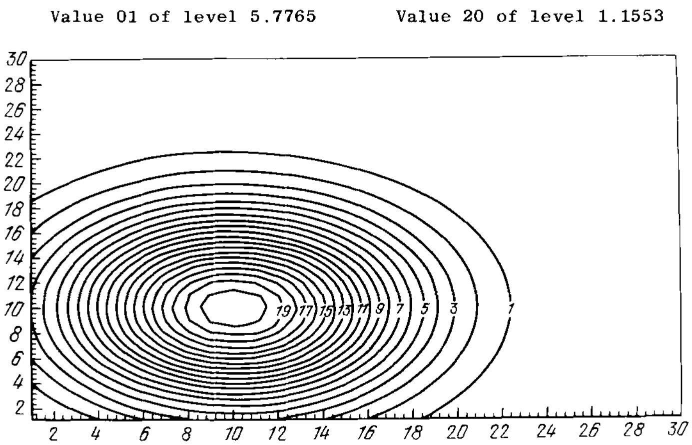


FIGURE 2.8

2.3. Uniqueness of the Solution for the Adjoint Problem

We now demonstrate that the solution for adjoint problem (2.15) is unique. To this end, we multiply the equation of (2.15) by ϕ^* and integrate the result over the entire domain of the solution. Then we have

$$- \int_0^T dt \int_G \phi^* \frac{\partial \phi^*}{\partial t} \, dG - \int_0^T dt \int_G \phi^* \operatorname{div} \underline{u}\phi^* \, dG + \int_0^T dt \int_G \sigma \phi^{*2} dG -$$

$$- \int_0^T dt \int_G \phi^* \frac{\partial}{\partial z} \nu \frac{\partial \phi^*}{\partial z} dG - \mu \int_0^T dt \int_G \phi^* \Delta\phi^* dG = \int_0^T dt \int_G p\phi^* dG. \qquad (3.1)$$

Similarly to the above considerations, we transform the integrals as follows:

$$\int_0^T dt \int_G \phi^* \operatorname{div} u\phi^* dG = \int_0^T dt \int_G \operatorname{div} u \frac{\phi^{*2}}{2} dG = \int_0^T dt \int_\Sigma \frac{u_n \phi^{*2}}{2} d\Sigma, \qquad (3.2)$$

$$\int_0^T dt \int_G \phi^* \frac{\partial}{\partial z} \nu \frac{\partial \phi^*}{\partial z} dG = \int_0^T dt \int_{\Sigma_H} \nu\phi^* \frac{\partial \phi^*}{\partial z} d\Sigma - \int_0^T dt \int_{\Sigma_o} \nu\phi^* \frac{\partial \phi^*}{\partial z} d\Sigma -$$

$$- \int_0^T dt \int_G \nu \left(\frac{\partial \phi^*}{\partial z}\right)^2 dG, \qquad (3.3)$$

$$\mu \int_0^T dt \int_G \phi^* \Delta\phi^* dG = \mu \int_0^T dt \int_\Sigma \phi^* \frac{\partial \phi^*}{\partial n} d\Sigma - \mu \int_0^T dt \int_G (\nabla\phi^*)^2 dG, \qquad (3.4)$$

where

$$\nabla\phi = \frac{\partial \phi}{\partial x} \underline{i} + \frac{\partial \phi}{\partial y} \underline{j}, \quad (\nabla\phi)^2 = \left(\frac{\partial \phi}{\partial x}\right)^2 + \left(\frac{\partial \phi}{\partial y}\right)^2.$$

Using (3.2)-(3.4), we reduce (3.1) to the form

$$- \int_0^T dt \int_G \frac{1}{2} \frac{\partial \phi^{*2}}{\partial t} dG + \int_0^T dt \left\{ \int_G \left(\sigma\phi^{*2} + \nu \left(\frac{\partial \phi^*}{\partial z}\right)^2 + \mu(\nabla\phi^*)^2\right) dG - \right.$$

$$- \int_\Sigma \phi^* \left(- \frac{u_n \phi^*}{2} + u_n\phi^* + \mu \frac{\partial \phi^*}{\partial n}\right) d\Sigma - \int_{\Sigma_H} \nu\phi^* \frac{\partial \phi^*}{\partial z} d\Sigma + \qquad (3.5)$$

$$\left. + \int_{\Sigma_o} \nu\phi^* \frac{\partial \phi^*}{\partial z} d\Sigma \right\} = \int_0^T dt \int_G p\phi^* dG.$$

Since the problem is periodic, we have

$$\int_0^T dt \int_G \frac{\partial \phi^{*2}}{\partial t} dG = 0. \qquad (3.6)$$

Next, by virtue of the condition

$$\phi^* = 0 \quad \text{on } \Sigma \quad \text{for } u_n < 0 \tag{3.7}$$

we have

$$\int_0^T dt \int_{\Sigma^-} \phi^* \left(-\frac{u_n^- \phi^*}{2} + u_n^- \phi^* + \mu \frac{\partial \phi^*}{\partial n} \right) d\Sigma = 0, \tag{3.8}$$

and by virtue of the condition

$$u_n \phi^* + \mu \frac{\partial \phi^*}{\partial n} = 0 \quad \text{on } \Sigma \quad \text{for } u_n \geqq 0 \tag{3.9}$$

we obtain

$$\int_0^T dt \int_{\Sigma^+} u_n^+ \phi^{*2} \, d\Sigma + \int_0^T dt \int_{\Sigma^+} \mu \phi^* \frac{\partial \phi^*}{\partial n} d\Sigma = 0. \tag{3.10}$$

As for the last but one terms on the left-hand side of (3.5), we have according to the boundary conditions on Σ_o and Σ_H,

$$\int_0^T dt \int_{\Sigma_H} \nu \phi^* \frac{\partial \phi^*}{\partial z} d\Sigma = 0, \qquad \int_0^T dt \int_{\Sigma_o} \nu \phi^* \frac{\partial \phi^*}{\partial z} d\Sigma = \int_0^T dt \int_{\Sigma} \nu \alpha \phi^{*2} \, d\Sigma . \tag{3.11}$$

Thus, with an allowance for (3.7)-(3.11), relation (3.5) takes the form

$$\int_0^T dt \int_{\Sigma} \frac{u_n^+ \phi^{*2}}{2} d\Sigma + \int_0^T dt \int_G \sigma \phi^{*2} \, dG + \int_0^T dt \int_G \nu \left(\frac{\partial \phi^*}{\partial z} \right)^2 dG +$$

$$+ \mu \int_0^T dt \int_G (\nabla \phi^*)^2 \, dG + \alpha \nu \int_0^T dt \int_{\Sigma_o} \phi^{*2} \, d\Sigma = \int_0^T dt \int_G p \phi^* \, dG. \tag{3.12}$$

Relation (3.12) will be basically used to prove the uniqueness of the solution for problem (2.15). Indeed, let this problem have two equal solutions, ϕ_1^* and ϕ_2^*. Then for the difference $\omega^* = \phi_1^* - \phi_2^*$ we have the homogeneous problem

$$- \frac{\partial \omega^*}{\partial t} - \operatorname{div} u\omega^* + \sigma \omega^* - \frac{\partial}{\partial z} \nu \frac{\partial \omega^*}{\partial z} - \mu \, \Delta \omega^* = 0,$$

$$\mu \frac{\partial \omega^*}{\partial n} + u_n \omega^* = 0 \quad \text{on } \Sigma \quad \text{for } u_n \geqq 0, \tag{3.13}$$

$$\omega^* = 0 \quad \text{on } \Sigma \quad \text{for } u_n < 0$$

$$\frac{\partial \omega^*}{\partial z} = \alpha\omega^* \quad \text{on} \quad \sum_o$$

$$\frac{\partial \omega^*}{\partial z} = 0 \quad \text{on} \quad \sum_H$$

$$\omega^* (\underline{r}, T) = \omega^* (\underline{r}, 0).$$

The relation of the form (3.12), corresponding to this problem, is

$$\int_0^T dt \int_\Sigma \frac{u_n^+ \omega^{*2}}{2} d\Sigma + \int_0^T dt \int_G \sigma\omega^{*2} dG + \int_0^T dt \int_G \nu\left(\frac{\partial \omega^*}{\partial z}\right)^2 dG +$$

$$+ \mu \int_0^T dt \int_G (\nabla\omega^*)^2 dG + \alpha\nu \int_0^T dt \int_{\Sigma_o} \omega^{*2} d\Sigma = 0. \tag{3.14}$$

Since $\sigma, \nu, \mu, \alpha \geqq 0$, this relation holds only for $\omega^* = 0$, i.e. when $\phi_1^* = \phi_2^*$. Thus, the uniqueness of the problem solution is proved. Of course, in the proof we have tacitly assumed that all the functions involved are smooth, which ensured the validity of all the transformations made. Similarly, we might prove the uniqueness theorem for a mixed problem as well, but in that case we should have to set $\phi^* = \phi_T^*$ for $t = T$ and solve the problem for decreasing t. Precisely under these conditions the solution algorithm gives correct results.

In conclusion, it is pertinent to point out that both the basic and the *adjoint problems also admit a unique solution when the conditions* $\phi = 0$ on Σ for $u_n < 0$, $\partial\phi/\partial n = 0$ on Σ for $u_n \geqq 0$ given by (2.1), and the conditions $\mu\, \partial\phi^*/\partial n + u_n\phi^* = 0$ on Σ for $u_n \geqq 0$, $\phi^* = 0$ on Σ for $u_n < 0$ given by (2.15) are replaced by the conditions $\phi = 0$ on Σ and $\phi^* = 0$ on Σ for all u_n.

2.4. Adjoint Equation and Lagrange Identity

In the preceding sections of this chapter we suggested a method of deriving adjoint equations for the equations of aerosol transport and diffusion. These equations can also be obtained from general considerations using the Lagrange identity. Let us analyse the procedure for deriving adjoint equations for a general evolution equation. Thus, we shall handle the problem

$$\frac{\partial \phi}{\partial t} + A\phi = f, \tag{4.1}$$

$$\phi = \phi_o \quad \text{at} \quad t = 0$$

where the linear operator A in the Hilbert space is defined on the set of functions $\phi \in \Phi$. Each element of this operator meets the smoothness conditions, some additional (say, boundary) conditions, and other requirements inherent in the problem. This point will be illustrated below by way of several examples.

Let the scalar product of two functions, g and h, in the Hilbert space Φ be defined as follows:

$$(g,\ h) = \int_0^T dt \int_G gh\ dG, \tag{4.2}$$

where $[0,\ T]$ is the range of the variable t, and G is the range of the spatial variables. Suppose, for certainty, that the problem is periodic and put $\phi\ (\underline{r},\ T) =$ $= \phi\ (\underline{r},\ 0)$.

Let Eq.(4.1) be formalized further by writing

$$L\phi = f, \tag{4.3}$$

where $L = \frac{\partial}{\partial t} + A$. With the linear operator L we associated the adjoint operator L^* through the Lagrange identity

$$(g,\ Lh) = (h,\ L^*g), \tag{4.4}$$

where the operator L and the functions g and h are assumed to be real. Putting $h = \phi$, $g = \phi^*$, we have

$$(\phi^*,\ L\phi) = (\phi,\ L^*\phi^*). \tag{4.5}$$

Since Eq.(4.3) is valid, the formal expression

$$L^*\phi^* = p, \tag{4.6}$$

(p being still an unknown function) leads to the following form of (4.5):

$$(\phi^*,\ f) = (\phi,\ p). \tag{4.7}$$

If p is a characteristic of measurement (say, of an instrument) or of a system of measurements (say, the sum of measurements), our basic functional is

$$J = (\phi,\ p). \tag{4.8}$$

Expression (4.7) implies the dual formula

$$J = (\phi^*,\ f). \tag{4.9}$$

We now employ this method to solve a particular problem.

$$\begin{gathered} \frac{\partial\phi}{\partial t} + \operatorname{div} \underline{u}\phi + \sigma\phi = \frac{\partial}{\partial z}\nu\frac{\partial\phi}{\partial z} + \mu\Delta\phi + f, \\ \phi = 0 \quad \text{on} \quad \Sigma \\ \frac{\partial\phi}{\partial z} = \alpha\phi \quad \text{on} \quad \Sigma_0 \end{gathered} \tag{4.10}$$

$$\frac{\partial \phi}{\partial z} = 0 \qquad \text{on} \quad \Sigma_H$$

$$\phi\ (\underline{r},\ T) = \phi\ (\underline{r}, 0)$$

As previously, we assume that the components u, v, and w satisfy the conditions

$$\begin{gathered} \operatorname{div} \underline{u} = 0 \\ w = 0 \quad \text{for } z = 0,\ z = H. \end{gathered} \tag{4.11}$$

Consider the space Φ of quadratically summable functions which have derivatives with respect to all the variables, generalized second-order derivatives with respect to z, x, and y, and which meet conditions (4.10). The scalar product is defined by

$$(g,\ h) = \int_0^T dt \int_G gh\ dG.$$

We write (4.10) for the functions of the Hilbert space Φ in the form

$$\frac{\partial \phi}{\partial t} + A\phi = f, \tag{4.12}$$

where

$$A = \operatorname{div}(\underline{u}\cdot) + \sigma - \frac{\partial}{\partial z}\nu\frac{\partial}{\partial z} - \mu\Lambda.$$

Using Lagrange identity (4.4) and writing out its left-hand side explicitly, we obtain

$$(g,\ Lh) = \int_0^T dt \int_G g\left(\frac{\partial h}{\partial t} + \operatorname{div} \underline{u}h + \sigma h - \frac{\partial}{\partial z}\nu\frac{\partial h}{\partial z} - \mu\Delta h\right) dG =$$

$$\begin{aligned} &= \int_G g_T h_T\ dG - \int_G g_o h_o\ dG + \int_0^T dt \int_\Sigma u_n gh\ d\Sigma + \sigma\int_0^T dt \int_G gh\ dG - \\ &- \int_0^T dt \int_{\Sigma_H} \nu g\frac{\partial h}{\partial z}\ d\Sigma + \int_0^T dt \int_{\Sigma_o} \nu g\frac{\partial h}{\partial z}\ d\Sigma + \int_0^T dt \int_{\Sigma_H} \nu h\frac{\partial g}{\partial z}\ d\Sigma - \\ &- \int_0^T dt \int_{\Sigma_o} \nu h\frac{\partial g}{\partial z}\ d\Sigma - \int_0^T dt \int_G h\frac{\partial}{\partial z}\nu\frac{\partial g}{\partial z}\ dG - \mu\int_0^T dt \int_\Sigma g\frac{\partial h}{\partial n}\ d\Sigma + \end{aligned} \tag{4.13}$$

$$+ \mu \int_0^T dt \int_\Sigma h \frac{\partial g}{\partial n} d\Sigma - \int_0^T dt \int_G \mu h \Delta g \, dG - \int_0^T dt \int_G h \frac{\partial g}{\partial t} dG -$$

$$- \int_0^T dt \int_G h \operatorname{div} \underline{u} g \, dG.$$

Identity (4.13) goes over into the expression

$$(g, Lh) = \int_0^T dt \int_G h \left(- \frac{\partial g}{\partial t} - \operatorname{div} \underline{u} g + \sigma g - \frac{\partial}{\partial z} \nu \frac{\partial g}{\partial z} - \mu \Delta g \right) dG. \quad (4.14)$$

The operator acting on the function g in the expression enclosed in parentheses will be denoted by

$$L^* = - \frac{\partial}{\partial t} - \operatorname{div} (\underline{u} \cdot) + \sigma - \frac{\partial}{\partial z} \nu \frac{\partial}{\partial z} + \mu \Delta. \quad (4.15)$$

Then, the right-hand side of (4.14) is a scalar product of the form (h, L^*g). Hence, we naturally arrive at identity (4.4) and adjoint operator (4.15) in the space Φ.

Let us define formally the adjoint problem as

$$L^* \phi^* = p, \quad (4.16)$$

or in explicit form

$$- \frac{\partial \phi^*}{\partial t} - \operatorname{div} \underline{u} \phi^* + \sigma \phi^* - \frac{\partial}{\partial z} \nu \frac{\partial \phi^*}{\partial z} - \mu \Delta \phi^* = p,$$

$$\begin{aligned} &\phi^* = 0 \quad \text{on } \Sigma \\ &\frac{\partial \phi^*}{\partial z} = \alpha \phi^* \quad \text{on } \Sigma_o \\ &\frac{\partial \phi^*}{\partial z} = 0 \quad \text{on } \Sigma_n \\ &\phi^*(\underline{r}, T) = \phi^*(\underline{r}, 0) \end{aligned} \quad (4.17)$$

In that case, we obtain any particular functional J, depending on the choice of p. Really, if we take $h = \phi$, $g = \phi^*$, then, according to (4.7), we have functionals (4.8) and (4.9).

Chapter 3. NUMERICAL SOLUTION OF BASIC AND ADJOINT EQUATIONS

This chapter discusses the methods used to solve evolution problems as applied to substance transport and diffusion in the atmosphere. It will be assumed that the problem solution satisfies homogeneous conditions on the boundary of the region. As regards the equation itself, it is naturally inhomogeneous. The splitting method is the main algorithm for solving such problems.

3.1. Elements of General Splitting Theory

A complicated problem encountered in mathematical physics can be reduced in many cases to simpler problems solvable successively and effectively by a computer. This reduction proves feasible if the initial positive semidefinite operator can be represented as the sum of simple positive semidifinite operators. Such methods will be referred to as splitting-up methods. The methods for splitting nonstationary problems were originally developed by G.Douglas, D.Peaceman, and H.Rachford. Subsequently, they were greatly advanced by Soviet mathematicians K.A.Bagrinovsky and S.K.Godunov, N.N.Yanenko, A.A.Samarsky, E.G.Dyakonov, V.K.Saulev, G.I.Marchuk.

At first, the splitting-up methods were formulated and substantiated theoretically for simple problems with commutative positive definite operators. Clearly, as applied to problems of this kind in the studies of various authors, the splitting-up methods proved either almost similar or equivalent but differing only in the scheme of their implementation. Since these methods have become nearly classical today, we will not personify them here. Those wishing to delve more deeply into the details of the algorithms may start with the references to original literature. Later on, the range of non-trivial problems solved by the splitting methods was considerably extended. Currently, the splitting-up methods provide powerful mathematics used to solve very complicated problems of mathematical physics. Since the splitting-up method theory has been elaborated most comprehensively for the case where the initial operator is given as the sum of two simpler operators, we will start with the exposition of precisely this case.

Despite the availability of multinumerous splitting-up methods, the most universal and generally applied is, in the opinion of the author, component splitting. We hope that this circumstance will be duly considered by the reader of this chapter. As for the other methods outlined below, they are rather of methodical nature.

Let us consider the evolution problem

$$\begin{aligned} \frac{\partial\phi}{\partial t} + A\phi &= f, \\ \phi &= g \quad \text{in } D \text{ at } t = 0 \end{aligned} \tag{1.1}$$

with the operator $A \geq 0$ represented in the form

$$A = A_1 + A_2 \tag{1.2}$$

where

$$A_1 \geq 0, \quad A_2 \geq 0. \tag{1.3}$$

Assume that the solution of problem (1.1) is sufficiently smooth.

We now consider the component splitting-up methods under the assumption that problem (1.1) has already been reduced to a difference form and, hence, the operators A, A_1, and A_2 are matrices. Let $A_1(t) \geq 0$, $A_2(t) \geq 0$. Examine the approximations of these matrices on the interval $t_j \leq t \leq t_{j+1}$

$$\Lambda_\alpha^j = A_\alpha(t_{j+1/2}), \quad \Lambda^j = \Lambda_1^j + \Lambda_2^j,$$

assuming that the elements of A_1 and A_2 are sufficiently smooth. We write the difference system of equations suggested by N.N.Yanenko, which consists of successive solutions of simple Cranck-Nickolson schemes*

$$\begin{aligned} &\frac{\phi^{j+1/2} - \phi^j}{\tau} + \Lambda_1^j \frac{\phi^{j+1/2} + \phi^j}{2} = 0, \\ &\frac{\phi^{j+1} - \phi^{j+1/2}}{\tau} + \Lambda_2^j \frac{\phi^{j+1} + \phi^{j+1/2}}{2} = 0. \end{aligned} \tag{1.4}$$

Eliminating the auxiliary function $\phi^{j+1/2}$ from the system of difference Eqs.(1.4), we can reduce it to a single equation

$$\phi^{j+1} = T_j \phi^j, \tag{1.5}$$

where

$$T_j = \left(E + \frac{\tau}{2}\Lambda_2^j\right)^{-1}\left(E - \frac{\tau}{2}\Lambda_2^j\right)\left(E + \frac{\tau}{2}\Lambda_1^j\right)^{-1}\left(E - \frac{\tau}{2}\Lambda_1^j\right). \tag{1.6}$$

First, we examine the approximation problem. Expand the operator T_j in the powers of τ, assuming that $\frac{\tau}{2}||\Lambda_\alpha^i|| \leq 1$. Simple transformation yields

$$T_j = E - \tau\Lambda^j + \frac{\tau^2}{2}((\Lambda_1^j)^2 + 2\Lambda_2^j\Lambda_1^j + (\Lambda_2^j)^2) - \ldots \tag{1.7}$$

If the operators Λ_α^j are commutative, i.e. if $\Lambda_1\Lambda_2 = \Lambda_2\Lambda_1$, expansion (1.7) can be written as

$$T_j = E - \tau\Lambda^j + \frac{\tau^2}{2}(\Lambda^j)^2 - \ldots \tag{1.8}$$

Thus, if $A_1(t) \geq 0$, $A_2(t) \geq 0$, then difference scheme (1.4) is absolutely stable for sufficiently smooth matrix elements and solution ϕ of problem (1.1)-(1.3) (this follows from the inequality $||T_j|| < 1$ which is valid, accord-

*Theoretical substantiation and modifications of the scheme were reported by the author at the Symposium on Numerical methods for solving partial differential equations, which was held in the USA in 1970.

ing to the Kellog lemma). The scheme approximates the initial Eq.(1.1) to the second order in τ, if Λ_1^j, Λ_2^j are commutative, and to the first order in τ, if they are not commutative.

Suppose now that the operators $A_1(t)$ and $A_2(t)$ are approximated in the interval $t_{j-1} \leq t \leq t_{j+1}$ (rather than in the interval $t_j \leq t < t_{j+1}$ as was the case with (1.4) by $\Lambda_\alpha^j = A_\alpha(t_j)$.

Consider the following two systems of difference equations:

$$\begin{aligned} &\frac{\phi^{j-1/2} - \phi^{j-1}}{\tau} + \Lambda_1^j \frac{\phi^{j-1/2} + \phi^{j-1}}{2} = 0, \\ &\frac{\phi^{j} - \phi^{j-1/2}}{\tau} + \Lambda_2^j \frac{\phi^{j} + \phi^{j-1/2}}{2} = 0; \end{aligned} \tag{1.9}$$

$$\begin{aligned} &\frac{\phi^{j+1/2} - \phi^{j}}{\tau} + \Lambda_2^j \frac{\phi^{j} + \phi^{j+1/2}}{2} = 0, \\ &\frac{\phi^{j+1} - \phi^{j+1/2}}{\tau} + \Lambda_1^j \frac{\phi^{j+1} + \phi^{j+1/2}}{2} = 0. \end{aligned} \tag{1.10}$$

Computation procedure is precisely the successive use of difference schemes (1.9) and (1.10). Similarly to the above considerations, it is easy to show that a complete computation procedure involving (1.9) and (1.10) gives

$$\phi^{j+1} = T^j \phi^j, \tag{1.11}$$

where

$$\begin{aligned} T^j = {} & (E + \tfrac{\tau}{2}\Lambda_1^j)^{-1}(E - \tfrac{\tau}{2}\Lambda_1^j)(E + \tfrac{\tau}{2}\Lambda_2^j)^{-1}(E - \tfrac{\tau}{2}\Lambda_2^j)\ (E + \tfrac{\tau}{2}\Lambda_2^j)^{-1} \cdot \\ & \cdot (E - \tfrac{\tau}{2}\Lambda_2^j)(E + \tfrac{\tau}{2}\Lambda_1^j)^{-1}(E - \tfrac{\tau}{2}\Lambda_1^j) = E - 2\tau\,\Lambda^j + \frac{(2\tau)^2}{2}(\Lambda^j)^2 - \ldots \end{aligned} \tag{1.12}$$

Comparison of the operator T^j with the step operator in the Cranck-Nickolson scheme

$$\frac{\phi^{j+1} - \phi^{j-1}}{2\tau} + \Lambda^j \frac{\phi^{j+1} + \phi^{j-1}}{2} = 0, \tag{1.13}$$

shows that in a two-cycle splitting scheme the former operator coincides, up to τ^2, with the latter operator as applied to a double time interval, no matter whether the operators A_α are commutative or not. Thus, this method relaxes significantly the requirement for operator commutation.

Let us now discuss computation stability provided by the method. For this purpose, we estimate relation (1.5) in terms of the energy norm

$$\left\| \phi^{j+1} \right\| \leq \left\| T_j \right\| \left\| \phi^j \right\|.$$

Since $\|T_j\| \leq 1$ for $A_\alpha \geq 0$, the estimate is

$$\|\phi^{j+1}\| \leq \|\phi^j\|, \tag{1.14}$$

whence

$$\|\phi^j\| \leq \|g\|. \tag{1.15}$$

If we deal with a two-cycle method, each step of the cycle involves estimations of the type (1.14). This means that the two-cycle method is absolutely stable, too. It should be noted that a similar symmetrization technique was suggested independently by J. Strang who considered the method of variable directions.

Consequently, if $A_1(t) \geq 0$, $A_2(t) \geq 0$, systems of difference Eqs. (1.9) and (1.10) are absolutely stable and scheme (1.11) approximates initial Eq.(1.1) up to τ^2, provided the solution ϕ of problem (1.1)-(1.3) and the elements of $A_1(t)$ and $A_2(t)$ are sufficiently smooth.

We now turn to the inhomogeneous problem and seek its solution by a complete two-cycle splitting. To this end, we analyse a system of difference equations of the form (1.9), (1.10) expressed more conveniently as

$$\begin{aligned}
(E + \frac{\tau}{2}\Lambda_1^j)\,\phi^{j-1/2} &= (E - \frac{\tau}{2}\Lambda_1^j)\,\phi^{j-1},\\
(E + \frac{\tau}{2}\Lambda_2^j)(\phi^j - \tau f^j) &= (E - \frac{\tau}{2}\Lambda_2^j)\,\phi^{j-1/2},\\
(E + \frac{\tau}{2}\Lambda_2^j)\,\phi^{j+1/2} &= (E - \frac{\tau}{2}\Lambda_2^j)(\phi^j + \tau f^j),\\
(E + \frac{\tau}{2}\Lambda_1^j)\,\phi^{j+1} &= (E - \frac{\tau}{2}\Lambda_1^j)\,\phi^{j+1/2},
\end{aligned} \tag{1.16}$$

where $f^j = f(t_j)$. Solving these equations for ϕ^{j+1}, we obtain

$$\phi^{j+1} = T^j\phi^{j-1} + 2\tau T_1^jT_2^jf^j, \tag{1.17}$$

where

$$T^j = T_1^jT_2^jT_2^jT_1^j, \tag{1.18}$$

$$T_\alpha^j = (E + \frac{\tau}{2}\Lambda_\alpha^j)^{-1}(E - \frac{\tau}{2}\Lambda_\alpha^j), \quad \alpha = 1,2. \tag{1.19}$$

Expanding (1.17) in the powers of the small parameter τ, we reduce this expression to

$$\phi^{j+1} = [E - 2\tau\Lambda^j + \frac{(2\tau)^2}{2}(\Lambda^j)^2]\phi^{j-1} + 2\tau(E - \tau\Lambda^j)f^j + O(\tau^3), \tag{1.20}$$

then transform it to

$$\frac{\phi^{j+1} - \phi^{j-1}}{2\tau} + \Lambda^j (E - \tau\Lambda^j)\phi^{j-1} = (E - \tau\Lambda^j) f^j + O(\tau^2) \tag{1.21}$$

and eliminate ϕ^{j-1}. To this end, we expand the solution in a Taylor series in the neighborhood of the point t_{j-1}. We have, up to τ^2,

$$\phi^j = \phi^{j-1} + \left(\frac{\partial\phi}{\partial t}\right)^{j-1} \tau + O(\tau^2). \tag{1.22}$$

The derivative $\partial\phi/\partial t$ is eliminated by the equality

$$\left(\frac{\partial\phi}{\partial t}\right)^{j-1} = - \Lambda^j \phi^{j-1} + f^j + O(\tau). \tag{1.23}$$

Substituting (1.23) into (1.22), we obtain

$$\phi^j = (E - \tau\Lambda^j)\phi^{j-1} + \tau f^j + O(\tau^2),$$

whence

$$(E - \tau\Lambda^j)\phi^{j-1} = \phi^j - \tau f^j + O(\tau^2). \tag{1.24}$$

Substituting now (1.24) into (1.21), we find

$$\frac{\phi^{j+1} - \phi^{j-1}}{2\tau} + \Lambda^j \phi^j = f^j + O(\tau^2). \tag{1.25}$$

Evidently, (1.25) approximates initial Eq.(1.1) in the interval $t_{j-1} \leq t \leq t_{j+1}$ to the second order in t. Thus, using a two-cycle method, we have accomplished a second-order difference approximation of an inhomogeneous evolution equation.

It is a simple matter to prove the stability of the method in terms of the energy norm. Indeed, let us estimate ϕ^{j+1} from (1.17) with respect to the norm

$$\phi^{j+1} \leq \|T^j\| \, \|\phi^{j-1}\| + 2\tau \|T_1\| \, \|T_2\| \, \|f^j\|. \tag{1.26}$$

Allowing for $\|T_\alpha\| \leq 1$ and, hence, for $\|T^j\| \leq \|T_1\| \, \|T_2\| \, \|T_2\| \, \|T_1\| \leq 1$, we have

$$\|\phi^{j+1}\| \leq \|\phi^{j-1}\| + 2\tau \|f^j\|. \tag{1.27}$$

Using recurrence relation (1.17), we obtain

$$\|\phi^j\| \leq \|g\| + \tau j \|f\|, \tag{1.28}$$

where $\|f\| = \max \|f^j\|$. Relation (1.28) implies the computational stability of the scheme in any finite time interval.

The system of Eqs.(1.16) can also be expressed in the following equivalent form:

$$
\begin{aligned}
(E + \frac{\tau}{2}\Lambda_1^j)\phi^{j-2/3} &= (E - \frac{\tau}{2}\Lambda_1^j)\phi^{j-1},\\
(E + \frac{\tau}{2}\Lambda_2^j)\phi^{j-1/3} &= (E - \frac{\tau}{2}\Lambda_2^j)\phi^{j-2/3},\\
\phi^{j+1/3} &= \phi^{j-1/3} + 2\tau f^j, \qquad (1.29)\\
(E + \frac{\tau}{2}\Lambda_2^j)\phi^{j+2/3} &= (E - \frac{\tau}{2}\Lambda_2^j)\phi^{j+1/3},\\
(E + \frac{\tau}{2}\Lambda_1^j)\phi^{j+1} &= (E - \frac{\tau}{2}\Lambda_1^j)\phi^{j+2/3}.
\end{aligned}
$$

Eliminating the unknown quantities with fractional indices, we arrive at a resolved equation

$$\phi^{j+1} = T_1T_2T_2T_1\phi^{j-1} + 2\tau T_1T_2f^j, \qquad (1.30)$$

which coincides with (1.17). Sometimes, it is more preferable to write the equations in the form (1.29) rather than in the form (1.16).

Thus, if the matrices $A_1(t)$, $A_2(t) \geqq 0$, and if the solution ϕ_1, the function $f(t)$, and the elements of $A_1(t)$, $A_2(t)$ are sufficiently smooth, the system of difference Eqs.(1.16) is absolutely stable in the interval $0 \leqq t \leqq T$ and it approximates the initial equation up to the second order in τ.

We have assumed so far that the initial operator A can be represented as the sum of two simpler operators. When tackling complicated problems of mathematical physics, one has frequently to split operators into a large number of components. Generally, we have

$$A = \sum_{\alpha=1}^{n} A_\alpha, \qquad (1.31)$$

with $A_\alpha \geqq 0$. Since the case of $n = 2$ was treated in detail earlier, we shall concentrate here only on the situation where $n > 2$.

First of all, one is readily convinced that straight forward extension of above splitting-up methods (for $n = 2$) is, generally, impossible. That is why we shall try to extend the component splitting algorithms to the case $n > 2$ under the assumptions that make such an extension possible.

An attempt will be undertaken to develop a difference analogue to the problem of the second-order approximation with respect to τ, which is absolutely stable in time. According to the assumption of a multicomponent splitting, we write

$$\Lambda^j = \sum_{\alpha=1}^{n} \Lambda_\alpha^j, \tag{1.32}$$

where all Λ_α^j are positive semidefinite operators and, therefore, $\Lambda_\alpha^j \geq 0$. Consider the system of equations

$$(E + \frac{\tau}{2}\Lambda_\alpha^j)\, \phi^{j+\alpha/n} = (E - \frac{\tau}{2}\Lambda_\alpha^j)\phi^{j+(\alpha-1)/n}, \tag{1.33}$$

$$\alpha = 1, 2, \ldots, n$$

When $\Lambda_\alpha^j \geq 0$, the operators Λ_α are commutative and either $\Lambda_\alpha^j = A_\alpha^{j+1/2}$ or $\Lambda_\alpha^j = \frac{1}{2}(A^{j+1} + A^j)$, scheme (1.33) is absolutely stable and is a second-order approximation. This can be demonstrated in an elementary way using the Fourier transformation method. Evidently, for non-commutative operators Λ_α^j scheme (1.33) is, generally, of the first order in τ and, therefore, less attractive for application than the following second-order scheme suggested by E.G.Dyakonov:

$$\begin{gathered} \phi^{j+\alpha/(2n)} = (E - \frac{\tau}{2}\Lambda_\alpha^j)\phi^{j+(\alpha-1)/(2n)}, \\ \alpha = 1,2, \ldots, n \\ (E + \frac{\tau}{2}\Lambda_{2n-\alpha+1}^j)\phi^{j+\alpha/(2n)} = \phi^{j+(\alpha-1)/(2n)}, \\ \alpha = n+1, n+2, \ldots, 2n. \end{gathered} \tag{1.34}$$

In what follows we shall try to give a specific description of the complete splitting method based on (1.33) which admits a solution to the Cauchy problem for positive semidefinite and non-commutative operators Λ_α^j and which provides a second-order approximation. This would actually be a definitive solution to the splitting problem.

Note that system (1.33) is reduced to a single equation

$$\phi^{j+1} = \prod_{\alpha=1}^{n} (E + \frac{\tau}{2}\Lambda_\alpha^j)^{-1}(E - \frac{\tau}{2}\Lambda_\alpha^j)\phi^j, \tag{1.35}$$

which can be used to obtain an estimate with respect to the norm

$$\|\phi^{j+1}\| \leq \prod_{\alpha=1}^{n} \|(E + \frac{\tau}{2}\Lambda_\alpha^j)^{-1}(E - \frac{\tau}{2}\Lambda_\alpha^j)\| \, \|\phi^j\|. \tag{1.36}$$

From the Kellog lemma we have

$$\|\phi^{j+1}\| \leq \|\phi^j\| \leq \ldots \leq \|g\|. \tag{1.37}$$

If the operator is antisymmetric, then we have

$$\|\phi^{j+1}\| = \|\phi^j\| = \dots \|g\|.$$

Thus, we have proved that the scheme is absolutely stable.

To determine the order of approximation, we expand the expression

$$T^j = \prod_{\alpha=1}^{n} (E + \frac{\tau}{2} \Lambda_\alpha^j)^{-1} (E - \frac{\tau}{2} \Lambda_\alpha^j). \tag{1.38}$$

in the powers of the small parameter τ (assuming that $\frac{\tau}{2} \|\Lambda_\alpha\| < 1$). Since $T^j = \prod_{\alpha=1}^{n} T_\alpha^j$, we first expand the operator T^j:

$$T_\alpha^j = E - \tau\Lambda_\alpha^j + \frac{\tau^2}{2} (\Lambda_\alpha^j)^2 \dots; \tag{1.39}$$

We have

$$T^j = E - \tau\Lambda^j + \frac{\tau^2}{2} \left[(\Lambda^j)^2 + \sum_{\alpha=1}^{n} \sum_{\beta=\alpha+1}^{n} (\Lambda_\alpha^j \Lambda_\beta^j - \Lambda_\beta^j \Lambda_\alpha^j) \right] + 0(\tau^3) \tag{1.40}$$

If the operators Λ_α^j are commutative, the expression under the double sum vanishes and we obtain

$$T^j = E - \tau\Lambda^j + \frac{\tau^2}{2} (\Lambda^j)^2 + 0(\tau^3). \tag{1.41}$$

Comparison of (1.41) with the similar expansion for the Cranck-Nickolson scheme indicates that in this particular case scheme (1.33) is a second-order approximation in τ. If the operators Λ_α^j are not commutative, the splitting scheme gives only a first-order approximation in τ. To develop a second-order scheme in τ for the non-commutative case, one should modify scheme (1.33) as follows:

$$\phi^j = \prod_{\alpha=1}^{n} T_\alpha^j \phi^{j-1}, \quad \phi^{j+1} = \prod_{\alpha=n}^{1} T_\alpha^j \phi^j. \tag{1.42}$$

From the algorithmic standpoint, this means that we first solve system (1.33) in the interval $t_{j-1} \leqq t \leqq t_j$ for $\alpha = 1,2, \dots, n$ and then solve the same system in the interval $t_j \leqq t \leqq t_{j+1}$, but in the reverse order ($\alpha = n, n-1, \dots, 1$):

$$\begin{gathered} (E + \frac{\tau}{2} \Lambda_\alpha^j)\phi^{j+\alpha/(n-1)} = (E - \frac{\tau}{2} \Lambda_\alpha^j)\phi^{j+(\alpha-1)/(n-1)}, \\ \alpha = 1, 2, \dots, n \\ (E + \frac{\tau}{2} \Lambda_\alpha^j)\phi^{j+1-(\alpha-1)/n} = (E - \frac{\tau}{2} \Lambda_\alpha^j)\phi^{j+1-\alpha/n}, \\ \alpha = n, n-1, \dots, 1. \end{gathered} \tag{1.43}$$

Evidently, a complete cycle of computations in (1.43) requires that

$$\phi^{j+1} = T^j \phi^{j-1}.$$

where

$$T^j = \prod_{\alpha=1}^{n} T_\alpha^j \prod_{\alpha=n}^{1} T_\alpha^j = E - 2\tau\Lambda^j + \frac{(2\tau)^2}{2}(\Lambda^j)^2 + O(\tau^3).$$

Thus, scheme (1.43) gives a second-order approximation in τ on the interval $t_{j-1} \leqq t \leqq t_{j+1}$, provided for Λ_α^j we take one of the analogues defined by (1.22)-(1.24). This follows from the comparison of (1.43) and (1.33) for the double time interval.

In conclusion, we should like to note that difference scheme (1.43) is absolutely stable for $\Lambda_\alpha^j \geqq 0$. Hence, we have obtained an optimum algorithm of multicomponent splitting. For the non-homogeneous problem

$$\begin{aligned} \frac{\partial\phi}{\partial t} + A\phi &= f, \\ \phi = g \quad \text{at} \quad t &= 0, \end{aligned} \tag{1.44}$$

where $A(t) \geqq 0$, $A = \sum_{\alpha=1}^{n} A_\alpha$, $A_\alpha(t) \geqq 0$ the following splitting scheme holds in the interval $t_{j-1} \leqq t \leqq t_{j+1}$:

$$\begin{aligned}
(E + \tfrac{\tau}{2}\Lambda_1^j)\phi^{j-(n-1)/n} &= (E - \tfrac{\tau}{2}\Lambda_1^j)\phi^{j-1}, \\
&\cdots\cdots\cdots\cdots \\
(E + \tfrac{\tau}{2}\Lambda_n^j)(\phi^j - \tau f^j) &= (E - \tfrac{\tau}{2}\Lambda_n^j)\phi^{j-1/n}, \\
(E + \tfrac{\tau}{2}\Lambda_n^j)\phi^{j+1/n} &= (E - \tfrac{\tau}{2}\Lambda_n^j)(\phi^j + \tau f^j), \\
&\cdots\cdots\cdots\cdots \\
(E + \tfrac{\tau}{2}\Lambda_1^j)\phi^{j-1} &= (E - \tfrac{\tau}{2}\Lambda_1^j)\phi^{j-(n-1)/n},
\end{aligned} \tag{1.45}$$

Here $\Lambda_\alpha^j = A_\alpha(t_j)$. One can easily see that the scheme gives a second-order approximation in τ and is absolutely stable under the assumption that ϕ is sufficiently smooth.

Similarly to the case of $\alpha = 2$, system (1.45) can be written in an equivalent form

$$(E + \frac{\tau}{2}\Lambda_\alpha^j)\phi^{j-\frac{(n+1)-\alpha}{n+1}} = (E - \frac{\tau}{2}\Lambda_\alpha^j)\phi^{j-\frac{(n+1)-\alpha+1}{n+1}},$$

$$\alpha = 1, 2, \ldots, n,$$

$$\phi^{j+1/(n+1)} = \phi^{j-1/(n+1)} + 2\tau f^j, \tag{1.46}$$

$$(E + \frac{\tau}{2}\Lambda^j_{n-\alpha+2})\phi^{j+\alpha/(n+1)} = (E - \frac{\tau}{2}\Lambda^j_{n-\alpha+2})\phi^{j+(\alpha-1)/(n+1)},$$

$$\alpha = 2, 3, \ldots, n + 1$$

Let us now turn to the splitting-up method for implicit difference approximations. To this end, we handle the problem

$$\frac{\partial\phi}{\partial t} + A\phi = 0,$$
$$\phi = g \quad \text{at} \quad t = 0. \tag{1.47}$$

Suppose $A = \sum_{\alpha=1} A_\alpha$, $A_\alpha \geqq 0$, and A_α do not depend on time. Then the splitting algorithm is of the form

$$\frac{\phi^{j+1/n} - \phi^j}{\tau} + A_1\phi^{j+1/n} = 0,$$
$$\cdots\cdots\cdots\cdots\cdots \tag{1.48}$$
$$\frac{\phi^{j+1} - \phi^{j+(n-1)/n}}{\tau} + A_n\phi^{j+1} = 0.$$

It will be shown that this algorithm is absolutely stable. Consider the equation

$$\frac{\phi^{j+\alpha/n} - \phi^{j+(\alpha-1)/n}}{\tau} + A_\alpha\phi^{j+\alpha/n} = 0; \tag{1.49}$$

and multiply it scalarly by $\phi^{j+\alpha/n}$:

$$(\phi^{j+\alpha/n} - \phi^{j+(\alpha-1)/n}, \phi^{j+\alpha/n}) + \tau(A_\alpha\phi^{j+\alpha/n}, \phi^{j+\alpha/n}) = 0.$$

Since the operators A_α are positive semidefinite, we obtain*

$$(\phi^{j+\alpha/n} - \phi^{j+(\alpha-1)/n}, \phi^{j+\alpha/n}) \leqq 0,$$

or

$$(\phi^{j+\alpha/n}, \phi^{j+\alpha/n}) \leqq (\phi^{j+\alpha/n}, \phi^{j+(\alpha-1)/n}).$$

On the other hand,

$$(\phi^{j+\alpha/n}, \phi^{j+(\alpha-1)/n}) \leqq \tfrac{1}{2}[(\phi^{j+\alpha/n}, \phi^{j+\alpha/n}) + (\phi^{j+(\alpha-1)/n}, \phi^{j+(\alpha-1)/n})],$$

whence

$$\|\phi^{j+\alpha/n}\|^2 \leq \|\phi^{j+(\alpha-1)/n}\|^2, \quad \alpha = 1, 2, \ldots, n$$

*For methodic reasons, only homogeneous boundary conditions are considered.

By virtue of this recurrence inequality we have

$$\|\phi^{j+1}\| \leq \|\phi^{j}\|. \tag{1.50}$$

This means that under the above assumptions, computation by splitting scheme (1.48) is absolutely stable. One can readily see that (1.48) approximates the initial problem to the first order in τ.

We now consider the non-homogeneous problem

$$\begin{aligned} &\frac{\partial\phi}{\partial t} + A\alpha = f \\ &\phi = g \quad \text{at} \quad t = 0 \end{aligned} \tag{1.51}$$

The splitting scheme for this problem is defined as

$$\begin{aligned} &\frac{\phi^{j+1/n} - \phi^{j}}{\tau} + A_1\phi^{j+1/n} = 0, \\ &\dots\dots\dots\dots\dots \\ &\frac{\phi^{j+1} - \phi^{j+(n-1)/n}}{\tau} + A_n\phi^{j+1} = f^{j}. \end{aligned} \tag{1.52}$$

This scheme approximates the initial non-homogeneous equation to within the first-order in τ.

The stability of the scheme can be proved as follows. Multiply each equation scalarly by $\phi^{j+1/n}, \dots, \phi^{j+1}$, respectively. Similarly to the above, we have

$$\|\phi^{j+\alpha/n}\| \leq \|\phi^{j+(\alpha-1)/n}\|, \quad \alpha = 1,2, \dots, n-1 \tag{1.53}$$

Examine the last equation of (1.52) more closely. We have

$$(\phi^{j+1}, \phi^{j+1}) = (\phi^{j+(n-1)/n}, \phi^{j+1}) - \tau(A_n\phi^{j+1}, \phi^{j+1}) + \tau(f^{j}, \phi^{j+1}).$$

Since $A_n \geq 0$, we obtain

$$(\phi^{j+1}, \phi^{j+1}) \leq (\phi^{j+(n-1)/n}, \phi^{j+1}) + \tau(f^{j}, \phi^{j+1}).$$

By virtue of the Cauchy-Bunyakovsky inequality, we have

$$|(\phi^{j+(n-1)/n}, \phi^{j+1})| \leq \|\phi^{j+(n-1)/n}\| \, \|\phi^{j+1}\|,$$

$$|(f^{j}, \phi^{j+1})| \leq \|f^{j}\| \, \|\phi^{j+1}\|.$$

Consequently,

$$\|\phi^{j+1}\|^2 \leq \|\phi^{j+(n-1)/n}\| \, \|\phi^{j+1}\| + \tau\|f^{j}\| \, \|\phi^{j+1}\|.$$

Cancellation of $\|\phi^{j+1}\|$ leads to the inequality

$$\|\phi^{j+1}\| \leq \|\phi^{j+(n-1)/n}\| + \tau\|f^j\|.$$

Eliminating solutions with fractional indices, we get

$$\|\phi^{j+1}\| \leq \|\phi^j\| + \tau\|f^j\|. \tag{1.54}$$

Allowing for $\|\phi^o\| = \|g\|$ and eliminating intermediate solutions, we obtain

$$\|\phi^{j+1}\| \leq \|g\| + \tau_j \|f\|, \tag{1.55}$$

where $\|f\| = \max \|f^j\|$. This implies absolute stability of the difference scheme for any moment within the interval $0 \leq t_j \leq T$.

This splitting algorithm can be extended to the case of a time-dependent operator A. Here, in the computation cycle performed by the splitting scheme, A should be replaced by a suitable difference approximation of this operator in each interval $t_j \leq t \leq t_{j+1}$.

3.2. Splitting of a Problem According to Physical Processes

We will assume that each element of the Hilbert space Φ, where the basic problem solution is sought, is sufficiently smooth and meets some requirements related to the boundary conditions on $\sum$, $\sum_o$, and $\sum_H$. Then the solution of the basic problem satisfies the evolution problem

$$\frac{\partial\phi}{\partial t} + \frac{\partial u\phi}{\partial x} + \frac{\partial v\phi}{\partial y} + \frac{\partial w\phi}{\partial z} - \frac{\partial}{\partial z}\nu\frac{\partial\phi}{\partial z} - \mu\Delta\phi + \sigma\phi = f, \tag{2.1}$$

$$\phi = g \quad \text{at} \quad t = 0.$$

As previously, we assume that for u, v, and w the following relations are valid:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0,$$

$$w = 0 \quad \text{at} \quad z = 0, \quad z = H. \tag{2.2}$$

Generally speaking, problem (2.1) describes two essentially different processes. One is substance transport (with conservation) along a trajectory. This process is described by the equation

$$\frac{\partial\phi}{\partial t} + \frac{\partial u\phi}{\partial x} + \frac{\partial v\phi}{\partial y} + \frac{\partial w\phi}{\partial z} = 0,$$

$$\phi = g \quad \text{at} \quad t = 0, \tag{2.3}$$

$$\phi = 0 \quad \text{on} \ \sum \ \text{for} \quad u_n < 0.$$

The other physical process is related to substance diffusion and absorption in the course of propagation. This process is fitted by the problem

$$\frac{\partial\phi}{\partial t} + \sigma\phi = \frac{\partial}{\partial z}\nu\frac{\partial\phi}{\partial t} + \mu\Delta\phi + f,$$
$$\phi = g \quad \text{at} \quad t = 0,$$
$$\phi = 0 \quad \text{on} \quad \Sigma \tag{2.4}$$
$$\frac{\partial\phi}{\partial z} = \alpha\phi \quad \text{on} \quad \Sigma_o$$
$$\frac{\partial\phi}{\partial z} = 0 \quad \text{on} \quad \Sigma_H.$$

Here we have chosen the simplest boundary conditions. They could be replaced (as pointed out in chapter 1) by the following conditions:

$$\phi = 0 \quad \text{on} \quad \Sigma \quad \text{for} \quad u_n < 0,$$
$$\frac{\partial\phi}{\partial n} = 0 \quad \text{on} \quad \Sigma \quad \text{for} \quad u_n \geqq 0,$$
$$\frac{\partial\phi}{\partial z} = \alpha\phi \quad \text{on} \quad \Sigma_o$$
$$\frac{\partial\phi}{\partial z} = 0 \quad \text{on} \quad \Sigma_H$$

From the computational viewpoint, however, the problem with such boundary conditions does not differ, in principle, from the problem formulated above.

These processes are two limiting cases of problem (2.1). Indeed, putting $\nu = 0$, $\mu = 0$, $\sigma = 0$ in (2.1), we arrive at problem (2.3), whereas setting $u = 0$, $v = 0$, $w = 0$, we come to problem (2.4). Therefore, in later sections of the book we shall examine solutions of these physically elementary problems at greater length.

Now we will try to relate problems (2.3) and (2.4). It turns out that this can be done approximately due to local additivity of the processes. Choose a sufficiently small interval $t_j \leqq t \leqq t_{j+1}$ and solve in this interval the problem

$$\frac{\partial\phi_1}{\partial t} + \frac{\partial u\phi_1}{\partial x} + \frac{\partial v\phi_1}{\partial y} + \frac{\partial w\phi_1}{\partial z} = 0. \tag{2.5}$$

$$\phi_1 = \phi_2^j \quad \text{for} \quad t = t_j$$

$$\phi_1 = 0 \quad \text{on } \sum \text{ if } u_n \leq 0,$$

where ϕ_2^j is defined below. As a result, we find $\phi_1^{j+1} = \phi_1(\underline{r}, t_{j+1})$.

Next, we solve another problem in the same interval

$$\begin{aligned}
&\frac{\partial \phi_2}{\partial t} + \sigma\phi_2 = \frac{\partial}{\partial z}\nu\frac{\partial \phi_2}{\partial z} + \mu\Delta\phi_2 + f,\\
&\phi_2 = \phi_1^{j+1}\\
&\phi_2 = 0 \quad \text{on } \sum\\
&\frac{\partial \phi_2}{\partial z} = \alpha\phi_2 \quad \text{on } \sum\nolimits_o\\
&\frac{\partial \phi_2}{\partial z} = 0 \quad \text{on } \sum\nolimits_H
\end{aligned} \tag{2.6}$$

Then, $\phi_2^{j+1} = \phi_2(\underline{r}, t_{j+1})$ is an approximate solution for problem (2.1). To demonstrate this, we integrate (2.5) within the limits (t_j, t)

$$\phi_1 = \phi_2^j - \int_{t_j}^{t} \operatorname{div} \underline{u}\phi_1 \, dt. \tag{2.7}$$

Here we employed the condition $\phi_1 = \phi_2^j$ at $t = t_j$. Eliminate ϕ_1 under the integral sign in (2.7) (using the same formula)

$$\phi_1 = \phi_2^j - (t - t_j)\operatorname{div} \underline{u}\phi_2^j + \int_{t_j}^{t} \operatorname{div}(\underline{u} \int_{t_j}^{t} \operatorname{div} \underline{u}\phi_1 \, dt) \, dt, \tag{2.8}$$

or

$$\phi_1 = \phi_2^j - (t - t_j) \operatorname{div} \underline{u}\phi_2^j + 0(\tau^2), \tag{2.9}$$

where $\tau = t_{j+1} - t_j$. Using (2.9), we obtain

$$\phi_1^{j+1} = \phi_2^j - \tau\operatorname{div} \underline{u}\phi_2^j + 0(\tau^2). \tag{2.10}$$

Let us now consider problem (2.6). Integrate the equation over the interval $t_j \leq t \leq t_{j+1}$ with the initial conditions $\phi_2^j = \phi_1^{j+1}$. The result is

$$\phi_2^{j+1} = \phi_1^{j+1} + \int_{t_j}^{t_{j+1}} \left(\frac{\partial}{\partial z} \nu \frac{\partial \phi_2}{\partial z} + \mu\Delta\phi_2 - \sigma\phi_2 + f\right)dt. \tag{2.11}$$

Using a simple explicit approximation, we obtain

$$\phi_2^{j+1} = \phi_1^{j+1} + \tau\left(\frac{\partial}{\partial z} \nu \frac{\partial \phi_2^j}{\partial z} + \mu\Delta\phi_2^j - \sigma\phi_2^j + f\right) + O(\tau^2). \tag{2.12}$$

Substituting ϕ_1^{j+1} (from 2.10), we have

$$\phi_2^{j+1} = \phi_2^j - \tau\left(\mathrm{div}\, \underline{u}\phi_2^j - \frac{\partial}{\partial z} \nu \frac{\partial \phi_2^j}{\partial z} - \mu\Delta\phi_2^j - \sigma\phi_2^j - f\right) + O(\tau^2). \tag{2.13}$$

Dividing (2.13) by τ and calculating the limit of the expression thus derived for $\tau \to 0$, we arrive at the equation

$$\frac{\partial \phi_2}{\partial t} + \mathrm{div}\, \underline{u}\phi_2 + \sigma\phi_2 = \frac{\partial}{\partial z} \nu \frac{\partial \phi_2}{\partial z} + \mu\Delta\phi_2 + f.$$

Hence, it follows that $\phi_2 \to \phi$, when $\tau \to 0$. Thus, we have shown that a combination of problems (2.5) and (2.6) does yield an approximate solution for problem (2.1) in a small time interval τ, provided all the functions involved are sufficiently smooth.

It should be noted that our estimates are fairly crude. Hence, the above analysis can be regarded as a proof of a fundamental result pertaining to approximation. Actually, the approximation of the initial problem by the split problem provides much better results. To make sure of it, we consider a model spatial two-dimensional problem corresponding to (2.1) for constant values of u, v. In this case, we have

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} + v\frac{\partial \phi}{\partial y} + \sigma\phi = \mu\Delta\phi, \tag{2.14}$$

$$\phi = g \quad \text{at} \quad t = 0.$$

Let $g(x, y)$ be defined in the entire plane (x, y) and decrease rather rapidly at infinity, so that the solution can be given as the Fourier integral

$$\phi = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Phi(m, n, t)e^{imx+iny}\, dm\, dn. \tag{2.15}$$

In a similar way,

$$g = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} A(m, n)\, e^{imx+iny}\, dm\, dn. \tag{2.16}$$

Multiplying the equation and the initial data of (2.14) by $\frac{1}{4\pi^2} e^{imx-iny}$ and integrating the result with respect to x and y, we obtain the problem for the Fourier coefficients

$$\frac{\partial\Phi}{\partial t} + [-imu - inv + \sigma + \mu(m^2 + n^2)]\Phi = 0, \tag{2.17}$$

$$\Phi = A \quad \text{at} \quad t = 0,$$

The solution of this problem is of the form

$$\Phi = A \exp\{[imu + inv - \sigma - \mu(m^2 + n^2)]t\}. \tag{2.18}$$

Substitution of (2.18) into (2.15) yields the exact solution

$$\phi = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} A(m, n) \exp\{im(x + ut) + in(y + vt) - [\sigma + \mu(m^2 + n^2)]t\}\cdot \tag{2.19}$$

$$\cdot dm\, dn.$$

take a time interval $0 \leqq t \leqq \tau$ and write on it two problems:

$$\frac{\partial\phi_1}{\partial t} + u\frac{\partial\phi_1}{\partial x} + v\frac{\partial\phi_1}{\partial y} = 0,$$

$$\phi_1 = g \quad \text{at} \quad t = 0.$$

$$\frac{\partial\phi}{\partial t} = \mu\Delta\phi - \sigma\phi, \tag{2.21}$$

$$\phi = \phi(x, y, \tau).$$

Let the function $g(x, y)$ be of the form (2.16). Consider similar Fourier integrals for the functions ϕ_1 and ϕ. Then, just as in the above consideration, we come to two problems:

$$\frac{d\Phi_1}{dt} - (imu + inv)\Phi_1 = 0, \tag{2.22}$$

$$\Phi_1 = A \quad \text{at} \quad t = 0;$$

for the Fourier coefficients Φ_1 of problem (2.20)

$$\frac{d\Phi}{dt} + [\sigma + \mu(m^2 + n^2)]\Phi = 0, \tag{2.23}$$

$$\Phi = \Phi_1(\tau) \quad \text{at} \quad t = \tau.$$

for the Fourier coefficients Φ of problem (2.21).

The solution for (2.22) is

$$\Phi_1(t) = A \exp \{(imu + inv)t\}; \tag{2.24}$$

and that for (2.23) is

$$\Phi(t) = \Phi_1(\tau) \exp \{-[\sigma + \mu(m^2 + n^2)]t\}. \tag{2.25}$$

Putting $t = \tau$ in (2.24) and substituting $\Phi_1(\tau)$ into (2.25), we have

$$\Phi(\tau) = A \exp \{(imu + inv)\tau - [\sigma + \mu(m^2 + n^2)]t\}. \tag{2.26}$$

Finally, putting $t = \tau$ in (2.26), we obtain

$$\Phi(\tau) = A \exp \{[imu + inv - \sigma - \mu(m^2 + n^2)]\tau\},$$

and, hence,

$$\phi = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} A(m, n) \exp \{im(x + u\tau) + in(y + v\tau) - \\ - [\sigma + \mu(m^2 + n^2)]\tau\} \, dm \, dn. \tag{2.27}$$

The value of τ has not so far been fixed. Suppose it is chosen arbitrarily. Let $t = \tau$ in (2.19). Then, (2.19) and (2.27) are just identical (for any τ). It is evident, however, that these solutions coincide only when $t = \tau$. If we endeavored to find a solution within the interval $0 \leq t \leq \tau$ using a split problem, the result would be only an approximate estimate. So, if we seek a solution for a discrete set of points $t = t_j$, we should successively solve the split problems, i.e. the problems

$$\frac{\partial\phi_1}{\partial t} + u\frac{\partial\phi_1}{\partial x} + v\frac{\partial\phi_1}{\partial y} = 0, \\ \phi_1 = \phi^j \quad \text{for} \quad t = t_j; \tag{2.28}$$

$$\frac{\partial\phi}{\partial t} = \mu\Delta\phi - \sigma\phi, \\ \phi = \phi_1^{j+1} \quad \text{for} \quad t = t_j. \tag{2.29}$$

This remarkable fact underlies the splitting of problems according to physical processes. Since in actual situations the coefficients u and v are, as a rule, time-dependent quantities, the splitting algorithm does not yield an exact solution for $t = t_j$ ($j = 1, 2, \ldots$). To obtain more accurate results, the time intervals should be taken sufficiently small, thereby ensuring a better approximation under substantial variation of the coefficients u, v. We have analyzed a two-dimensional case, but the same calculations apply to a general three-dimensional case as well.

Let us now examine problem (2.28), provided $u = \text{const}$, $v = \text{const}$. This problem will be solved in two stages. First, we solve the problem

$$\frac{\partial \phi_{11}}{\partial t} + u \frac{\partial \phi_{11}}{\partial x} = 0, \qquad \phi_{11} = \phi_1^j \quad \text{for} \quad t = t_j, \tag{2.30}$$

and then, the problem

$$\frac{\partial \phi_{12}}{\partial t} + v \frac{\partial \phi_{12}}{\partial y} = 0, \qquad \phi_{12} = \phi_{11}^{j+1} \quad \text{for} \quad t = t_j. \tag{2.31}$$

Similarly to the foregoing discussion, we can show, using the Fourier analysis, that the solutions for the initial problem (2.28) in the interval $t_j \leqq t \leqq t_{j+1}$ and for split problem (2.30), (2.31) coincide at $t = t_{j+1}$:

$$\phi_{12}^{j+1} = \phi_1^{j+1} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Phi_1^j(m, n) \exp\{im(x + u\tau) + in(y + v\tau)\} \, dm \, dn. \tag{2.32}$$

Here Φ_1^j is the Fourier transform of the function ϕ_1^j.

Now, let us solve problem (2.29) by the component splitting method. We split this problem into two parts:

for the variable x

$$\frac{\partial \phi_{21}}{\partial t} = \mu \frac{\partial^2 \phi_{21}}{\partial x^2} - \frac{\sigma}{2} \phi_{21}, \qquad \phi_{21} = \phi_{12}^{j+1} \quad \text{at} \quad t = t_j; \tag{2.33}$$

and for the variable y

$$\frac{\partial \phi_{22}}{\partial t} = \mu \frac{\partial^2 \phi_{22}}{\partial y^2} - \frac{\sigma}{2} \phi_{22}, \qquad \phi_{22} = \phi_{21}^{j+1} \quad \text{at} \quad t = t_j. \tag{2.34}$$

Solving these problems by the Fourier transformation method, we obtain the expression

$$\phi_{22}^{j+1} \equiv \phi^{j+1} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \Phi_1^{j+1}(m, n) \exp\{imx + iny - \\ - [\sigma + \mu(m^2 + n^2)]\tau\}\, dm\, dn, \tag{2.35}$$

which is an exact solution to the problem in the interval $t_j \leq t \leq t_{j+1}$.

And finally, we consider a more general case of splitting when problem (2.14) is split into the following components:

the first problem

$$\frac{\partial\phi_1}{\partial t} + u\frac{\partial\phi_1}{\partial x} + \frac{\sigma}{2}\phi_1 = \mu\frac{\partial^2\phi_1}{\partial x^2}, \\ \phi_1 = \phi_2^j \quad \text{at} \quad t = t_j; \tag{2.36}$$

the second problem

$$\frac{\partial\phi_2}{\partial t} + v\frac{\partial\phi_2}{\partial y} + \frac{\sigma}{2}\phi_2 = \mu\frac{\partial^2\phi_2}{\partial y^2}, \\ \phi_2 = \phi_1^{j+1} \quad \text{at} \quad t = t_j. \tag{2.37}$$

Fourier transformation yields a solution for problems (2.36), (2.37) which is just identical to the solution of problem (2.14) the interval $t_j \leq t \leq t_{j+1}$:

$$\phi_2^{j+1} \equiv \phi = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \Phi^j(m, n) \exp\{im(x + u\tau) + in(y + v\tau) - \\ - [\sigma + \mu(m^2 + n^2)]\tau\}\, dm\, dn. \tag{2.38}$$

As can be seen, the splitting of problem (2.38) falls under a variety of possibilities and in each case there exists an exact solution at a given moment t_j. An uncertainty that may arise under actual conditions is only due to variations in the values of u, v. To minimize a possible splitting error, the time interval should be taken rather small. Precisely for this purpose, it is reasonable to split general problem (2.14) on each interval $t_j \leq t \leq t_{j+1}$, $\tau = t_{j+1} - t_j$ into two problems related to different physical processes, since each of the processes generally involves particular physical balance relations which must not be violated even in the stage of the development of difference approximations. As regards the difference analogues of split systems, they should be solved by the multicomponent cyclic reduction outlined in the previous section.

Using the splitting method, we can also obtain solutions identical to the solution of problems like

$$\frac{\partial\phi}{\partial t} + A\phi = 0, \tag{2.39}$$

where $A = \sum_{i=1}^{n} A_i$, A_i are pairwise-commutative simple-shape matrices. In this case, the splitting scheme is as follows:

$$\frac{\partial\phi_1}{\partial t} + A_1\phi_1 = 0, \quad \phi_1 = \phi_n^j \quad \text{at } t = t_j; \tag{2.40}$$

$$\frac{\partial\phi_2}{\partial t} + A_2\phi_2 = 0, \quad \phi_2 = \phi_1^{j+1} \quad \text{at } t = t_j; \tag{2.41}$$

$$\cdots\cdots\cdots\cdots$$

$$\frac{\partial\phi_n}{\partial t} + A_n\phi_n = 0, \quad \phi_n = \phi_{n-1}^{j+1} \quad \text{at } t = t_j. \tag{2.42}$$

It is clear from the above analysis why the splitting method ensures such remarkably exact results in solving problems related to substance transport and diffusion, theory of climate, etc. Naturally, all this refers equally to a three-dimensional case, too.

3.3. Equation of Motion

The equation of substance transport along trajectories, which will be hereinafter called, for the sake of brevity, an *equation of motion*, is one of the simplest problems in mathematical physics. Its numerical solution, however, is hardly a simple task and requires careful choice of the solution algorithm.

Let us consider the equation of motion as a constituent of a more general problem (2.14). We have

$$\frac{d\phi}{dt} = 0,$$

where

$$\frac{d}{dt} = \frac{\partial}{\partial t} + u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y} + w\frac{\partial}{\partial z}.$$

This equation will be solved under an additional condition

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0.$$

The initial data will be taken as

$$\phi = g \quad \text{at} \quad t = 0.$$

The simplest problem of this type is a one-dimensional transport of a substance ϕ

$$\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} = 0,$$
$$\phi = g(x) \quad \text{at} \quad t = 0 \tag{3.1}$$

where u is the velocity, $g(x)$ is the initial distribution. The functions $\phi(x,y)$ and $g(x)$ are assumed to be 2π-periodic in x. If u = const, problem (3.1) has an obvious solution

$$\phi(x, t) = g(x - ut) \tag{3.2}$$

provided $g(x)$ is a differentiable function. Solution (3.2) describes the propagation of the initial perturbation along the characteristic curve $x - ut$ = const. This means that $\phi(x,y)$ = const on any straight line $x - ut$ = const. Thus, when $u > 0$, problem (3.1) defines perturbation propagation towards increasing values of x.

These well-known concepts should be borne in mind while elaborating difference analogues of problem (3.1). If the velocity $u = u(x,t)$ is variable, problem (3.1) cannot, in general, be solved analytically. Precisely in these cases, numerical methods based on difference approximations appear to be very useful.

We now consider simple difference schemes with c = const. Let us assume, for certainty, that $u > 0$. Then we have the explicit scheme

$$\frac{\phi_k^{j+1} - \phi_k^j}{\tau} + u \frac{\phi_k^j - \phi_{k-1}^j}{\Delta x} = 0 \tag{3.3}$$

and the implicit scheme

$$\frac{\phi_k^{j+1} - \phi_k^j}{\tau} + u \frac{\phi_k^{j+1} - \phi_{k-1}^{j+1}}{\Delta x} = 0, \tag{3.4}$$

where $\phi_k^j = (x_k, t_j)$.

One can see that scheme (3.3) becomes absolutely stable if it is modified as

$$\frac{\phi_k^{j+1} - \phi_k^j}{\tau} + u \frac{\phi_n^j - \phi_{n-1}^j}{\Delta x} = 0,$$

where $n = k\text{-entier}\,(\tau/\Delta x)$.

But if the difference expressions for $u\partial\phi/\partial x$ in (3.3) are taken in the form

$$u\,\frac{\phi_k^j - \phi_{k-1}^j}{\Delta x},$$

instead of

$$u\,\frac{\phi_{k+1}^j - \phi_k^j}{\Delta x}$$

the resultant scheme is unstable for any relation between the steps.

The two schemes are approximate to the first order in Δx and τ. Indeed, suppose the initial values of $g(x)$ and $\phi(x,t)$ are sufficiently smooth functions. We expand the solution of Eq.(3.1) in a Taylor series in the neighborhood of the point $x = x_k$, $t = t_j$:

$$\phi(x,\ t) = (\phi)_k^j + (\phi_t)_k^j(t - t_j) + (\phi_x)_k^j(x - x_k) + \ldots \tag{3.5}$$

Substituting (3.5) into (3.3), we obtain

$$\frac{\partial\phi}{\partial t} + u\,\frac{\partial\phi}{\partial x} = \frac{u\Delta x}{2}\,\frac{\partial^2\phi}{\partial x^2} - \frac{\tau}{2}\,\frac{\partial^2\phi}{\partial t^2}, \tag{3.6}$$

the discarded terms being of a higher order of smallness. It follows from (3.1) that

$$\frac{\partial^2\phi}{\partial t^2} = u^2\,\frac{\partial^2\phi}{\partial x^2}. \tag{3.7}$$

Then (3.6) takes the form

$$\frac{\partial\phi}{\partial t} + u\,\frac{\partial\phi}{\partial x} = \frac{u\Delta x - \tau u^2}{2}\,\frac{\partial^2\phi}{\partial x^2} \quad \text{for} \quad x = x_k, \quad t = t_j. \tag{3.8}$$

This analysis of difference schemes was suggested by A.I.Zhukov. When $u\tau/\Delta x < 1$, relation (3.8) can be interpreted as an equation with the solution range $x_{k-1} \leqq x \leqq x_k$, $t_j \leqq t \leqq t_{j+1}$.

Assuming that the discarded terms in (3.8) are small, we arrive at the heat conduction equation

$$\frac{\partial\phi}{\partial t} + u\,\frac{\partial\phi}{\partial x} = \mu\,\frac{\partial^2\phi}{\partial x^2},$$

where $\mu = (u\Delta x - u^2\tau)/2$ is the so-called coefficient of artificial or computation viscosity. It should be noted that if $u\tau/\Delta x = 1$, then $\mu = 0$ and all the other discarded terms are zero, i.e. explicit scheme (3.3) becomes a scheme of an infinite-order approximation in x and τ.

Of special interest is the case of $u\tau/\Delta x > 1$, where the equation

$$\frac{\partial\phi}{\partial t} + u\,\frac{\partial\phi}{\partial x} = -|\mu|\,\frac{\partial^2\phi}{\partial x^2}. \tag{3.9}$$

holds true.

One can easily see that Eq.(3.9) with the initial condition

$$\phi = \phi^{o}(x) \quad \text{at} \quad t = 0 \tag{3.10}$$

leads to an ill-defined Hadamard's problem whose solution is unstable under small variations of the initial data. In deriving difference equations for problem (3.1), we should take into account the condition $\mu = u\tau/\Delta x \leq 1$ that the problem is well-defined.

Let us now examine the computation stability of scheme (3.3). First, we consider the spectral problem

$$(A^{h}\omega)_{k} = u \frac{\omega_{k} - \omega_{k-1}}{\Delta x} = \lambda\omega_{k} \tag{3.11}$$

in an infinite-difference interval $D_h = -\infty < x_k < \infty$. The solution of (3.11), which is bounded in D_h, is

$$\omega_{k} = e^{ikp\Delta x}, \tag{3.12}$$

where p is an arbitrary integer. Substituting (3.12) into (3.11), we arrive at the formula for the eigenvalue

$$\lambda_{p} = \frac{u}{\Delta x} \left(2 \sin^2 \frac{p\Delta x}{2} + i \sin p\Delta x\right). \tag{3.13}$$

Write (3.3) in the operator form

$$\frac{\phi^{j+1} - \phi^{j}}{\tau} + A^{h}\phi^{j} = 0, \tag{3.14}$$

and seek a solution in the form

$$\phi^{j} = \sum_{p=-\infty}^{\infty} \phi_{p}^{j} e^{ikp\Delta x}, \tag{3.15}$$

where ϕ_p^j is the Fourier coefficient of the function ϕ^j. For the coefficients ϕ_p^j we obtain the equation

$$\frac{\phi_{p}^{j+1} - \phi_{p}^{j}}{\tau} + \lambda_{p}\phi_{p}^{j} = 0. \tag{3.16}$$

Hence,

$$\phi_{p}^{j+1} = T_{p}\phi_{p}^{j},$$

where $T_p = 1 - \tau\lambda_p$ is the transition factor for the Fourier coefficients.

The condition that none of the components ϕ_p^j increase in modulus is

$$|1 - \tau\lambda_p| \leq 1. \tag{3.17}$$

the inequality taking place if $u\tau/\Delta x \leq 1$. Indeed,

$$|1 - \tau\lambda_p|^2 = \left(1 - \frac{2u\tau}{\Delta x}\sin^2\frac{p\Delta x}{2}\right)^2 + \left(\frac{u\tau}{\Delta x}\right)^2 \sin^2 p\Delta x =$$

$$= 1 - 4\sin^2\frac{p\Delta x}{2}\left(\frac{u\tau}{\Delta x}\right)\left(1 - \frac{u\tau}{\Delta x}\right).$$

If $u\tau/\Delta x > 1$, then $|1 - \tau\lambda_p| > 1$. Therefore, it remains to consider the range of variation in $|1 - \tau\lambda_p|$ for $0 < u\tau/\Delta x \leq 1$ (recall that we assume $u > 0$). In the above interval, the function $\frac{u\tau}{\Delta x}(1 - \frac{u\tau}{\Delta x})$ takes a maximum value equal to 1/4 for $u\tau/\Delta x = 1/2$. In this case, $|1 - \tau\lambda_p| = 1 - \sin^2\frac{p\Delta x}{2} = \cos^2\frac{p\Delta x}{2}$. For other values of $u\tau/\Delta x$ in the interval $0 \leq u\tau/\Delta x \leq 1$, this positive function decreases and tends to zero at the extreme points $u\tau/\Delta x = 0$ and $u\tau/\Delta x = 1$. This means that we have the inequality

$$4\sin^2\frac{p\Delta x}{2}\left(\frac{u\tau}{\Delta x}\right)\left(1 - \frac{u\tau}{\Delta x}\right) \leq 1$$

which proves the statement. Thus, we have established the condition of computation stability of a difference scheme. Evidently, the stability criterion coincides in our case with the condition that Eq.(3.8) is well-defined.

Using the above method, we can readily show that scheme (3.4) also provides the first-order approximation in Δx and τ. Expansion into a Taylor series for $x = x_k$ and $t = t_j$ yields the equation similar to (3.8):

$$\frac{\partial\phi}{\partial t} + u\frac{\partial\phi}{\partial x} = \mu\frac{\partial^2\phi}{\partial x^2} + \ldots, \tag{3.18}$$

where $\mu = (u\Delta x - u^2\tau)/2$.

Even now we can see a fundamental difference between (3.8) and (3.18). The coefficient of computation viscosity is always positive in the latter equation. Consequently, Eq.(3.18) is always well-defined for the relevant sufficiently smooth initial data. It is a simple matter to show that difference Eq.(3.4) is stable for any relation between the steps, i.e. it is absolutely stable since the transition factor for each Fourier coefficient is $T_p \doteq 1/(1 + \tau\lambda_p)$. This implies that $|T_p| \leq 1$.

Among the most interesting and commonly used difference schemes, other than (3.3) and (3.4), we can point out the following two:

$$\frac{\phi_k^{j+1} - \phi_k^j}{\tau} + u\frac{\phi_{k+1}^{j+1} - \phi_{k-1}^{j+1}}{2\Delta x} = 0; \tag{3.19}$$

$$\frac{\phi_k^{j+1} - \phi_k^j}{\tau} + u\,\frac{\phi_{k+1}^{j+1/2} - \phi_{k-1}^{j+1/2}}{2\Delta x} = 0; \tag{3.20}$$

Here $\phi_k^{j+1/2} = \frac{1}{2}(\phi_k^{j+1} + \phi_k^j)$.

One can easily see that scheme (3.19) gives a first-order approximation in τ and a second-order approximation in Δx. The differential equation corresponding to this scheme is (3.18) where $\mu = u^2\tau/2$.

The scheme stability is determined by the transition operators for Fourier coefficients. We arrive, therefore, at the spectral problem

$$(A^h\omega)_k = u\,\frac{\omega_{k+1} - \omega_{k-1}}{2\Delta x} = \lambda\omega_k. \tag{3.21}$$

Its solution will be sought in the form (3.12). Thus, we have

$$\lambda_p = i\,\frac{u}{\Delta x}\sin p\Delta x, \tag{3.22}$$

hence we immediately obtain the equation for the Fourier coefficients

$$\frac{\phi_p^{j+1} - \phi_p^j}{\tau} + \lambda_p\phi_p^{j+1} = 0,$$

$$\phi_p^{j+1} = T_p\phi_p^j,$$

where

$$T_p = \frac{1}{1+\tau\lambda_p}. \tag{3.23}$$

With due regard to (3.22), we have $T_p = 1/(1 + i\,\frac{u\tau}{\Delta x}\sin p\Delta x)$ and, hence,

$$|T_p| = \left(\sqrt{1 + \left(\frac{u\tau}{\Delta x}\right)^2 \sin^2 p\Delta x}\right)^{-1} \leq 1.$$

This indicates an absolute computation stability of scheme (3.19).

Of particular interest to us, in view of applications, is the Cranck-Nickolson scheme (3.20). One is readily convinced that this scheme gives a second-order approximation in τ and Δx and is not dissipative. This means that in differential Eq.(3.18) $\mu = 0$ and the discarded terms are of the orders of $\tau\Delta x$, τ^2, and Δx^2. As regards the computation stability, we have in this case

$$T_p = \left(1 - i\,\frac{u\tau}{2\Delta x}\sin p\Delta x\right) / \left(1 + i\,\frac{u\tau}{2\Delta x}\sin p\Delta x\right),$$

and, hence, $|T_p| = 1$. Thus, this scheme is absolutely stable.

In conclusion, we consider another attractive method for numerical solution of problem (3.1) based on the so-called *running computation scheme* suggested by

L.D.Landau, N.N.Neiman, and I.M.Khalatnikov. The scheme is of the form

$$\frac{\phi_k^{j+1} - \phi_k^j}{\tau} + \frac{u}{\Delta x}\left[\left(\frac{\phi_k^{j+1} + \phi_k^j}{2}\right) - \left(\frac{\phi_{k-1}^{j+1} + \phi_{k-1}^j}{2}\right)\right] = 0. \qquad (3.24)$$

One can easily see that this scheme is approximate to the second order in τ and to the first order in x. It is defined by the recurrence relation

$$\phi_k^{j+1} = \frac{1 - u\tau/(2\Delta x)}{1 + u\tau/(2\Delta x)}\,\phi_k^j + \frac{u\tau/(2\Delta x)}{1 + u\tau/(2\Delta x)}\,(\phi_{k-1}^{j+1} + \phi_{k-1}^j). \qquad (3.25)$$

It can be readily demonstrated by the Fourier analysis of stability, in the sense of J.von Neumann, that scheme (3.24) is absolutely stable.

Similarly, we can elaborate an absolutely stable running computation scheme for a multidimensional problem of motion and prove that it is absolutely stable for an equation with constant coefficients.

We have always assumed above that the function u is time-constant and positive. If u is negative, then replacing x by $-x$, we arrive at the above equation. Of particular interest for applications, however, is the case of $u = u(x, t)$. Even a simple analysis reveals that in this situation computation stability can fail, despite the use of implicit dissipative schemes. This fact shows up especially in non-linear problems. The main point here is as follows. If the solution of a difference problem and the coefficient $u(x_k, t_j)$ are expanded in a Fourier series, the product of the Fourier series gives rise to harmonics which are either longer or shorter than the interacting harmonics. As a result, the energy related to rounding-off errors may sometimes be transferred from longer to shorter waves, thereby making the computation process unstable, although this difference scheme with a constant coefficient is computation-stable. This kind of instability is generally termed *non-linear instability*. Sometimes, it also arises in solving linear problems with variable coefficients. It is, therefore, of current interest to elaborate perturbation-stable difference schemes for non-linear equations or for equations with variable coefficients. In most cases, computation instability can be eliminated by using dissipative difference schemes with a suitable choice of the computation viscosity coefficient μ. But such schemes give, as a rule, a first-order approximate either in τ, or in Δx, or both in τ and in Δx.

Of particular interest to applications are equations of the form

$$\frac{\partial\phi}{\partial t} + \frac{\partial u\phi}{\partial x} = 0, \qquad (3.26)$$

where $u = u(x, t)$. The difference schemes for this type of equations, which are absolutely stable and provide a first-order or even a second-order approximation for some classes of coefficients, will be studied for multidimensional equations of the form (3.26).

Let us analyse the motion of a particle ensemble along given trajectories in the (x, y) plane. Within the framework of the mechanics of continuous media, we arrive at the problem

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} + v\frac{\partial \phi}{\partial y} = 0, \qquad \phi(x, y, 0) = g, \tag{3.27}$$

where $u = u(x, y, t)$, $v = v(x, y, t)$. Assume that the components of the velocity vector, u and v, at each moment satisfy the continuity equation

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0. \tag{3.28}$$

Let a solution be sought in the rectangular domain D, $\{0 \le x \le a, 0 \le y \le b\}$, and let the solution of problem (3.27) together with the coefficients u and v be periodic and take the same values on the opposing boundaries of the rectangle.

Write (3.27) in the operator form

$$\frac{\partial \phi}{\partial t} + A\phi = 0, \qquad \phi = g \quad \text{at} \quad t = 0 \tag{3.29}$$

where $A = u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y}$.

Evidently, for our problem the operator A satisfies the condition $(A\phi, \phi) = 0$. Indeed, introducing a scalar product, we write

$$(A\phi, \phi) = \int_0^a dx \int_0^b \left(u\frac{\partial \phi}{\partial x} + v\frac{\partial \phi}{\partial y}\right)\phi dy. \tag{3.30}$$

With due regard to (3.28), the integrand is transformed to

$$\left(u\frac{\partial \phi}{\partial x} + v\frac{\partial \phi}{\partial y}\right)\phi = \tfrac{1}{2}\left(\frac{\partial u\phi^2}{\partial x} + \frac{\partial v\phi^2}{\partial y}\right);$$

whence it follows that

$$(A\phi, \phi) = \int_0^a dx \int_0^b \tfrac{1}{2}\left(\frac{\partial u\phi^2}{\partial x} + \frac{\partial v\phi^2}{\partial y}\right) dy, \tag{3.31}$$

Hence, taking into account that the solution is periodic on the boundaries, we obtain

$$(A\phi, \phi) = 0. \tag{3.32}$$

Thus, the operator A can be reduced to an antisymmetric form, thereby permitting an elaboration of absolutely stable difference schemes.

Now we shall try to split the operator A in such a manner that each of the elementary operators A_α ($\alpha = 1, 2$) also satisfies the condition

$$(A_\alpha \phi, \phi) = 0. \tag{3.33}$$

In this case, the difference scheme of component splitting provides an absolutely stable scheme with a second-order approximation.

A formal decomposition of the operator A into constituents

$$A_1 = u \frac{\partial}{\partial x}, \quad A_2 = v \frac{\partial}{\partial y} \tag{3.34}$$

is not compatible with condition (3.33). One can easily see that the following relations are valid:

$$(A_1 \phi, \phi) = -\frac{1}{2} \int_0^a dx \int_0^b \phi^2 \frac{\partial u}{\partial x} dy,$$

$$(A_2 \phi, \phi) = -\frac{1}{2} \int_0^a dx \int_0^b \phi^2 \frac{\partial v}{\partial y} dy.$$

This means that we cannot use A_1 and A_2 as elementary operators in the elaboration of the successive splitting scheme.

Now let us choose the operators A_1 and A_2 in a more complicated form

$$A_1 \phi = u \frac{\partial \phi}{\partial x} + \frac{\phi}{2} \frac{\partial u}{\partial x}, \quad A_2 \phi = v \frac{\partial \phi}{\partial y} + \frac{\phi}{2} \frac{\partial v}{\partial y}. \tag{3.35}$$

It is evident that each of these operators satisfies condition (3.33) and their sum is exactly equal to A

$$(A_1 + A_2)\phi = u \frac{\partial \phi}{\partial x} + v \frac{\partial \phi}{\partial y} + \frac{\phi}{2} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) = u \frac{\partial \phi}{\partial x} + v \frac{\partial \phi}{\partial y} = A\phi.$$

Here we have employed the fact that the coefficients u and v satisfy Eq.(3.28).

So, all the necessary conditions for the splitting method applicability are now valid, and we come to the splitting scheme in the interval $t_{j-1} \leqq t \leqq t_{j+1}$

$$\frac{\phi^{j-1/2} - \phi^{j-1}}{\tau} + \left(u^j \frac{\partial}{\partial x} + \frac{1}{2} \frac{\partial u^j}{\partial x}\right) \frac{\phi^{j-1/2} + \phi^{j-1}}{2} = 0,$$

$$\frac{\phi^j - \phi^{j-1/2}}{\tau} + \left(v^j \frac{\partial}{\partial y} + \frac{1}{2} \frac{\partial u^j}{\partial y}\right) \frac{\phi^j + \phi^{j-1/2}}{2} = 0, \tag{3.36}$$

$$\frac{\phi^{j+1/2} - \phi^j}{\tau} + \left(v^j \frac{\partial}{\partial y} + \frac{1}{2}\frac{\partial u^j}{\partial y}\right)\frac{\phi^{j+1/2} + \phi^j}{2} = 0,$$

$$\frac{\phi^{j+1} - \phi^{j+1/2}}{\tau} + \left(u^j \frac{\partial}{\partial x} + \frac{1}{2}\frac{\partial u^j}{\partial x}\right)\frac{\phi^{j+1} + \phi^{j+1/2}}{2} = 0.$$

If the functions u and v as well as the solution ϕ are sufficiently smooth for all the variables, scheme (3.36) is approximate to the second order and is absolutely stable

$$\|\phi^{j+1}\| = \|\phi^{j-1}\| = \ldots = \|g\|. \tag{3.37}$$

This is an instructive example to show that a formal decomposition into operators (3.34) may compromise the very idea of splitting and that only some additional considerations may lead to schemes which are proved theoretically and effective in application.

Following this preliminary introduction, we will now elaborate difference schemes for solving problem (3.27) in space variables and in time. To this end, we first consider the optimal methods of approximating the operator A with respect to space variables x and y. As was already noted, a convenient method of approximating problems in mathematical physics which preserves the additive properties and qualitative features of the operator, is a coordinate approximation. Precisely this method will be used to elaborate difference schemes.

Suppose the coefficients u and v are sufficiently smooth and consider Eq.(3.27) in the divergent form

$$\begin{gathered}\frac{\partial\phi}{\partial t} + \frac{\partial u\phi}{\partial x} + \frac{\partial v\phi}{\partial y} = 0 \quad \text{in} \quad D \cdot D_t, \\ \phi = g \quad \text{in} \quad D \text{ for } t = 0.\end{gathered} \tag{3.38}$$

To construct the difference scheme, we shall use the operator defined as

$$A\phi = \frac{\partial u\phi}{\partial x} + \frac{\partial v\phi}{\partial y} - \frac{\phi}{2}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right), \tag{3.39}$$

and consider the following difference analogue of this relation:

$$\begin{aligned}(\Lambda^h\phi)_{k\ell} = {} & \frac{u_{k+1,\ell}\phi_{k+1,\ell} - u_{k-1,\ell}\phi_{k-1,\ell}}{2\Delta x} + \frac{v_{k,\ell+1}\phi_{k,\ell+1} - v_{k,\ell-1} - v_{k,\ell-1}\phi_{k,\ell-1}}{2\Delta y} - \\ & - \frac{\phi_{k\ell}}{2}\left(\frac{u_{k+1,\ell} - u_{k-1,\ell}}{2\Delta x} + \frac{v_{k,\ell+1} - v_{k,\ell-1}}{2\Delta y}\right).\end{aligned} \tag{3.40}$$

Evidently, difference expression (3.40) approximates (3.39) to the second order in Δx and Δy for sufficiently smooth functions u, v, and ϕ. But this expression has a substantial shortcoming, since in this form the operator Λ is no longer antisymmetric, i.e.

$$(\Lambda^h\phi,\ \phi) \neq 0. \tag{3.41}$$

This implies that the conventional approximation does not fit the form of the computation algorithm used to solve problem (3.27).

We now show that the approximation of (3.39) in the form

$$(\Lambda^h\phi)_{k\ell} = \frac{u_{k+1/2,\ell}\phi_{k+1,\ell} - u_{k-1/2,\ell}\phi_{k-1,\ell}}{2\Delta x} + \frac{v_{k,\ell+1/2}\phi_{k,\ell+1} - v_{k,\ell-1/2}\phi_{k,\ell-1}}{2\Delta y} \tag{3.42}$$

satisfies the basic relation

$$(\Lambda^h\phi,\ \phi) = 0 \tag{3.43}$$

and is of the second order in Δx and Δy. To this end, we shall approximate the coefficients as follows:

$$\begin{aligned}
u_{k+1/2,\ell} &= u_{k+1,\ell} - \frac{u_{k+1,\ell} - u_{k\ell}}{2},\\
v_{k,\ell+1/2} &= v_{k,\ell+1} - \frac{v_{k,\ell+1} - v_{k\ell}}{2},\\
u_{k-1/2,\ell} &= u_{k-1,\ell} + \frac{u_{k\ell} - u_{k-1,\ell}}{2},\\
v_{k,\ell-1/2} &= v_{k,\ell-1} + \frac{v_{k\ell} - v_{k,\ell-1}}{2}.
\end{aligned} \tag{3.44}$$

Substituting (3.44) into((3.42), we obtain after simple transformations

$$\begin{aligned}
(\Lambda^h\phi)_{k\ell} = {} & \frac{u_{k+1,\ell}\phi_{k+1,\ell} - u_{k-1,\ell}\phi_{k-1,\ell}}{2\Delta x} + \\
& + \frac{v_{k,\ell+1}\phi_{k,\ell+1} - v_{k\ell-1}\phi_{k,\ell-1}}{2\Delta y} - \frac{\phi_{k\ell}}{2}\left(\frac{u_{k+1,\ell}u_{k-1,\ell}}{2\Delta x} + \frac{v_{k,\ell+1} - v_{k,\ell-1}}{2\Delta y}\right) - \\
& - (\Delta x^2 R_{k\ell} + \Delta y^2 Q_{k\ell}),
\end{aligned} \tag{3.45}$$

where

$$R_{k\ell} \to \frac{1}{4}\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\frac{\partial \phi}{\partial x}\right), \quad Q_{k\ell} \to \frac{1}{4}\frac{\partial}{\partial y}\left(\frac{\partial v}{\partial y}\frac{\partial \phi}{\partial y}\right).$$

for $\Delta x \to 0$ and $\Delta y \to 0$.

Now let us assume that the coefficients $u_{k\ell}$, $v_{k\ell}$ satisfy the difference analogue of the continuity equation

$$\frac{u_{k+1,\ell} - u_{k-1,\ell}}{2\Delta x} + \frac{v_{k,\ell+1} - v_{k,\ell-1}}{2\Delta y} = 0\ (h^2). \tag{3.46}$$

If the coefficients u, v, and the solution ϕ have finite second-order derivatives with respect to x and y and if condition (3.46) is satisfied, expression (3.45) differs from (3.40) in the same order as (3.40) differs from (3.39). Thus, we have demonstrated that expression (3.42) approximates (3.39) to the second order in Δx and Δy.

We now demonstrate that the operator thus constructed meets condition (3.43) and, what is more, each of the operators Λ_1 and Λ_2 defined by

$$\begin{aligned}\Lambda_1\phi &= \frac{u_{k+1/2,\ell}\phi_{k+1,\ell} - u_{k-1/2,\ell}\phi_{k-1,\ell}}{2\Delta x},\\ \Lambda_2\phi &= \frac{v_{k,\ell+1/2}\phi_{k,\ell+1} - v_{k,\ell-1/2}\phi_{k,\ell-1}}{2\Delta y},\end{aligned} \tag{3.47}$$

also satisfies the condition

$$(\Lambda_\alpha\phi,\ \phi) = 0. \tag{3.48}$$

For this purpose, we define a scalar product for vector quantities $\underline{a}$, $\underline{b}$ as

$$(\underline{a},\ \underline{b}) = \sum_k \sum_\ell a_{k\ell} b_{k\ell} \Delta x\ \Delta y;$$

hence,

$$\begin{aligned}(\Lambda_1\underline{\phi},\ \underline{\phi}) &= \frac{1}{2} \sum_k \sum_\ell \Delta y (u_{k+1/2,\ell}\phi_{k+1,\ell} - u_{k-1/2,\ell}\phi_{k-1,\ell})\ \phi_{k\ell},\\ (\Lambda_2\underline{\phi},\ \underline{\phi}) &= \frac{1}{2} \sum_\ell \sum_k \Delta x (v_{k,\ell+1/2}\ \phi_{k,\ell+1} - v_{k,\ell-1/2}\ \phi_{k,\ell-1})\ \phi_{k\ell}.\end{aligned} \tag{3.49}$$

Collecting terms in (3.49), we obtain Eqs.(3.48) which directly imply condition (3.43). Thus, we have accomplished necessary space approximations. Now, our aim is to reduce in time the system of ordinary differential equations

$$\begin{aligned}\frac{\partial\underline{\phi}^h}{\partial t} + \Lambda\underline{\phi}^h &= 0,\\ \underline{\phi}^h &= \underline{g}^h,\end{aligned} \tag{3.50}$$

where $\Lambda = \Lambda_1 + \Lambda_2$, $\underline{\phi}$ is the vector function with the components $\phi_{k\ell}$, and $\Lambda_\alpha\phi$ satisfies condition (3.48). This means that problem (3.50) can be solved using the splitting method. Omitting the superscript h (as inessential) in the functions and operators we obtain the system

$$\frac{\phi^{j-1/2} - \phi^{j-1}}{\tau} + \Lambda_1^j \frac{\phi^{j-1/2} + \phi^{j-1}}{2} = 0,$$

$$\frac{\phi^{j} - \phi^{j-1/2}}{\tau} + \Lambda_2^j \frac{\phi^{j} + \phi^{j-1/2}}{2} = 0,$$

$$\frac{\phi^{j+1/2} - \phi^{j}}{\tau} + \Lambda_2^j \frac{\phi^{j+1/2} + \phi^{j}}{2} = 0, \tag{3.51}$$

$$\frac{\phi^{j+1} - \phi^{j+1/2}}{\tau} + \Lambda_1^j \frac{\phi^{j+1} + \phi^{j+1/2}}{2} = 0.$$

on the interval $t_{j-1} \leqq t \leqq t_{j+1}$.

Thus, problem (3.27) has been reduced to the system of simple one-dimensional difference equations which can be solved by factorizing three-point difference equations. Similarly, we can also solve the equation of motion in three-dimensional space, when $A = A_1 + A_2 + A_3$.

It is noteworthy that the solution of the equation of motion by coordinate splitting, with the space operator approximated by finite-difference operators in the form (3.40), is not a unique method admits a quadratic invariant in the difference form. We now give another example concerned with the solution of a (three-dimensional) transport equation based on separation of the barotropic component of the velocity. In this case, the problem is reduced to a series of plane problems for domain sections, which enables us to effectively employ the finite-element method to make the differential operators discrete.

So, we consider the equation

$$\frac{\partial\phi}{\partial t} + u\frac{\partial\phi}{\partial x} + v\frac{\partial\phi}{\partial y} + w\frac{\partial\phi}{\partial z} = 0, \tag{3.52}$$

$$\phi = g \quad \text{at} \quad t = 0$$

in the domain (0, T) G, where G is the three-dimensional cylinder with the base $\sum_o$, upper base $\sum_H$, and lateral surface $\sum$. As previously, the coefficients are assumed to obey the continuity equation

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0. \tag{3.53}$$

Besides, it is required that

$$u_n = 0 \quad \text{on} \quad \textstyle\sum_o, \ \sum_H, \ \sum \tag{3.54}$$

It is well known that processes taking place in the atmosphere or in the ocean are quasi-horizontal, i.e. the horizontal scales of motion and velocity markedly exceed,on the average, the vertical scales. Hence, horizontal motions play a dominant role in planetary-scale geographical processes. Nevertheless, vertical processes, though of a relatively small scale, should also be taken into consideration to ensure a correct description of the vertical distribution of the characteristics in the medium. By separating the barotropic component in this case we can distinguish between the motions of different quantities and scales and simplify considerably the solution of the problem.

Thus, we shall represent the velocity components as

$$u = \bar{u} + u', \quad v = \bar{v} + v', \quad w = w', \tag{3.55}$$

where

$$\bar{u} = \frac{1}{H} \int_0^H u \, dz, \quad \bar{v} = \frac{1}{H} \int_0^H v \, dz.$$

Then, $\bar{\underline{u}}$, $\bar{v}$, u', v' will satisfy the continuity equations of the form

$$\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} = 0, \tag{3.56}$$

$$\frac{\partial u'}{\partial x} + \frac{\partial v'}{\partial y} + \frac{\partial w}{\partial z} = 0. \tag{3.57}$$

Using Eq.(3.56), we can define a *stream function* Ψ by the relations

$$\bar{u} = -\frac{\partial \Psi}{\partial y}, \quad \bar{v} = \frac{\partial \Psi}{\partial x} \tag{3.58}$$

or

$$\Delta\Psi = \mathrm{rot}\, \bar{\underline{u}}, \quad \Psi|_{\Sigma} = 0. \tag{3.59}$$

We shall employ (3.57) to find the vertical velocity component w. Integrating (3.57) along the vertical between z and H and allowing for the fact that $w_H = 0$, we obtain

$$w = \frac{\partial}{\partial x} \int_z^H u' dz + \frac{\partial}{\partial y} \int_z^H v' \, dz. \tag{3.60}$$

Introducing the notation

$$\hat{u} = \int_z^H u' \, dz, \quad \hat{v} = \int_z^H v' \, dz \tag{3.61}$$

and substituting (3.56), (3.58), (3.61) into (3.52), we arrive at the equation

$$\frac{\partial \phi}{\partial t} - \frac{\partial}{\partial x} \Psi \frac{\partial \phi}{\partial y} + \frac{\partial}{\partial y} \Psi \frac{\partial \phi}{\partial x} - \frac{\partial}{\partial z} \hat{u} \frac{\partial \phi}{\partial x} + \frac{\partial}{\partial x} \hat{u} \frac{\partial \phi}{\partial z} - \frac{\partial}{\partial z} \hat{v} \frac{\partial \phi}{\partial y} + \frac{\partial}{\partial y} \hat{v} \frac{\partial \phi}{\partial z} = 0. \tag{3.62}$$

Consider the space operator of this equation. It can be represented in the form

$$A = A_{xy} + A_{xz} + A_{yz},$$

where

$$A_{xy} = -\frac{\partial}{\partial x}\Psi\frac{\partial}{\partial y} + \frac{\partial}{\partial y}\Psi\frac{\partial}{\partial x},$$
$$A_{xz} = -\frac{\partial}{\partial z}\hat{u}\frac{\partial}{\partial x} + \frac{\partial}{\partial x}\hat{u}\frac{\partial}{\partial z}, \tag{3.63}$$
$$A_{yz} = -\frac{\partial}{\partial z}\hat{v}\frac{\partial}{\partial y} + \frac{\partial}{\partial y}\hat{v}\frac{\partial}{\partial z}.$$

Analysing the functional of energy for A_{xy}, A_{xz}, A_{yz}, we can prove that

$$(A_{xy}\phi, \phi) = 0, \quad (A_{xz}\phi, \phi) = 0, \quad (A_{yz}\phi, \phi) = 0. \tag{3.64}$$

Thus, the operator A is again represented as the sum of antihermitian operators. Hence, we can solve (3.62) for time, using the above two-cycle splitting scheme. Then, for each interval we obtain a set of problems to be solved successively

$$\begin{aligned}
&\frac{\phi^{j-2/3} - \phi^{j-1}}{\tau} + A^j_{xy}\frac{\phi^{j-2/3} + \phi^{j-1}}{2} = 0,\\
&\frac{\phi^{j-1/3} - \phi^{j-2/3}}{\tau} + A^j_{xz}\frac{\phi^{j-1/3} + \phi^{j-2/3}}{2} = 0,\\
&\frac{\phi^{j} - \phi^{j-1/3}}{\tau} + A^j_{yz}\frac{\phi^{j} + \phi^{j-1/3}}{2} = 0,\\
&\frac{\phi^{j+1/3} - \phi^{j}}{\tau} + A^j_{yz}\frac{\phi^{j+1/3} + \phi^{j}}{2} = 0,\\
&\frac{\phi^{j+2/3} - \phi^{j+1/3}}{\tau} + A^j_{xz}\frac{\phi^{j+2/3} + \phi^{j+1/3}}{2} = 0,\\
&\frac{\phi^{j+1} - \phi^{j+2/3}}{\tau} + A^j_{xy}\frac{\phi^{j+1} + \phi^{j+2/3}}{2} = 0.
\end{aligned} \tag{3.65}$$

Since conditions (3.64) are satisfied for the operators A_{xy}, A_{xz}, A_{yz}, scheme (3.65) is absolutely stable.

Let us now consider the method of spatial discretization of two-dimensional operators A_{xy}, A_{xz}, and A_{yz}. In this case, approximations on sections parallel to the coordinate planes are carried out best of all by the *finite element method*, which yields difference operators obeying an analogue of the conservation law.

Let us illustrate the application of this method for a two-dimensional equation containing A_{xy} as a space operator defined by the first of relations (3.63)

$$\frac{\partial \phi}{\partial t} + A_{xy}\phi = 0, \qquad \phi = g \quad \text{at} \quad t = 0 \tag{3.66}$$

in a rectangular domain $G = \{(x, y) \mid 0 \le x \le a,\ 0 \le y \le b\}$ with the boundary $\sum$.

As we know, the finite element method is the Galerkin method for coordinate functions with a finite support. To define the coordinate functions, we introduce in G a network domain G^h with steps Δx and Δy along the coordinate directions

$$G^h = \{(x_i, y_j) \mid x_i = i\Delta x,\ y_j = j\Delta y,\ i = \overline{0, M},\ \ j = \overline{0, N},\ \ M = a/\Delta x,\ N = b/\Delta y\}.$$

The cells of the network G are triangulated by positive diagonals. Let us define in G continuous functions $\omega_{mn}(x, y)$ which are linear in each triangle and such that

$$\omega_{mn}(x_i, y_j) = \begin{cases} 1, & (i, j) = (m, n), \quad i, m = \overline{0, M}, \\ 0, & (i, j) \ne (m, n), \quad j, n = \overline{0, N}. \end{cases}$$

The functions $\omega_{mn}(x, y)$ have a hexagon as a carrier (figure 3.1), and the functions themselves are shown in figure 3.2.

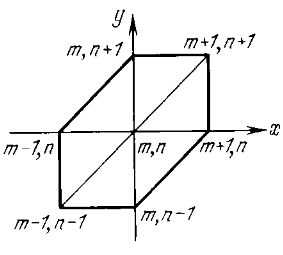


FIGURE 3.1

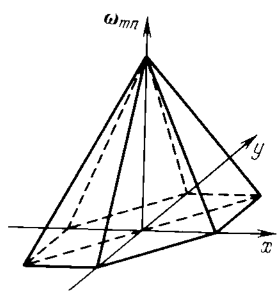


FIGURE 3.2

According to the Galerkin method, an approximate solution is sought as a linear combination of the coordinate functions

$$\bar{\phi} = \sum_{m=0}^{M} \sum_{n=0}^{N} \phi_{mn}(t) \quad \omega_{mn}(x, y). \tag{3.67}$$

Then, using a quadrature formula to calculate the evolution term, we can write the equations for the coefficients $\phi_{mn}(t)$

$$\left(\iint_G \omega_{mn} \, dx \, dy \right) \frac{\partial \phi_{mn}}{\partial t} + \iint_G \left(\Psi \frac{\partial \bar{\phi}}{\partial y} \frac{\partial \omega_{mn}}{\partial x} - \Psi \frac{\partial \bar{\phi}}{\partial x} \frac{\partial \omega_{mn}}{\partial y} \right) dx \, dy = 0, \tag{3.68}$$

$$\phi_{mn}(0) = g.$$

Substituting (3.67) into (3.68), we obtain

$$\kappa_{mn} \frac{\partial \phi_{mn}}{\partial t} + \int_G \left\{ \Psi \frac{\partial}{\partial y} \left(\sum_{i,j}^{M,N} \phi_{ij} \omega_{ij} \right) \frac{\partial \omega_{mn}}{\partial x} - \Psi \frac{\partial}{\partial x} \left(\sum_{i,j}^{M,N} \phi_{ij} \omega_{ij} \right) \cdot \frac{\partial \omega_{mn}}{\partial y} \right\} dx \, dy = 0, \tag{3.69}$$

where $\kappa_{mn} = \int_D \omega_{mn} \, dx \, dy$. Since the functions ω_{mn} are linear, their derivatives on the triangles T^i_{mn} take the values presented in table 3.1.

TABLE 3.1

	T^1_{mn}	T^2_{mn}	T^3_{mn}	T^4_{mn}	T^5_{mn}	T^6_{mn}
$\frac{\partial \omega_{mn}}{\partial x}$	$-\frac{1}{\Delta x}$	0	$\frac{1}{\Delta x}$	$\frac{1}{\Delta x}$	0	$-\frac{1}{\Delta x}$
$\frac{\partial \omega_{mn}}{\partial y}$	0	$-\frac{1}{\Delta y}$	$-\frac{1}{\Delta y}$	0	$\frac{1}{\Delta y}$	$\frac{1}{\Delta y}$

Evaluating the integrals in (3.69) and collecting terms, we finally arrive at a problem which can be expressed in the matrix form

$$\kappa \frac{\partial \phi_h}{\partial t} + \Lambda \phi_h = 0, \tag{3.70}$$

$$\phi = g \quad \text{at} \quad t = 0.$$

Here $[\phi_h]_{mn} = \phi_{mn} \int_D \omega_{mn} \, dx \, dy$ and Λ is the difference operator which is of the form

$$[\Lambda \phi_h]_{mn} = \frac{1}{\Delta x \Delta y} [(\bar{\Psi}^{(2)}_{mn} - \bar{\Psi}^{(3)}_{mn}) \phi_{m,n+1} + (\bar{\Psi}^{(5)}_{mn} - \bar{\Psi}^{(6)}_{mn}) \phi_{m,n-1} +$$
$$+ (\bar{\Psi}^{(6)}_{mn} - \bar{\Psi}^{(1)}_{mn}) \phi_{m+1,n} + (\bar{\Psi}^{(3)}_{mn} - \bar{\Psi}^{(4)}_{mn}) \phi_{m-1,n} + \tag{3.71}$$
$$+ (\bar{\Psi}^{(1)}_{mn} - \bar{\Psi}^{(2)}_{mn}) \phi_{m+1,n+1} + (\bar{\Psi}^{(4)}_{mn} - \bar{\Psi}^{(5)}_{mn}) \phi_{m-1,n-1}],$$

$$\overline{\Psi}^{(i)}_{mn} = \int\limits_{T^i_{mn} \cap D} \Psi \, dx\, dy.$$

at the point (x_m, y_n).

To verify how problem (3.70) approximates the initial problem (3.52), we substitute a smooth function into (3.52) and expand this function as well as the coefficients of (3.70) into a Taylor series in the neighborhood of the point (x_m, y_n). Performing all calculations, we find that problem (3.70) approximates (3.52) up to the terms of the order Δx^2.

If each Eq.(3.70) is multiplied by ϕ_{mn} and summed over all $m = \overline{0, M}$, $n = \overline{0, N}$, we get the relation

$$\frac{\kappa}{2} \frac{\partial(\phi_h, \phi_h)_h}{\partial t} = 0,$$

which is a difference representation of the quadratic conservation law for (3.70). This follows from the fact that

$$(\Lambda\phi_h, \phi_h)_h = 0. \tag{3.72}$$

Let us prove the validity of this relation. Examining (3.71), we see that the coefficients of the operator satisfy the following relations:

$$\begin{aligned}
(\overline{\Psi}^{(2)}_{mn} - \overline{\Psi}^{(3)}_{mn}) &= -(\overline{\Psi}^{(5)}_{m,n+1} - \overline{\Psi}^{(6)}_{m,n+1}), \\
(\overline{\Psi}^{(6)}_{mn} - \overline{\Psi}^{(1)}_{mn}) &= -(\overline{\Psi}^{(3)}_{m+1,n} - \overline{\Psi}^{(4)}_{m+1,n}), \\
(\overline{\Psi}^{(1)}_{mn} - \overline{\Psi}^{(2)}_{mn}) &= -(\overline{\Psi}^{(4)}_{m+1,n+1} - \overline{\Psi}^{(5)}_{m+1,n+1}).
\end{aligned} \tag{3.73}$$

Rearranging the terms of (3.72) one can easily demonstrate that

$$\begin{aligned}
(\Lambda\phi_h, \phi_h)_h = \sum_{m=0}^{M} \sum_{n=0}^{N} \frac{1}{\Delta x \Delta y} [& (\overline{\Psi}^{(2)}_{mn} - \overline{\Psi}^{(3)}_{mn}) \phi_{m,n+1} + (\overline{\Psi}^{(5)}_{mn} - \overline{\Psi}^{(6)}_{mn}) \phi_{m,n-1} + \\
& + (\overline{\Psi}^{(6)}_{mn} - \overline{\Psi}^{(1)}_{mn}) \phi_{m+1,n} + (\overline{\Psi}^{(3)}_{mn} - \overline{\Psi}^{(4)}_{mn}) \phi_{m-1,n} + \\
& + (\overline{\Psi}^{(1)}_{mn} - \overline{\Psi}^{(2)}_{mn}) \phi_{m+1,n+1} + (\overline{\Psi}^{(4)}_{mn} - \overline{\Psi}^{(5)}_{mn}) \phi_{m-1,n-1}] \phi_{mn} = 0.
\end{aligned}$$

Consider the structure of the operator Λ. It is evident from (3.71) that this operator can be represented as the sum of one-dimensional operators

$$\Lambda = \Lambda_1 + \Lambda_2 + \Lambda_3,$$

where

$$[\Lambda_1\phi_h]_{mn} = (\overline{\Psi}^{(2)}_{mn} - \overline{\Psi}^{(3)}_{mn})\phi_{m,n+1} + (\overline{\Psi}^{(5)}_{mn} - \overline{\Psi}^{(6)}_{mn})\phi_{m,n-1},$$

$$[\Lambda_2\phi_h]_{mn} = (\overline{\Psi}^{(6)}_{mn} - \overline{\Psi}^{(1)}_{mn})\phi_{m+1,n} + (\overline{\Psi}^{(3)}_{mn} - \overline{\Psi}^{(4)}_{mn})\phi_{m-1,n}, \tag{3.74}$$

$$[\Lambda_3\phi_h]_{mn} = (\overline{\Psi}^{(1)}_{mn} - \overline{\Psi}^{(2)}_{mn})\phi_{m+1,n+1} + (\overline{\Psi}^{(4)}_{mn} - \overline{\Psi}^{(5)}_{mn})\phi_{m-1,n-1},$$

As for the operator Λ, the relations

$$(\Lambda_1\phi_h, \phi_h) = 0, \ (\Lambda_2\phi_h, \phi_h) = 0, \ (\Lambda_3\phi_h, \phi_h) = 0. \tag{3.75}$$

are also valid for the operators Λ_1, Λ_2, and Λ_3. This means that to solve (3.70) for time, we can employ the splitting method, which will be absolutely stable. In each step, the operator is reversed by the factorization method.

In the interval $t_{j-1} \leqq t \leqq t_{j+1}$ the scheme is

$$\begin{aligned}
&\kappa\frac{\phi_h^{j-2/3} - \phi_h^{j-1}}{\tau} + \Lambda_1\frac{\phi_h^{j-2/3} + \phi_h^{j-1}}{2} = 0,\\
&\kappa\frac{\phi_h^{j-1/3} - \phi_h^{j-2/3}}{\tau} + \Lambda_2\frac{\phi_h^{j-1/3} + \phi_h^{j-2/3}}{2} = 0,\\
&\kappa\frac{\phi_h^{j} - \phi_h^{j-1/3}}{\tau} + \Lambda_3\frac{\phi_h^{j} + \phi_h^{j-1/3}}{2} = 0,\\
&\kappa\frac{\phi_h^{j+1/3} - \phi_h^{j}}{\tau} + \Lambda_3\frac{\phi_h^{j+1/3} + \phi_h^{j}}{2} = 0,\\
&\kappa\frac{\phi_h^{j+2/3} - \phi_h^{j+1/3}}{\tau} + \Lambda_2\frac{\phi_h^{j+2/3} + \phi_h^{j+1/3}}{2} = 0,\\
&\kappa\frac{\phi_h^{j+1} - \phi_h^{j+2/3}}{\tau} + \Lambda_1\frac{\phi_h^{j+1} + \phi_h^{j+2/3}}{2} = 0.
\end{aligned} \tag{3.76}$$

Similarly, we can approximate the operators A_{xz} and A_{yz} on the vertical sections of the domain G.

Thus, problem (3.52) is reduced to a successive solution of a set of one-dimensional difference equations.

3.4. Diffusion Equation

In accordance with the splitting method, we reduce the basic problem of substance diffusion in the interval $t_j \leqq t \leqq t_{j+1}$

$$\frac{\partial\phi}{\partial t} = \frac{\partial}{\partial z}\nu\frac{\partial}{\partial z} + \mu\Delta\phi + f,$$

$$\phi = \phi^j \quad \text{at} \quad t = 0$$

$$\phi = 0 \quad \text{on} \quad \Sigma$$

$$\frac{\partial \phi}{\partial z} = \alpha\phi \quad \text{on} \quad \Sigma_o \tag{4.1}$$

$$\frac{\partial \phi}{\partial z} = 0 \quad \text{on} \quad \Sigma_H$$

to three problems. The first describes diffusion along the z-axis

$$\frac{\partial \phi_1}{\partial t} = \frac{\partial}{\partial z} \nu \frac{\partial \phi_1}{\partial z} + f,$$

$$\phi_1 = \phi^j \quad \text{at} \quad t = 0$$

$$\frac{\partial \phi_1}{\partial z} = \alpha\phi \quad \text{on} \quad \Sigma_o \tag{4.2}$$

$$\frac{\partial \phi_1}{\partial z} = 0 \quad \text{on} \quad \Sigma_H$$

the second problem - along the x-axis

$$\frac{\partial \phi_2}{\partial t} = \mu \frac{\partial^2 \phi_2}{\partial x^2},$$

$$\phi_2 = \phi_1^{j+1} \quad \text{at} \quad t = t_j \tag{4.3}$$

$$\phi_2 = 0 \quad \text{on} \quad \Sigma$$

and the third problem - along the y-axis

$$\frac{\partial \phi_3}{\partial t} = \mu \frac{\partial^2 \phi_3}{\partial y^2},$$

$$\phi_3 = \phi_2^{j+1} \quad \text{at} \quad t = t_j \tag{4.4}$$

$$\phi_3 = 0 \quad \text{on} \quad \Sigma$$

Assume that the solution for problem (4.1) with $t = t_{j+1}$ is sought either in the layer $-\infty < x < \infty$, $-\infty < y < \infty$, $0 \leq z \leq H$ or in the parallelepiped $-a \leq x \leq a$, $-b \leq y \leq b$, $0 \leq z \leq H$, where a and b can be infinite in a particular case. Then, for the strip-shaped region the solution can be represented as a Fourier integral with respect to x, y and a Fourier series in z; for the parallelepiped the solution is represented as a Fourier series with respect to all the three variables (x, y, z). In both cases, for $f = 0$ and $t = t_{j+1}$ the splitting method yields an exact solution of (4.1), i.e. $\phi_3^{j+1} = \phi^{j+1}$; in the remaining cases, the solution is approximate.

We have assumed so far that we deal with a differential statement of the problem. In actual situations, however, we usually replace differential equations by finite-difference analogues. This means that instead of (4.1) we consider the problem

$$\frac{\partial \phi}{\partial t} + (\Lambda_1 + \Lambda_2 + \Lambda_3)\phi = f, \tag{4.5}$$

where

$$\Lambda_1 \phi = -\frac{\mu}{\Delta x^2}(\phi_{k+1} - 2\phi_k + \phi_{k-1}),$$

$$\Lambda_2 \phi = -\frac{\mu}{\Delta y^2}(\phi_{\ell+1} - 2\phi_\ell + \phi_{\ell-1}), \tag{4.6}$$

$$\Lambda_3 \phi = \frac{2}{\Delta z_m + \Delta z_{m+1}} \left\{ -\frac{\nu_{m+1/2}}{\Delta z_{m+1}}(\phi_{m+1} - \phi_m) + \frac{\nu_{m-1/2}}{\Delta z_m}(\phi_m - \phi_{m-1}) \right\},$$

$$k = \overline{1,\ n},\ \ell = \overline{1,p},\ m = \overline{0,s};\ \Delta z_m = z_m - z_{m-1},\ \Delta z_o = \Delta z_{s+1} = 0.$$

For simplicity, we assume here that the x-y network is uniform with steps Δx and Δy, respectively. For convenience, we have also omitted the indices which are not essential for the operators $\Lambda\alpha$ in (4.5) and (4.6).

Note that in the neighborhood of the boundary points expressions (4.6) are somewhat modified in accordance with the boundary conditions

$$\phi_k = 0 \quad \text{at} \quad k = 0,\ k = n + 1,$$

$$\phi_\ell = 0 \quad \text{at} \quad \ell = 0,\ \ell = p + 1,$$

$$\frac{\phi_m - \phi_{m-1}}{\Delta z_m} = \alpha\phi_m \quad \text{at} \quad m = 0,$$

$$\frac{\phi_{m-1} - \phi_m}{\Delta z_{m+1}} = 0 \quad \text{at} \quad m = 3.$$

One can readily see that different operators Λ_1, Λ_2, and Λ_3 on the functions $\phi_{k\ell m}$ satisfying boundary conditions (4.7) are positevely definite. Indeed, multiply respective Eqs. (4.6) by $\phi_k\,\Delta x$, $\phi_\ell\Delta\phi$, and $\phi_m(\Delta z_m + \Delta z_{m+1})/2$ and sum up every result over nodes of the network. Taking into account the boundary conditions, we derive

$$(\Lambda_1\phi,\ \phi) = \frac{\mu}{\Delta x}\sum_{k=1}^{n}(\phi_{k+1} - \phi_k)^2 > 0,$$

$$(\Lambda_2\phi,\ \phi) = \frac{\mu}{\Delta y}\sum_{\ell=1}^{p}(\phi_{\ell+1} - \phi_\ell)^2 > 0, \tag{4.8}$$

$$(\Lambda_3\phi,\ \phi) = \nu_{-1/2}\,\alpha\phi_o^2 + \sum_{m=0}^{s-1} \frac{\nu_{m+1/2}}{\Delta z_{m+1}} (\phi_{m+1} - \phi_m)^2 > 0.$$

As previously, here indices are used only for essential variables.

Thus, we have approximated (4.1) in the space variables. It remains to approximate (4.5) with respect to time. To this end, we employ the splitting method:

$$\begin{aligned}
&\frac{\phi^{j+1/6} - \phi^j}{\tau} + \Lambda_1 \frac{\phi^{j+1/6} + \phi^j}{2} = 0,\\
&\frac{\phi^{j+2/6} - \phi^{j+1/6}}{\tau} + \Lambda_2 \frac{\phi^{j+2/6} + \phi^{j+1/6}}{2} = 0,\\
&\frac{\phi^{j+3/6} - \phi^{j+2/6}}{\tau} + \Lambda_3 \frac{\phi^{j+3/6} + \phi^{j+2/6}}{2} = f_2^j,\\
&\frac{\phi^{j+4/6} - \phi^{j+3/6}}{\tau} + \Lambda_3 \frac{\phi^{j+4/6} + \phi^{j+3/6}}{2} = f_2^j,\\
&\frac{\phi^{j+5/6} - \phi^{j+4/6}}{\tau} + \Lambda_2 \frac{\phi^{j+5/6} + \phi^{j+4/6}}{2} = 0,\\
&\frac{\phi^{j+1} - \phi^{j+5/6}}{\tau} + \Lambda_1 \frac{\phi^{j+1} + \phi^{j+5/6}}{2} = 0.
\end{aligned} \tag{4.9}$$

As was shown earlier, splitting in the form (4.9) ensures a second-order approximation in τ, whereas the order of approximation in x, y, z, which was adopted previously, provides accuracy to the second order in Δz, Λx, and Δy.

3.5. General Numerical Algorithm

As was already pointed out, it is sometimes reasonable to solve problem (2.1) by the *component splitting-up method*, which comes about as follows. Problem (2.1) is written as

$$\frac{\partial\phi}{\partial t} + (A_1 + A_2 + A_3)\phi = f, \tag{5.1}$$

where

$$\begin{aligned}
A_1\phi &= \frac{\partial u\phi}{\partial x} - \mu \frac{\partial^2\phi}{\partial x^2},\\
A_2\phi &= \frac{\partial v\phi}{\partial y} - \mu \frac{\partial^2\phi}{\partial y^2},\\
A_3\phi &= \frac{\partial w\phi}{\partial z} - \frac{\partial}{\partial z}\nu\frac{\partial\phi}{\partial z} + \sigma\phi.
\end{aligned} \tag{5.2}$$

Using difference approximations outlined in the foregoing discussion, we reduce problem (5.1) to the system of ordinary differential equations

$$\frac{\partial\phi}{\partial t} + (\Lambda_1 + \Lambda_2 + \Lambda_3)\phi = f, \tag{5.3}$$

where Λ_1, Λ_2, Λ_3, are the difference operators approximating A_1, A_2, A_3, respectively. Evolution problem (5.3) is reduced by component splitting to successive solutions of a number of problems

$$\begin{aligned}
&\frac{\phi^{j+1/6} - \phi^j}{\tau} + \Lambda_1 \frac{\phi^{j+1/6} + \phi^j}{2} = 0,\\
&\frac{\phi^{j+2/6} - \phi^{j+1/6}}{\tau} + \Lambda_2 \frac{\phi^{j+2/6} + \phi^{j+1/6}}{2} = 0,\\
&\frac{\phi^{j+3/6} - \phi^{j+2/6}}{\tau} + \Lambda_3 \frac{\phi^{j+3/6} + \phi^{j+2/6}}{2} = \frac{f^{j+1/2}}{2},\\
&\frac{\phi^{j+4/6} - \phi^{j+3/6}}{\tau} + \Lambda_3 \frac{\phi^{j+4/6} + \phi^{j+3/6}}{2} = \frac{f^{j+1/2}}{2},\\
&\frac{\phi^{j+5/6} - \phi^{j+4/6}}{\tau} + \Lambda_2 \frac{\phi^{j+5/6} + \phi^{j+4/6}}{2} = 0,\\
&\frac{\phi^{j+1} - \phi^{j+5/6}}{\tau} + \Lambda_1 \frac{\phi^{j+1} + \phi^{j+5/6}}{2} = 0.
\end{aligned} \tag{5.4}$$

As shown in 3.1, system (5.4) gives a second-order approximation in τ.

3.6. Numerical Solution of Adjoint Problems

Algorithmically, the solution of *adjoint problems* does not differ from the solution of basic problems if the procedure is performed in the reverse time direction, i.e. the problem

$$\begin{aligned}
&-\frac{\partial\phi^*}{\partial t} - \operatorname{div} \underline{u}\phi^* = \frac{\partial}{\partial z}\nu\frac{\partial\phi^*}{\partial z} + \mu\Delta\phi^* + p,\\
&\phi^* = g^* \quad \text{at} \quad t = T\\
&\phi^* = 0 \quad \text{on} \quad \Sigma\\
&\frac{\partial\phi^*}{\partial z} = \alpha\phi^* \quad \text{on} \quad \Sigma_o\\
&\frac{\partial\phi^*}{\partial z} = 0 \quad \text{on} \quad \Sigma_H
\end{aligned} \tag{6.1}$$

should be solved, beginning at $t = T$, towards decreasing values of t. In this case, the numerical algorithm is well-defined. Problem (6.1) can be reduced to the form typical of basic equations by substituting $t' = T - t$ for the independent variable t and the function $\underline{u}' = -\underline{u}$ for $\underline{u}$. Then it goes over to the problem

$$\frac{\partial\phi^*}{\partial t'} + \operatorname{div} \underline{u}'\phi^* = \frac{\partial}{\partial z}\nu\frac{\partial\phi^*}{\partial z} + \mu\Delta\phi^* + p,$$

$$\begin{aligned} &\phi^* = g^* \quad \text{at} \quad t' = 0 \\ &\phi^* = 0 \quad \text{on} \quad \textstyle\sum \\ &\frac{\partial \phi^*}{\partial z} = -\alpha\phi^* \quad \text{on} \quad \textstyle\sum_o \\ &\frac{\partial \phi^*}{\partial z} = 0 \quad \text{on} \quad \textstyle\sum_H \end{aligned} \tag{6.2}$$

Clearly, the operator of adjoint problem (6.2) in the new variables formally coincides with the operator of the direct problem. For this reason, all the numerical algorithms used to solve the direct problem apply automatically to the solution of the adjoint problem.

3.7. Comments on Difference Approximation of Basic and Adjoint Problems

The ideas and methods used by up-to-date computational mathematics make it possible to elaborate many qualitative difference schemes and algorithms both for direct (2.1) and adjoint (6.1), (6.2) equations. But the use of adjoint equations for numerical solution of this class of problems imposes certain constraints on the choice of operators approximating an adjoint problem. This section deals with the methods of elaborating a difference analogue of an adjoint problem with due account of the requirement that the functionals involved admit dual representation. Thus, suppose with the problem

$$\begin{aligned} &\frac{\partial \phi}{\partial t} + A\phi = f, \\ &\phi = \phi^o \quad \text{at} \quad t = 0, \end{aligned} \tag{7.1}$$

where A is a linear operator in the Hilbert space defined on the set of sufficiently smooth functions, there associates the difference analogue

$$\begin{aligned} &\frac{\underline{\phi}^{j+1} - \underline{\phi}^j}{\tau} + A^h \underline{\phi}^j = \underline{f}, \\ &\underline{\phi}^j = \underline{\phi}^o \quad \text{at} \quad j = 0, \end{aligned} \tag{7.2}$$

Here $\underline{\phi}' = (\phi_1^j, \ldots \phi_n^j)^T$ is the vector function defined at points (with numbers $k = \overline{1, n}$) of some region G and at points (with numbers $j = \overline{1, r}$) of the time axis; A^h is the matrix operator defined in the space of network functions

$$\Phi_1 = \{\underline{\phi}^j = (\phi_1^j, \ldots, \phi_n^j)^T\}; \tag{7.3}$$

the superscript T refers to transposition.

Let us introduce the space of network functions

$$\Phi_2 = \{\underline{\phi} = \{\phi^j\}, \quad j = \overline{0,r}\} \tag{7.4}$$

and define the scalar product in the spaces Φ_1 and Φ_2 by

$$(\underline{\phi}^j, \underline{\tilde{\phi}}^j)_1 = (D\underline{\phi}^j, \underline{\tilde{\phi}}^j) = \sum_{k=1}^{n} \phi_k^j \tilde{\phi}_k^j d_k, \tag{7.5}$$

$$(\underline{\phi}, \underline{\tilde{\phi}})_2 = \sum_{j=0}^{r} (\underline{\phi}^j, \underline{\tilde{\phi}}^j)\tau; \tag{7.6}$$

Here $D = \text{diag}\,[d_k]$ is the positive definite matrix. In the simplest case, $d_k = \Delta x$ $(k = \overline{1, n})$.

With respect to the function space Φ_2, Eq.(7.2) can be formalized as follows:

$$L^h \underline{\phi} = \underline{f}, \tag{7.7}$$

where the structures of the operator L^h and vector $\underline{f}$ depend on the form of (7.2). Multiplying (7.7) scalarly by the function $\underline{\tilde{\phi}}$, we obtain

$$(L^h\underline{\phi} - \underline{f}, \underline{\tilde{\phi}})_2 = \sum_{j=1}^{r} [(\underline{\phi}^j - \underline{\phi}^{j-1}, \underline{\tilde{\phi}}^j)_1 + \tau(A^h\underline{\phi}^{j-1}, \underline{\tilde{\phi}}^j)_1 - \tau(\underline{f}, \underline{\tilde{\phi}}^j)_1] = 0. \tag{7.8}$$

Considering that the operator adjoint to a real-element matrix is a transposed matrix and allowing for the form of scalar product (7.5), we can transform (7.8) to

$$\begin{gathered} -(\underline{\phi}^o, \underline{\tilde{\phi}}^o)_1 + (\underline{\phi}^r, \underline{\tilde{\phi}}^r)_1 + \sum_{j=1}^{r} [(\underline{\tilde{\phi}}^{j-1} - \underline{\tilde{\phi}}^j + \tau D^{-1}(A^h)^T D\underline{\tilde{\phi}}^j, \underline{\phi}^{j-1})_1 - \\ - \tau\,(\underline{f}, \underline{\tilde{\phi}}^j)_1] = 0. \end{gathered} \tag{7.9}$$

Let the adjoint function $\underline{\tilde{\phi}}^j$ $(j = \overline{r, 1})$ satisfy the equation

$$\begin{gathered} \frac{\underline{\tilde{\phi}}^{j-1} - \underline{\tilde{\phi}}^j}{\tau} + D^{-1}(A^h)^T D\underline{\tilde{\phi}}^j = \underline{p}, \\ \underline{\tilde{\phi}}^r = \underline{\tilde{\phi}}^{r+1} = 0. \end{gathered} \tag{7.10}$$

Then, relation (7.9) takes the form

$$(\underline{f}, \underline{\tilde{\phi}})_2 + (\underline{\phi}^o, \underline{\tilde{\phi}}^o)_1 = (\underline{p}, \underline{\phi})_2. \tag{7.11}$$

Eq.(7.10) is adjoint to (7.2) in metric (7.6) and its solution yields a dual representation of the functional

$$J = (\underline{p}, \underline{\phi})_2. \tag{7.12}$$

Adjoint equations for any other approximation in the variable t, as well as for the splitting can be derived in a similar way scheme. It should be stressed that the equation adjoint to the difference analogue of problem (2.1) must be made consistent with the approximation of the direct problem and with the metric of the network function space, using the method which permits dual representation of the functionals.

Chapter 4. OPTIMUM LOCATION OF INDUSTRIAL PLANTS

The present-day rate of economic development demands construction of more and more efficient industrial installations and complexes. Such industrial projects are generally built in or close to thickly populated areas capable of meeting requirements for man power. This imposes particular limitations on the location of works or plants that discharge into the air aerosols harmful to man and disturb the ecological system in the region. Optimal location of industrial plants is a multi-aspect and algorithmically rather complex problem. To solve this problem, the author had to develop a body of mathematics for adjoint problems whose solutions are typical functions of effects caused by aerosol pollution of the environment. In this chapter, the results of investigations given in chapters 1 and 2 have been applied to a definite object for studying optimum location of plants; diverse mathematical models of most typical situations have been examined. The chapter also contains methods of solving optimization problems and an interpretation of results. The ideas and methods described herewith will be further developed in subsequent chapters.

4.1. Statement of the Problem

Suppose that a new industrial plant has to be constructed close to populated areas, recreation zones, and other ecologically important zones so that their total annual pollution with noxious industrial substances will not exceed the values stipulated by sanitary requirements and the total ecological burden on the whole region $\sum_o$ due to pollution will be minimum or within the range specified in global sanitary requirements.

Suppose that an industrial plant discharges per time unit and with intensity Q noxious aerosol at a height $z = h$, which is then carried away by air mass and spreads under the action of low-scale turbulence. Assume that the aerosol source is located in a neighborhood of point $\underline{r}_o = (x_o, y_o, h)$. Then it can be described by function

$$f(\underline{r}) = Q\delta\,(\underline{r} - \underline{r}_o) \tag{1.1}$$

and we arrive at the equation

$$\frac{\partial\phi}{\partial t} + \operatorname{div} \underline{u}\phi + \sigma\phi = \frac{\partial}{\partial z}\,\nu\,\frac{\partial\phi}{\partial z} + \mu\Delta\phi + Q\delta(\underline{r} - \underline{r}_o). \tag{1.2}$$

As boundary conditions we take

$$\phi = 0 \quad \text{on} \quad \sum$$

$$\frac{\partial\phi}{\partial z} = \alpha\phi \quad \text{on} \quad \sum\nolimits_o \qquad (1.3)$$

$$\frac{\partial\phi}{\partial z} = 0 \quad \text{on} \quad \sum\nolimits_H$$

We shall find a solution to problem (1.2), (1.3) on a set of sufficiently smooth periodic functions with period T in variable t:

$$\phi(\underline{r}, T) = \phi(\underline{r}, o) \qquad (1.4)$$

The task is to select a zone $\omega_G \subset G$ where the plant can be located so that the global and local sanitary requirements for pollution will be observed both for the whole region $\sum_o$ and the chosen zone Ω_k. In solving a problem concerning transfer and diffusion of pollutants the components of the velocity vector in the planetary boundary layer of the atmosphere in the given region are computed by the methods used in mesometeorology (see Appendix). Having gathered necessary information on the wind field, direct modelling methods are employed for solving problems of spreading of industrial aerosol emissions at the given point $\underline{r}_o \in G$. For this purpose we take average weakly climatic data on wind velocity components obtained by mesometeorological methods. Thereafter, problem (1.2)-(1.4) is solved.

Figures 4.1 and 4.4 show how problem (1.2)-(1.4) is solved on the basis of

Value of 01 level 2.2755 Value of 20 level 11.332

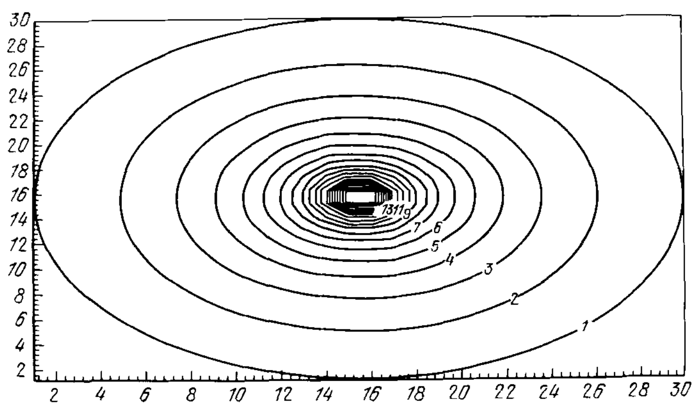


FIGURE 4.1

statistical model discussed in chapter 1. These figures depict the isolines of the function

$$\overline{\Phi}(x,\ y) = \frac{1}{TH}\int_0^T\int_0^H \phi(x,\ y,\ z,\ t)\ dt$$

for different types of air mass motion. Figure 4.1 conforms to the case $u = v = w = 0$, and figure 4.2, to the case $u = 5$ m/s, $v = w = 0$. Figure 4.3

Value of 01 level 0.19473 Value of 20 level 3.4992

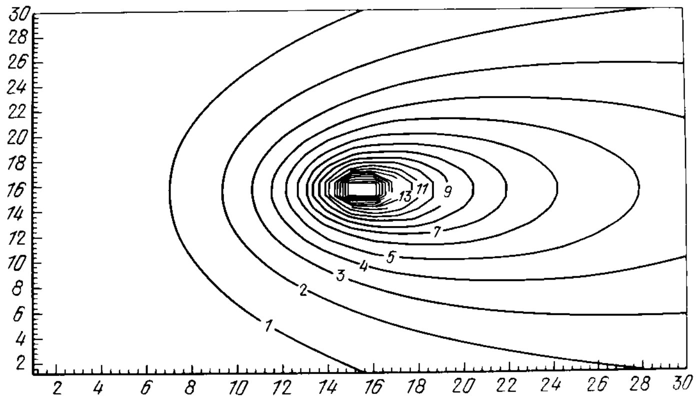


FIGURE 4.2

Value of 01 level 0.38945 Value of 20 level 6.9983

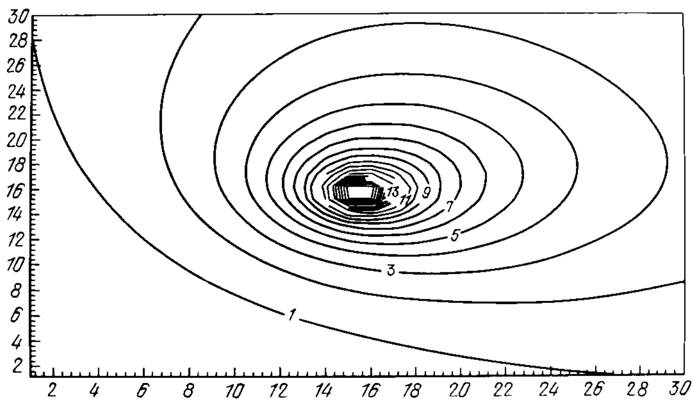


FIGURE 4.3

illustrates a case when the components of the wind velocity vector are equal to $u = 5$ m/s, $v = w = 0$ in $[0, T/2]$, and $u = 0$, $v = 5$ m/s, $w = 0$ in $[T/2, T]$. Figure 4.4 was obtained for the following components of the wind velocity vector:

$$u = \begin{cases} 5, & t \in [0, T/3), \\ 0, & t \in [T/3, 2T/3], \\ -5, & t \in [2T/3, T]; \end{cases}$$

$$v = \begin{cases} 0, & t \in [0, T/3), \\ 5, & t \in [T/3, 2T/3), \\ 0, & t \in [2T/3, T]; \end{cases}$$

$$w = 0.$$

Value of 01 level 0.77289 Value of 20 level 11.037

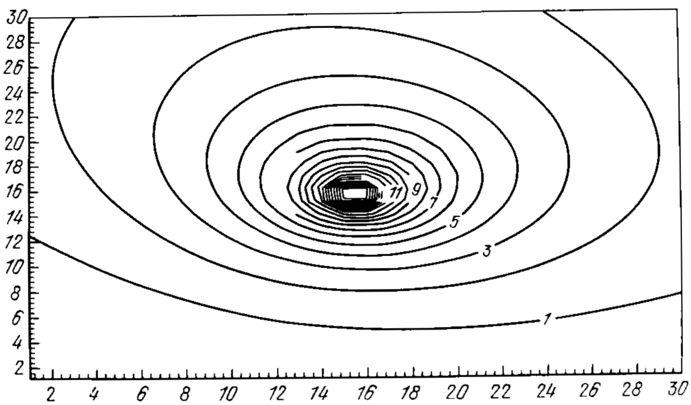


FIGURE 4.4

The solution obtained is integrated within the annual interval limits $0 \leq t \leq T$. Then either the average, for period T, amount of aerosol in a unit cylinder over an ecologically significant zone $\Omega_k \subset \sum_o$:

$$J_k^B = b \int_0^T dt \int_{G_k} \phi \, dG, \qquad (1.5)$$

or the total amount of aerosol that has settled on the Earth's surface in that very zone $\Omega_k \subset \sum_o$ is estimated:

$$J_k^A = a \int_0^T dt \int_{\Omega_k} \phi \, d\sum . \qquad (1.6)$$

Here b = 1/T; constant a takes into account the fraction of the aerosol that gets into the soil (first of all, these are heavy aerosols which fall on Earth under gravity and also a fraction of light particles that fall on Earth due to vertical diffusion). As shown in section 1.5, in this case

$$a = \overline{w}_g + \alpha\nu \qquad (1.7)$$

Note that both functionals are important for estimating pollution and its impact on the ecological conditions of zone Ω_k. Thus, functional (1.5) is significant for statistical estimation of the direct effect on animate nature consuming oxygen, and functional (1.6) - for judging about the pollution of soil cover and water bodies whose effect on the environmental ecology may also be appreciable, though of indirect nature within the corresponding lines of biocenosis.
As noted earlier, functionals (1.5) and (1.6) are particular cases of a more general functional

$$J_p = \int_0^T dt \int_G p\phi \, dG, \qquad (1.8)$$

whose use is expedient to estimate pollution in different cases with known values of p. Assuming that

$$p = \begin{cases} b, & \underline{r} \in G_k \\ o, & \underline{r} \in G_k \end{cases}$$

we arrive at functional (1.5). Assuming that

$$p = \begin{cases} a\ (z), & \underline{r} \in \Omega_k, \\ 0, & \underline{r} \in \Omega_k, \end{cases}$$

we arrive at functional (1.6). Recall that $\Omega_k \quad \sum_o$ is the basis of the cylindrical range G_k on plane z = 0.

The calculation has to be repeated when the industrial plant is located at a different point $\underline{r}_1 \in G$. This implies that a large number of variants have to be examined for finding an optimum location of a plant; subsequent comparison of functions J_k^A and J_k^B or their linear combinations with definite constants a and b is also necessary

$$J_k = J_k^A + J_k^B \qquad (1.9)$$

Keeping in view that pollution estimate is, in the final analysis, associated with the combination of functionals J_k^A and J_k^B, we introduce a generalized functional

$$J_k = \int_0^T dt \int_{G_k} [b + a\delta(z)]\,\phi\,dG, \qquad (1.10)$$

which can be written as functional (1.8) provided

$$p_k = \begin{cases} b + a\delta(z) & \text{in } G_k \\ 0 & \text{outside } G_k \end{cases}$$

Therefore, in our further consideration we shall deal with functional (1.10) only. We introduce also an important functional J_{pk}:

$$J_{pk} = \sum_{k=1}^{m} \int_0^T dt \int_{G_k} [b_k + a_k\delta(z)]\phi\,dG. \qquad (1.11)$$

Here we have assumed that constants a_k and b_k can be different for different (non-intersecting) zones G_k and may depend, for example, on the nature of the underlying surface. Then, functional(1.11) can be rewritten as

$$J_p = \int_0^T dt \int_G p\phi\,dG. \qquad (1.12)$$

where

$$p = \begin{cases} b_k + a_k\,\delta(z) & \text{on } G_k,\ k = 1, \ldots, m, \\ 0 & \text{outside } \bigcup_{k=1}^{m} G_k. \end{cases}$$

Functional J_p has the following physical interpretation: the functional yields over all ecologically significant regions G_k an integral effect of the environmental pollution, provided the industrial emission source is in a point $\underline{r}_o \in G$. Clearly, this is a global functional, in a certain sense, for every range G and all regions G_k.

Parallel with (1.11) we consider another global functional

$$Y_p = \int_0^T dt \int_G p_c\phi\,dG, \qquad (1.13)$$

in which

$$p_c = \begin{cases} B_k + A_k\,\delta(z), & \underline{r} \in G_k,\quad k = 1, \ldots, m, \\ 0 & \text{outside } \bigcup_{k=1}^{m} G_k. \end{cases}$$

Here A_k and B_k stand for values related to the sanitary (physiological) impact of industrial emissions over the whole district $G_k \subset G$. They can be selected by different methods. For example, constants B_k can express correlation between the amount of aerosols present in G_k and either their sanitary hazard or their direct action on various objects (including living ones) in region G_k. This is also true of constants A_k. Such findings are obtained on the basis of experimental data collected for several years.

Finally we give one more generalization. Suppose that we have every necessary information about physiological impacts not only in the most important ecological zones Ω_k, but also in all other points $\underline{r} \in \sum_o$. Then the values A and B turn into functions: $A = A(x,y)$, $B = B(x,y)$. Let us compare functional Y_p with the value

$$p_c = B + A\delta\ (z) \quad \text{in } G \tag{1.14}$$

We shall use functionals (1.13), (1.14) to estimate ecological burden on a region due to pollution. The task is to find a point $\underline{r}_o \in G$ such that

$$Y_p = \min_{\underline{r}_o \in G} \tag{1.15}$$

As mentioned earlier, this problem is solved with the help of basic problem (1.2)-(1.4) by exhaustion of $\underline{r}_o$ in G. Such an exhaustion demands large computations and is difficultly realized using even modern computers. This is the reason why in a real-life situation purposeful exhaustion is used taking into account a wind rose and other considerations of statistical nature. However, as we will show later, problem (1.15) can be solved uniquely by only one variant of computing an adjoint problem. This proves to be possible due to one of the most remarkable properties of duality. Let us now go over to the consideration of this algorithm.

4.2. Adjoint Equations and Optimization Problem

Inasmuch as we have taken the main functional of the problem in the form

$$\begin{gathered} Y_p = \int_0^T dt \int_G p_c \phi \, dG, \\ p_c = B + A\delta\ (z) \text{ in } G \end{gathered} \tag{2.1}$$

the following will be an adjoint problem with respect to the main one in accord with the results of chapter 2

$$
\begin{gathered}
-\frac{\partial\phi^*}{\partial t} - \operatorname{div} \underline{u}\phi^* + \sigma\phi^* = \frac{\partial}{\partial z}\nu\frac{\partial\phi^*}{\partial z} + \mu\Delta\phi^* + p_c, \\
\phi^* = 0 \quad \text{on } \textstyle\sum, \\
\frac{\partial\phi^*}{\partial z} = \alpha\phi^* \quad \text{on } \textstyle\sum_0, \\
\frac{\partial\phi^*}{\partial z} = 0 \quad \text{on } \textstyle\sum_H, \\
\phi^*(\underline{r}, T) = \phi^*(\underline{r}, 0).
\end{gathered}
\tag{2.2}
$$

Multiplying (1.2) by ϕ^* and (2.2) by ϕ, integrating the results over the whole time interval and range G, subtracting one from the other, and using boundary values and initial data of (1.3), (1.4) and (2.2), we, in virtue of the problem conjugacy (see chapter 2), obtain the dual form of function Y_p (see (2.17) and (2.18) of chapter 2) after transformations and simplifications

$$
Y_p = \int_0^T dt \int_G p_c\phi \, dG, \tag{2.3}
$$

$$
Y_p = Q \int_0^T \phi^*(\underline{r}_o, t) dt. \tag{2.4}
$$

Let us denote Y_p by $Y_p(\underline{r}_o)$ since this functional is parametrically dependent on location $\underline{r}_o \in G$ of the industrial plant.

Assume that the adjoint problem (2.2) is solved and a function $\phi^*(\underline{r},t)$ is found. Substituting it in (2.4), we obtain

$$
Y_p(\underline{r}) = Q \int_0^T \phi^*(\underline{r},t)\, dt. \tag{2.5}
$$

Now we use the auxiliary function $Y_p(\underline{r})$ for finding r_o from the condition

$$
Y_p(\underline{r}) = \min_{\underline{r} \in G} \tag{2.6}
$$

Here, the point minimizing $Y_p(\underline{r})$ will be $\underline{r}_o$.

Further, operations are evident. It is necessary to construct a field of function $Y_p(x,y,h)$ where h stands for emission height which is limited by the construction requirements. As a result, we obtain a field of isolines $Y_p(x,y,h) = \text{const}$ on the (x,y) plane.

Figures 4.5-4.8 represent fields of isolines of function $Y_p(x,y)$ (2.5) for the types of air mass motions shown in figures 4.1-4.4.

Value of 01 level 2.2755 Value of 20 level 11.332

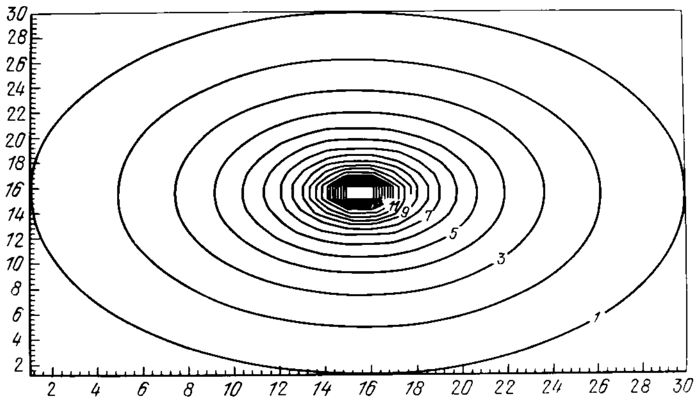


FIGURE 4.5

Value of 01 level 0.19473 Value of 20 level 3.4992

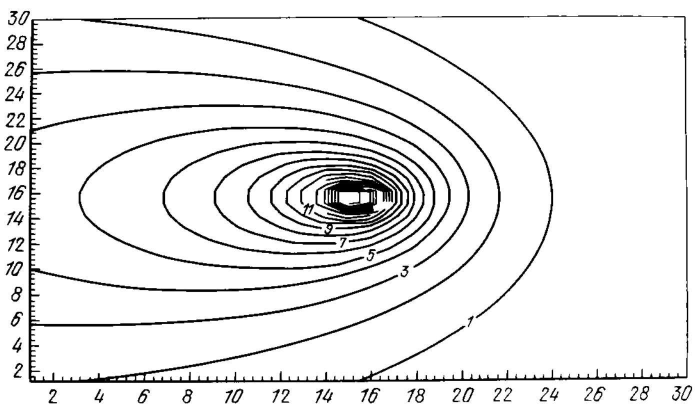


FIGURE 4.6

However, in most cases it is not required to have a unique solution of the optimization problem because the final solution requires that several limitations be met taking into account the region geology, proximity of manpower resources, water supply and various communication facilities. Therefore, it is necessary to choose a whole range values satisfying sanitary requirements. Let us denote by ω_G the region where the condition

$$Y_c \leq C \tag{2.7}$$

Value of 01 level 0.38945 Value of 20 level 6.9983

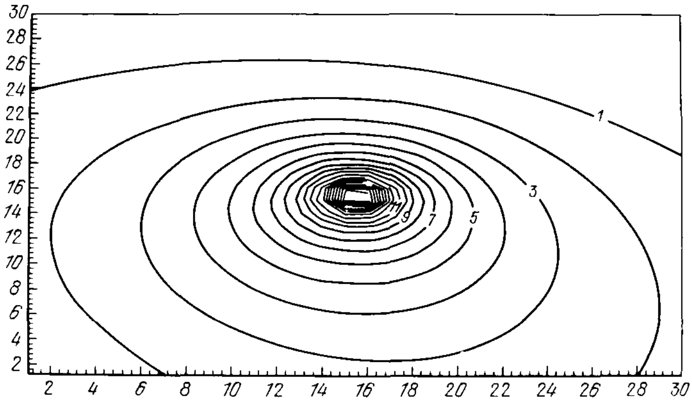


FIGURE 4.7

Value of 01 level 0.77289 Value of 20 level 11.037

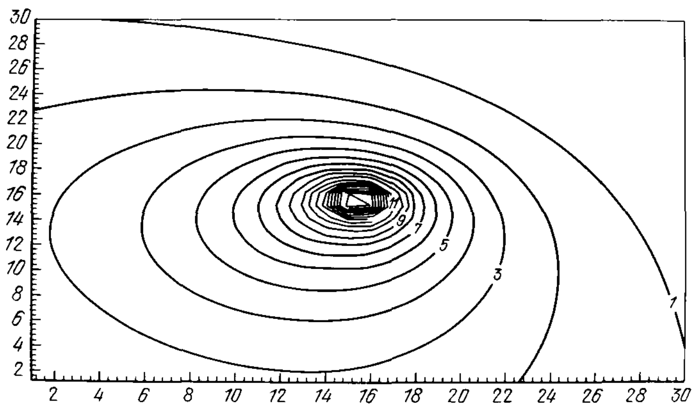


FIGURE 4.8

can be fulfilled, and which will be the solution to our problem.

Now we go back to the classical solution of the optimization problem. Suppose that $\underline{r}_0$ is found. Then for this fixed point it is necessary to solve the basic problem (1.2)-(1.3) (see figures 4.1-4.4) and obtain complete information on pollution fields not on the global but local scale, that is, to obtain information on pollution on different zones. If the pollution level in all zones does not exceed the maximum permissible doses, then the problem is solved. On the contrary, we shall have to solve a more complex and more informative multicriterional problem which will be considered in the following section.

4.3. Multicriterional Optimization Problem

In global estimation of safe pollution of the whole region $\sum_o$ with noxious industrial emissions certain ecologically important zones Ω_k may be polluted beyond the permissible level. To avoid this, we solve the following multicriterional problem.

Let Ω_k (k = 1,2, ..., m) be several ecologically important zones (human settlements, recreation zones, drinking water sources, etc.) picked up on plane z = 0 in $\sum_o$. Find an area where a new industrial plant can be located such that the pollution in all m zones of Ω_k will not exceed the maximum permissible values (if such an area exists in $\sum_o$). If it is impossible to find this area in $\sum_o$, then certain limitations can be imposed on the emission rate Q such that the plant location area will appear in $\sum_o$.

First we shall consider a simple problem when there is only one area $\Omega_k \subset \sum_o$. A priori we demand that safe pollution in this area should be less than the maximum permissible value C_k, that is,

$$Y_{pk} = \int_0^T dt \int_{G_k} p_{ck} \phi \; dG \leqq C_k , \tag{3.1}$$

where

$$p_{ck} = \begin{cases} b_k + a_k \, \delta(z) & \text{on } G_k \\ 0 & \text{outside } G_k \end{cases} \tag{3.2}$$

Unlike the case considered in section 4.2, integration in (3.1) is performed not over the whole region G, but over part of G_k. Then we have the following problem instead of (2.2):

$$\begin{gathered} -\frac{\partial \phi_k^*}{\partial t} - \operatorname{div} \underline{u}\phi_k^* + \sigma\phi_k^* = \frac{\partial}{\partial z} \nu \frac{\partial \phi_k^*}{\partial z} + \mu\Delta\phi_k^* + p_{ck} , \\ \phi_k^* = 0 \quad \text{on } \textstyle\sum , \\ \frac{\partial \phi_k^*}{\partial z} = \alpha\phi_k^* \quad \text{on } \textstyle\sum_o , \\ \frac{\partial \phi_k^*}{\partial z} = 0 \quad \text{on } \textstyle\sum_H , \\ \phi_k^* (\underline{r}, T) = \phi_k^*(\underline{r}, 0) , \end{gathered} \tag{3.3}$$

where p_{ck} is a function of type (3.2). Since the principle of duality holds

$$Y_{pk} = \int_0^T dt \int_{G_k} p_{ck}\phi \, dG,$$
$$Y_{pk} = Q \int_0^T \phi_k^* (\underline{r}_o, t) \, dt, \tag{3.4}$$

then along with (3.1) an equivalent condition is also valid

$$Y_{pk}(\underline{r}_o) = Q \int_0^T \phi_k^*(\underline{r}_o, t) \, dt \leq C_k. \tag{3.5}$$

It is this correlation that we use to define the area for a possible plant location. Indeed, we assume that problem (3.3) is solved and we have $\phi_k^*(\underline{r},t)$. Let us find $Y_{pk}(\underline{r})$ by formula

$$Y_{pk}(r) = Q \int_0^T \phi^*(r,t) \, dt \tag{3.6}$$

and draw isolines $Y_{pk}(\underline{r}) = \text{const}$.

Call the unknown area $\omega_k \subset \sum_o$. Thus, we clearly know the area ω_k where it is possible to locate an industrial plant. Further the ecological and other criteria of selecting the most suitable place for construction come into effect. If ω_k is found to lie outside $\sum_o$, then we can always bring ω_k into $\sum_o$ by decreasing Q. This, of course, imposes definite limitations on emissions and, possibl y, on the manufacturing technology of the plant. We also assume that there are several ecologically important zones Ω_k (k = 1,2, ..., m). In this case, we have to solve m adjoint problems of the type (3.3) and obtain $\phi_1^*, \phi_2^*, \ldots, \phi_m^*$. Using these solutions we formulate m functionals

$$Y_{pk}(\underline{r}_o) = Q \int_0^T dt \int_{G_k} \phi_k^*(\underline{r}_o,t) \, d\underline{r}, \quad k = 1,2, \ldots, m, \tag{3.7}$$

and obtain respectively m limitations

$$Y_{pk}(\underline{r}_o) \leq C_k, \quad k = 1,2, \ldots, m. \tag{3.7'}$$

Further, for each zone Ω_k we find ω_k. Intersection of these regions ω_k (k = 1,2, ..., m) is a region for constructing a sanitary safe plant for all zones Ω_k. This situation is represented in figures 4.9 through 4.12 where the fields of isolines are shown. These figures, similarly to figures 4.5 through

Value of 01 level 2.3874 Value of 10 level 10.866

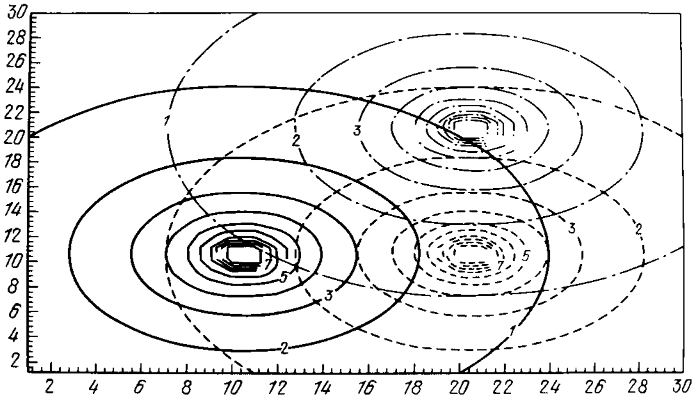


FIGURE 4.9

Value of 01 level 0.33878 Value of 10 level 3.3396

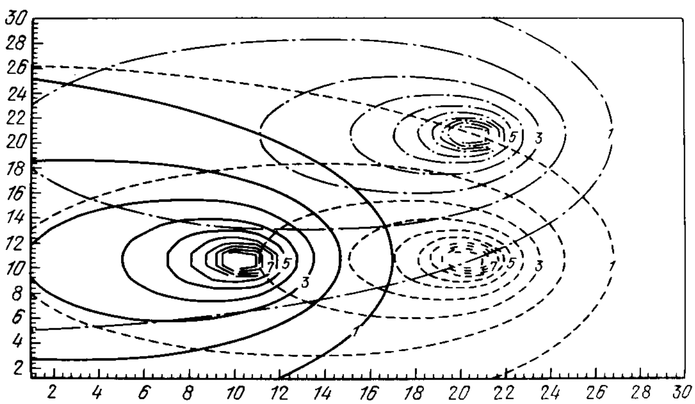


FIGURE 4.10

4.8., have been drawn for the case when there are several protection zones.

Thus, the area ω of possible location of an industrial plant is found. If this area does not exist for a given Q, it can be obtained by decreasing G.

Taking account of what has been described, it is quite real at present to set for every ecological region a program of locating industrial plants that discharge some of their wastes into atmosphere in the form of aerosols. For every region $\sum_0$ it is necessary to have climatic maps showing wind fields with due consideration of the characteristic features of local topography. On the basis

Value of 01 level 0.67755 Value 10 level 6.6793

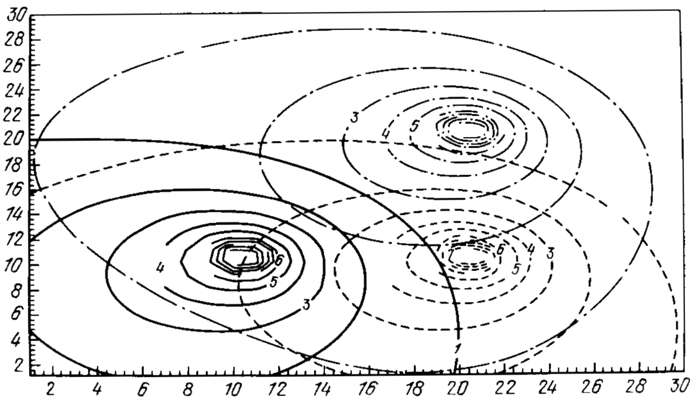


FIGURE 4.11

Value of 01 level 1.1526 Value of 10 level 10.535

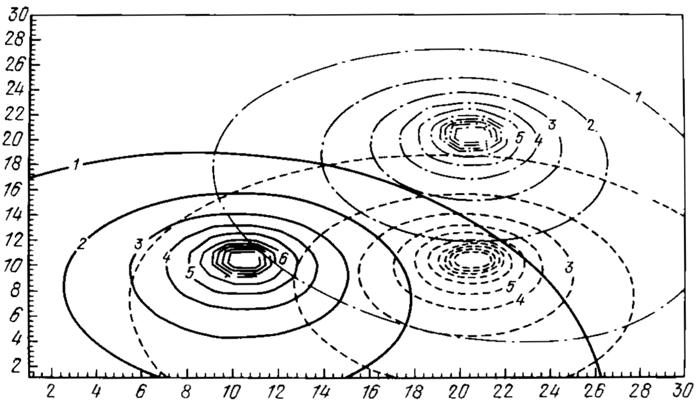


FIGURE 4.12

of these data we solve the adjoint problems and find functions ϕ_1^*, ϕ_2^*, ..., ϕ_m^*. The latter are used for obtaining functionals $Y_{pk}(\underline{r})$ which define the area of possible construction sites and determine the permissible emission level. This job, first of all, should be accomplished in planning construction sites in econimical regions which need to be developed and where decisions satisfying environment protection requirements can be taken. In future this will become a priority criterion.

4.4. Minimax Problem

The principles formulated in section 4.3 enable us to arrive at a solution to the minimax problem which we formulate as follows. Let G be a closed region of a space with boundary $S = \sum \cup \sum_o \cup \sum_H$. Inside G on $\sum_o$ m ecologically important zones needing special protection against industrial pollution are located. Let us denote them by $\Omega_1, \Omega_2, \ldots, \Omega_m$.

Value of 01 level 2.2084 Value of 20 level 11.328

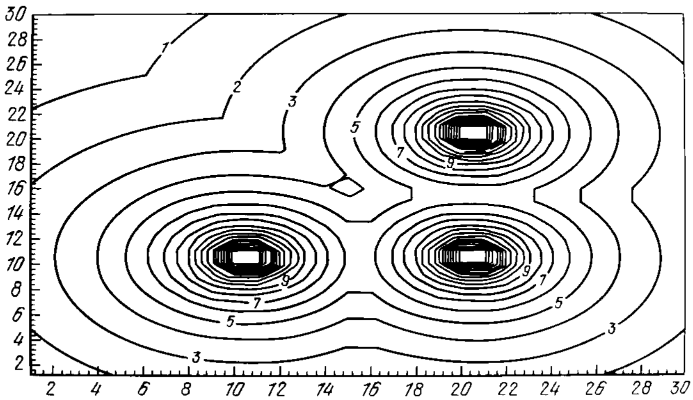


FIGURE 4.13

Value of 01 level 0.25707 Value of 20 level 3.5023

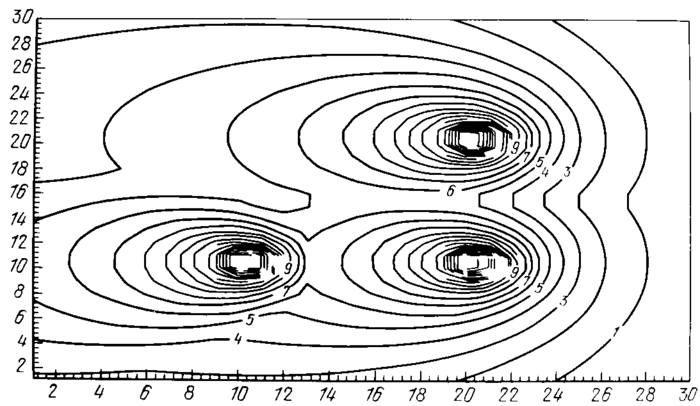


FIGURE 4.14

Value of 01 level 0.51413 Value of 20 level 7.0045

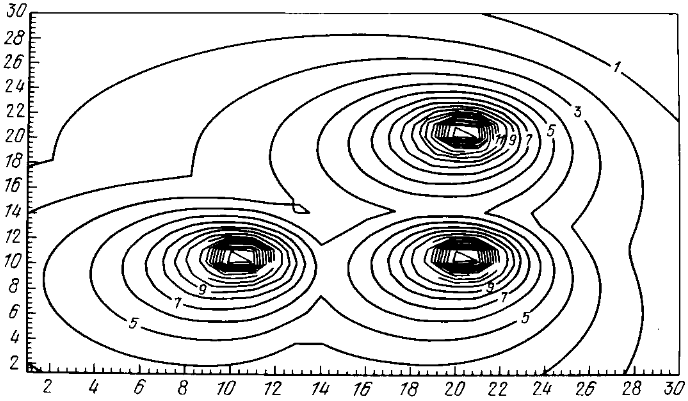


FIGURE 4.15

Value of 01 level 1.0881 Value of 20 level 11.053

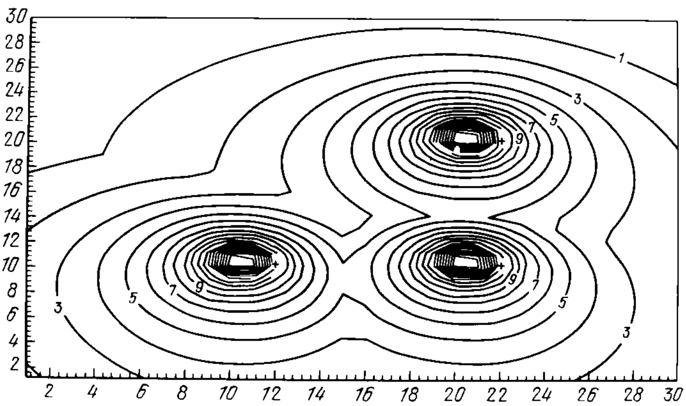


FIGURE 4.16

For every zone we construct functionals $Y_{p1}, \ldots, Y_{pm}$ using solutions of adjoint problems (3.3). Further, we consider the functional for every point $M(\underline{r}_o) \in G$ of possible location of an industrial plant which discharges aerosol at a rate Q and height h,

$$Y_p(\underline{r}) = \max_k Y_{pk}(\underline{r}). \tag{4.1}$$

Then, pollution in all zones Ω_k will be minimum when $M(\underline{r})$ is chosen from the condition

$$\max_{k} Y_{pk}(\underline{r}) = \min_{M \in \sum_o}, \tag{4.2}$$

Whence, by direct exhaustion of values of the functional $\max_k Y_{pk}(\underline{r})$ at all points of ω, we find a point $M_o(\underline{r}_o)$ where condition (4.2) is fulfilled. This is that very rare case when, based on single exhaustion of functionals, a minimax problem for a complex problem of mathematical physics is solved in an explicitform with an adjoint problem. The isolines of the functional $Y_p(x,y)$ which characterize the qualitative aspect of the problem, given three ecologically important zones, are shown in figures 4.13 through 4.16. Here, the types of wind circulations are similar to those in figures 4.1 through 4.4.

4.5. A Generalized Optimization Problem of Industrial Plant Location

Thus, we have arrived at two statements of the problem of chosing a region where a plant can possible be located with due consideration of its industrial emissions. Global estimation of pollution in an optimization problem is made for the whole region $\sum_o$, but it may not meet certain specific conditions for all of its ecologically important zones Ω_k. The multicriterional problem is solved in respect of all ecologically important zones, but it does not fully take account of pollution hazard in other areas of this region, though, in principle, the entire region $\sum_o$ can be covered with Ω_k zones such that $U\Omega_k = \sum_o$, and adjoint problems can be solved for all the zones, This is a possible but a difficult way because such zones may be numerous. Meanwhile a combination of both problems can meet us with success. Indeed, first a multicriterional problem is solved and a region ω_k of possible location of an industrial plant is found provided that sanitary requirements are observed for all Ω_k zones. Thereafter, the problem of global estimation of pollution of the entire region is solved. As a result, we obtain an area for possible location of industry in view of limiting ecological burden from environmental pollution of the region $\sum_o$. Let it be an area ω_G. Then the intersection of ω_k and ω_G will yield an area for which both conditions are satisfied. Denote it ω_G.

Figure 4.17 illustrates this procedure. Therein are shown the isolines of functionals obtained upon solving adjoint problems with the right-hand side of the form

$$p_1 = 1 \quad \text{when} \quad (x,y) \in G$$

$$p_2 = 1 \quad \text{when} \quad (x,y) \in G_1,$$

Value of 01 level 0.2718 - solid lines

Value of 10 level 1.8370 - solid lines

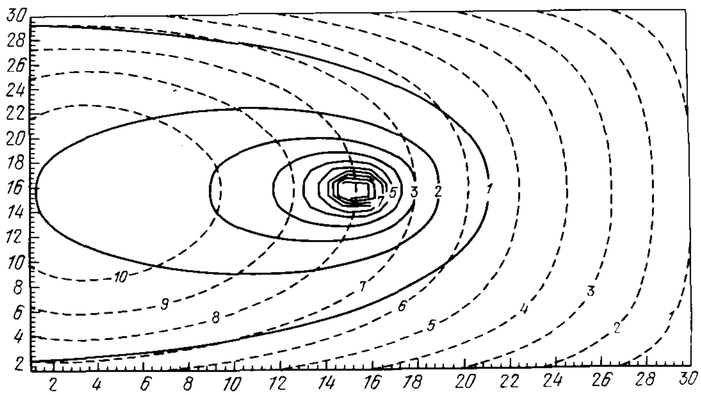


FIGURE 4.17

where G_1 is the protected zone in the middle of the figure. Solid lines correspond to the local criterion; dashed lines - the global criterion (1 level 1.0602, 10 level 2.0584). The velocity vector components were taken to be: $u = 10$ m/s, $v = 0$.

In conclusion it may be mentioned that we shall repeatedly return to the optimization problem by making the limitations more rigid at the expense of factors associated with the restoration of ecology of polluted environment and its depreciation. All of these problems are of economic nature and will be considered in the following chapter.

4.6. Some General Remarks

Up to now the aerosols density was assumed to be zero at the boundary of region G (on $\sum$). In most cases, this condition is not justified because aerosols of one region can be drifted to another through the boundary $\sum$. Therefore, account must be taken of this effect of internal pollution caused by industrial plants located in neighboring regions. Industrial plants discharging similar aerosols into atmosphere can now operate in the given region. The effect of this factor can be allowed for without disturbing the basic strategy of solving optimization problems described in the previous sections of this chapter. Let us consider a problem

$$\frac{\partial\phi'}{\partial t} + \operatorname{div} \underline{u}\phi' + \sigma\phi' = \frac{\partial}{\partial z}\nu\frac{\partial\phi'}{\partial z} + \mu\Delta\phi' + q + Q\delta(\underline{r} - \underline{r}_o),$$

$$\phi' = fs \qquad \text{on } \sum, \tag{6.1}$$

$$\frac{\partial\phi}{\partial z} = \alpha\phi' \qquad \text{on } \sum_o,$$

$$\frac{\partial \phi'}{\partial z} = 0 \quad \text{on } \sum_H$$

$$\phi' (\underline{r}, T) = \phi' (\underline{r}, 0),$$

where q(x,y,z) is an aerosol source of the plants in operation and f_s denotes the density of aerosols that are drifted through boundary G from the regions neighboring with $\sum_o$. In virtue of linearity of the problem the solution of (6.1) can be represented as a sum $\phi' = \phi^o + \phi$, where ϕ^o satisfies the problem

$$\frac{\partial \phi^o}{\partial t} + \operatorname{div} \underline{u}\, \phi^o + \sigma\phi^o = \frac{\partial}{\partial z} \nu \frac{\partial \phi^o}{\partial z} + \mu\Delta\phi^o + q,$$

$$\phi^o = f_s \quad \text{on } \sum,$$

$$\frac{\partial \phi^o}{\partial z} = \alpha\phi^o \quad \text{on } \sum_o, \tag{6.2}$$

$$\frac{\partial \phi^o}{\partial z} = 0 \quad \text{on } \sum_H,$$

$$\phi^o (\underline{r}, T) = \phi^o (\underline{r}, 0)$$

and ϕ satisfies the already known problem

$$\frac{\partial \phi}{\partial t} + \operatorname{div} \underline{u}\phi + \sigma\phi = \frac{\partial}{\partial z} \nu \frac{\partial \phi}{\partial z} + \mu\Delta\phi + Q\delta (\underline{r} - \underline{r}_o),$$

$$\phi = 0 \quad \text{on } \sum,$$

$$\frac{\partial \phi}{\partial z} = \alpha\phi \quad \text{on } \sum_o, \tag{6.3}$$

$$\frac{\partial \phi}{\partial z} = 0 \quad \text{on } \sum_H,$$

$$\phi (\underline{r}, T) = \phi (\underline{r}, 0).$$

It is now necessary to relate the functionals of (6.1) and similar functionals of (6.2), (6.3). Let us consider a functional

$$Y'_{pk} = \int_0^T dt \int_{G_k} p_{ck}\phi' \, dG, \tag{6.4}$$

where

$$p_{ck} = \begin{cases} b_k + a_k\delta (z) & \text{on } G_k, \\ 0 & \text{outside } G_k, \end{cases} \quad k = 1,2, \ldots, m.$$

Suppose that we have the following limitations for functionals Y'_{pk}

$$Y'_{pk} \leq C_k. \tag{6.5}$$

Inserting $\phi^o + \phi$ in (6.4) instead of ϕ' gives

$$Y'_{pk} = Y^o_{pk} + Y_{pk}, \tag{6.6}$$

where

$$Y^o_{pk} = \int_0^T dt \int_{G_k} p_{ck}\, \phi^o\, dG, \quad Y_{pk} = \int_0^T dt \int_{G_k} p_{ck}\phi\, dG. \tag{6.7}$$

Keeping in mind (6.6), condition (6.5) can be rewritten as

$$Y^o_{pk} + Y_{pk} \leq C_k \tag{6.8}$$

or $Y_{pk} \leq C_k - Y^o_{pk}$. Having denoted $C_k - Y^o_{pk} = \overline{C}_k$ we arrive at both the desired limitation for problem (6.3):

$$Y_{pk} \leq \overline{C}_k \tag{6.9}$$

and the problem we have considered though with new limitations. Functionals Y^o are found by solving problem (6.2).

The following remark relates to local in time functionals. Everywhere the basic functionals were assumed to be integral values over the entire time interval $0 \leq t \leq T$, that is, we proceeded from the assumption that the optimizing functional was connected with the total annual dose of aerosols, both in settled and suspended state over zone $\sum_k$. However, in this assumption no allowances were made for possible short-term but very intense aerosol emissions due to sudden changes in the direction and velocity of air mass motion. This can appreciably affect the pollution level in the zones of $\sum_o$, though the average annual safe dose of pollution with such aerosols will not exceed the stipulated value. This implies that local in time functionals (for the periods when variations in meteorological conditions are very likely) may also be considered along with the studied functionals of total annual value.

Suppose that in a given region, j_o typical variations in meteorological conditions occur and total annual duration of every condition is equal to t_j. Summing up over all $j = 1,2, \ldots, j_o$ we obtain

$$\sum_{j=1}^{j_o} \Delta t_j = T.$$

Neglecting transient processes, and assuming additivity, it is possible to consider the general process to be continuous with arbitrary alternation of different types of meteorological conditions and to solve j_o different basic problems (chapter 1):

$$\begin{aligned}
\operatorname{div} \underline{u}\phi_j + \sigma\phi_j &= \frac{\partial}{\partial z}\nu\frac{\partial \phi_j}{\partial z} + \mu\Delta\phi_j + Q\delta(\underline{r}-\underline{r}_o), \\
\phi_j &= 0 \quad \text{on } \textstyle\sum, \\
\frac{\partial \phi_j}{\partial z} &= \alpha\phi \quad \text{on } \textstyle\sum_o, \\
\frac{\partial \phi_j}{\partial z} &= 0 \quad \text{on } \textstyle\sum_H
\end{aligned} \tag{6.10}$$

Note that if transient effects are disregarded, then the solution to (6.10) can be obtained by the following nonstationary, but periodic problem:

$$\begin{aligned}
\frac{\partial \phi}{\partial t} + \operatorname{div} \underline{u}\phi + \sigma\phi &= \frac{\partial}{\partial z}\nu\frac{\partial \phi}{\partial z} + \mu\Delta\phi + Q\delta(\underline{r}-\underline{r}_o), \\
\phi &= 0 \quad \text{on } \textstyle\sum, \\
\frac{\partial \phi}{\partial z} &= \alpha\phi \quad \text{on } \textstyle\sum_o, \\
\frac{\partial \phi}{\partial z} &= 0 \quad \text{on } \textstyle\sum_H, \\
\phi(\underline{r}, t_{j+1}) &= \phi(\underline{r}, t_j),
\end{aligned} \tag{6.11}$$

where t_j, t_{j+1} are the limits of the generalized time interval Δt_j in which a typical meteorological situation develops. Then

$$\phi_j = \frac{1}{\Delta t_j}\int_{t_j}^{t_{j+1}} \phi \, dt. \tag{6.12}$$

Along with the basic problem (6.10) we shall consider the following adjoint problem:

$$\begin{aligned}
-\operatorname{div} \underline{u}\phi^*_{jk} + \sigma\phi^*_{jk} &= \frac{\partial}{\partial z}\nu\frac{\partial \phi^*_{jk}}{\partial z} + \mu\Delta\phi^*_{jk} + p_{ck}, \\
\phi^*_{jk} &= 0 \quad \text{on } \textstyle\sum, \\
\frac{\partial \phi^*_{jk}}{\partial z} &= \alpha\phi^*_{jk} \quad \text{on } \textstyle\sum_o, \\
\frac{\partial \phi^*_{jk}}{\partial z} &= 0 \quad \text{on } \textstyle\sum_H,
\end{aligned} \tag{6.13}$$

where

$$p_{ck} = \begin{cases} b_k + a_k \delta(z) & \text{on } G_k, \\ 0 & \text{outside } G_k. \end{cases}$$

The solution to problem (6.13) can be found by the nonstationary problem:

$$\begin{aligned} -\frac{\partial \phi_k^*}{\partial t} - \operatorname{div} \underline{u}\phi_k^* + \sigma\phi_k^* &= \frac{\partial}{\partial z} \nu \frac{\partial \phi_k^*}{\partial z} + \mu\Delta\phi_k^* + p_{ck}, \\ \phi_k^* &= 0 \quad \text{on } \textstyle\sum, \\ \frac{\partial \phi_k^*}{\partial z} &= \alpha\phi_k^* \quad \text{on } \textstyle\sum_o, \\ \frac{\partial \phi_k^*}{\partial z} &= 0 \quad \text{on } \textstyle\sum_H, \end{aligned} \tag{6.14}$$

$$\phi_k^* (\underline{r}, t_{j+1}) = \phi_k^*(\underline{r}, t_j).$$

Then

$$\phi_{jk}^* = \frac{1}{\Delta t_j} \int_{t_j}^{t_{j+1}} \phi_k^* \, dt.$$

Let us consider also the functionals

$$Y_{pjk} = \int_{G_k} p_{ck}\phi_j \, dG, \quad Y_{pjk} = Q\phi_{jk}^* (\underline{r}_o), \tag{6.15}$$

$$j = 1,2, \ldots, j_o; \quad k = 1,2, \ldots, m.$$

Having a set of adjoint problems, we introduce as before the inequality

$$Y_{pjk} \leq G_{jk},$$

where C_{jk} are the maximum permissible doses of pollution. As a result, the problem is boiled down to finding regions ω_{kj} where an industrial plant can be constructed without violating sanitary requirements for zone Ω_k. Let us denote the intersection of regions ω_{kj} $(j = 1,2, \ldots, j_o)$ by $\overline{\omega}_k$. It is this region that will satisfy all of the requirements with consideration for all types of meteorological processes involved in the transfer and diffusion of aerosols.

It follows that the intersection of all $\overline{\omega}_k$ $(k = 1,2, \ldots, m)$ yields a region $\overline{\omega}_C$ where an industrial unit can safely be located from the viewpoint of sanitary requirements and with consideration for standardization of meteorological processes.

Chapter 5. ECONOMIC CRITERIA OF PLANNING, PROTECTION AND RESTORATION OF ENVIRONMENT

In the previous chapter we have discussed the problem of locating industrial units with consideration for maximum permissible doses of pollution for all ecologically important zones in a given region. Here, we shall introduce a new functional connected with economic expenditure on restoration of the environment polluted with industrial emissions. Together with the facts considered before, this functional gives a sufficiently complete image of possible consequences of biosphere pollution and the economic expenditure on ecological restoration of the environment.

5.1. Value of Biosphere Products Losses, due to Environmental Pollution with Indistrual Emissions

Since, with a rare exception, industrial emissions tend to oppress the animal and vegetable kingdom, including birds, fish, mollusc, insects, useful bacteria, and other components of the biosphere, it is quite natural to give some integral, over the entire region $\sum_o$, estimate of loss due to industrial emissions.

With this aim we shall consider differential characteristics that describe the amount of biomass of a given component ℓ lost due to aerosol pollution j referred to a unit area per time unit of unit aerosol concentration. Let us denote it by $n_\ell b_{j\ell}$ ($j = 1,2, \ldots, m$; $\ell = 1, \ldots, s$), where $n_\ell(x,y)$ is the density of the ℓ-th population in $\sum_o$ and b_{ij} is loss in the population biomass calculated per unit density. Then the total annual loss of the biomass component ℓ due to aerosol pollution at concentration ϕ_j in $\sum_o$ is defined by formula

$$\beta_{\ell j} = \int_0^T dt \int_{\Sigma_o} n_\ell b_{j\ell} \phi_j d\Sigma. \qquad (1.1)$$

Let β_ℓ be the value of a unit component of the biomass. The loss due to pollution in such a case will be equal to

$$c_{\ell j} = \int_0^T dt \int_{\Sigma_o} \beta_\ell \, n_\ell b_{j\ell} \phi_j \, d\Sigma. \qquad (1.2)$$

Summing up $c_{\ell j}$ over all components ℓ we obtain

$$c_j = \int_0^T dt \int_{\Sigma_o} p_o^j \, \phi_j \, d\Sigma, \qquad (1.3)$$

where

$$p_o^j = \sum_{\ell=1}^{s} n_\ell \beta_\ell \, b_{j\ell}. \tag{1.4}$$

The values $b_{j\ell}$ showing the level of physiological oppression of biosphere components by aerosols of a given type are obtained on the basis of experimental studies. It may be noted that at large concentrations of pollutants, $b_{j\ell}$ cease to be linear functions. Now if we sum up the results over all components of the aerosols discharged by industrial plants, we obtain total loss of biosphere in the region:

$$c = \sum_{j=1}^{m} \int_0^T dt \int_{\Sigma_o} p_o^j \phi_j \, d\Sigma. \tag{1.5}$$

Let us now formulate the optimization problem. To this end, we consider m problems corresponding to basic components of emissions:

$$\begin{aligned}
&\frac{\partial \phi_j}{\partial t} + \operatorname{div} \underline{u}\phi_j + \sigma_j \phi_j = \frac{\partial}{\partial z} \nu \frac{\partial \phi_j}{\partial z} + \mu \Delta \phi_j + Q_j \delta(\underline{r} - \underline{r}_o),\\
&\phi_j = 0 \qquad \text{on } \textstyle\sum,\\
&\frac{\partial \phi_j}{\partial z} = \alpha \phi_j \qquad \text{on } \textstyle\sum_o,\\
&\frac{\partial \phi_j}{\partial z} = 0 \qquad \text{on } \textstyle\sum_H,\\
&\phi_j(\underline{r},T) = \phi_j(\underline{r},0), \qquad j = 1, 2, \ldots, m,
\end{aligned} \tag{1.6}$$

and m adjoint problems:

$$\begin{aligned}
&-\frac{\partial \phi_j^*}{\partial t} - \operatorname{div} \underline{u}\phi_j^* + \sigma_j \phi_j^* = \frac{\partial}{\partial z} \nu \frac{\partial \phi_j^*}{\partial z} + \mu \Delta \phi_j^* + p_{oj} \delta(z),\\
&\phi_j^* = 0 \qquad \text{on } \textstyle\sum,\\
&\frac{\partial \phi_j^*}{\partial z} = \alpha \phi_j^* \qquad \text{on } \textstyle\sum_o,\\
&\frac{\partial \phi_j^*}{\partial z} = 0 \qquad \text{on } \textstyle\sum_H,\\
&\phi_j^* (\underline{r}, T) = \phi_o^* (\underline{r}, 0), \qquad j = 1, 2, \ldots, m.
\end{aligned} \tag{1.7}$$

We shall assume that problems (1.6) and (1.7) are solved. Let us now consider the functional

$$I_j = \int_0^T dt \int_{\Sigma_o} p_o^j \phi_j \, d\Sigma. \qquad (1.8)$$

Its dual form is written by solving an adjoint equation and takes the form

$$I_j = Q_j \int_0^T \phi_j^* (\underline{r}_o, t)\, dt. \qquad (1.9)$$

It is important to note that in the case of the functional in question problem (1.7) is solved only once for a fixed aerosol. Further we compute function $\phi^*(\underline{r}, t)$ and find a region ω_B where the loss of biomass due to polluted environment will be minimum. Thus, along with the region ω_C introduced in the previous chapter and ensuring satisfaction of sanitary requirements for ecologically important objects, there appears a region ω_B where conditions of permissible environmental losses for the region $\sum_o$ are fulfilled. The intersection of these regions gives the most suitable area for locating a new industrial plant (figure 5.1).

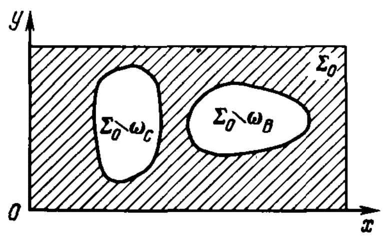


FIGURE 5.1

5.2. Value of Losses Due to Atmospheric Pollution with Multicomponent Aerosol

Let us consider a multicomponent mixture of a passive aerosol which undergoes no chemical changes upon scattering and therefore $\sigma_j = 0$. Assume that the aerosol is light and consists of oxides of different compounds. This implies that the entire mixture is scattered according to one law. In this case, problems (1.6) and (1.7) may immediately be formulated for the mixture density.

Suppose that the discharge of sources Q_j of given aerosol components is known and

$$Q_j/Q = \gamma_j, \quad j = 1, \ldots, m. \qquad (2.1)$$

Similarly we assume that

$$\phi_j = \gamma_j \phi, \quad \phi_j^* = \gamma_j \phi^*, \tag{2.2}$$

where

$$\sum_{j=1}^{m} \gamma_j = 1. \tag{2.3}$$

Taking into account (2.3) it follows from (2.1) and (2.2) that

$$\phi = \sum_{j=1}^{m} \phi_j, \quad \phi^* = \sum_{j=1}^{m} \phi_j^*, \quad Q = \sum_{j=1}^{m} Q_j, \tag{2.4}$$

Summing up every relation of (1.6) over j with the use of (2.4) we obtain an aerosol mixture scattering problem:

$$\begin{gathered}
\frac{\partial \phi}{\partial t} + \operatorname{div} \underline{u}\phi = \frac{\partial}{\partial z} \nu \frac{\partial \phi}{\partial z} + \mu\Delta\phi + Q\delta(\underline{r} - \underline{r}_o), \\
\phi = 0 \qquad \text{on } \Sigma, \\
\frac{\partial \phi}{\partial z} = \alpha\phi \qquad \text{on } \Sigma_o, \\
\frac{\partial \phi}{\partial z} = 0 \qquad \text{on } \Sigma_H, \\
\phi(\underline{r}, T) = \phi(\underline{r}, 0).
\end{gathered} \tag{2.5}$$

Analogously we arrive at an adjoint problem for the mixture:

$$\begin{gathered}
- \frac{\partial \phi^*}{\partial t} - \operatorname{div} \underline{u}\, \phi^* = \frac{\partial}{\partial z} \nu \frac{\partial \phi^*}{\partial z} + \mu\Delta\phi^* + p_o\delta(z), \\
\phi^* = 0 \qquad \text{on } \Sigma, \\
\frac{\partial \phi^*}{\partial z} = \alpha\phi^* \qquad \text{on } \Sigma_o, \\
\frac{\partial \phi^*}{\partial z} = 0 \qquad \text{on } \Sigma_H, \\
\phi^*(\underline{r}, T) = \phi^*(\underline{r}, 0),
\end{gathered} \tag{2.6}$$

where $p_o = \sum_{j=1}^{m} p_o^j$.

Thus, the functional under study - value of biosphere losses in region Σ_o - takes the form

$$I = \int_0^T dt \int_{\Sigma_o} p_o \phi \; d\Sigma \tag{2.7}$$

or

$$I = Q \int_0^T \phi^* (\underline{r}_o, t)\, dt; \tag{2.8}$$

Here

$$p_o = \sum_{j=1}^{m} \sum_{\ell=1}^{s} n_\ell \beta_\ell b_{\ell j} = \sum_{\ell=1}^{s} n_\ell \beta_\ell\, b_\ell,\ b_\ell = \sum_{j=1}^{m} b_{\ell j}. \tag{2.9}$$

After solving problem (2.6) and determining the location of the planned installation, we find a solution ϕ to problem (2.5). Further, using (2.2), recalculation is made in term of component-wise density $\phi_j = \gamma_j\ \phi(j= 1, \ldots, m)$. Together with this the differentiated distribution of aerosol densities in region $\sum_o$ is ascertained. If the propagation of aerosols ϕ_j follows different laws, then m problems will have to be solved for finding the total dose C.

In conclusion it may be noted that in such calculations the determination of coefficients b_{ij} is the most significant element of initial problems. This is a very nontrivial problem as it requires either simultaneous multi-year control over all biosphere components found in the polluted zone, or construction of complex biocoenosis mathematical models that would take account of biosphere components interaction as much as possible. Let us illustrate it. Suppose that an aerosol ϕ_j proves fatal for insects. This will entail a sharp decrease in the abundance of insectivorous birds and this, in its turn, will have an effect on birds-of-prey feeding on insectivorous birds and rodents. As a result, rodent population will increase and the loss of cereals in fields will grow, and the like. Therefore, much attention should be paid to the determination of coefficients b_{ij} since it is of prime importance in planning expansion of industry and forecasting its ecological effect on the environment.

5.3. Economic Aspects of Natural Resources Depreciation when Ecological Conditions are Disturbed Due to Environmental Pollution

Earlier we have touched upon values of losses in various biosphere components due to environmental pollution. This is only one way of looking at this problem. The other way resides in restoration jobs aimed at improving or, at least, maintaining ecological conditions of the regions. In fact, if for example, in polluted water bodies the fish breeding decreases due to the oppression of spawning, then fish hatcharing farms are established to restore fish population in a given water body up to the optimal level which is determined by available fish-feed resources. A decreased crop yield should be augmented by improving farming practices, applying organic and mineral fertilizers, and land reclamation. When abundance of beasts decreases, measures are taken to feed and look after them; hunting quotas are set, and so on.

Thus, the damage to nature, particularly to animate nature, should be compensated by planned additional deductions made from the operating profits of the enterprises. Such deductions should be made compulsary like depreciation deductions.

Let us formulate a mathematical model for estimating such compulsary expenses. Let p_ℓ be the cost of measures aimed at restoring a unit mass of the ℓ-th biosphere component, oppressed by noxious industrial emissions, to its initial level. Let us now calculate the loss of the j-th biosphere component:

$$\Delta M = \int_0^T dt \int_{\Sigma_o} n_\ell b_{j\ell}\phi_j \, d\Sigma. \tag{3.1}$$

Then the cost of restoration measures will equal to

$$R_{j\ell} = \int_0^T dt \int_{\Sigma_o} p_\ell n_\ell b_{j\ell}\phi_j \, d\Sigma. \tag{3.2}$$

Adding (3.2) over ℓ and j we obtain

$$R_g = \sum_{\ell=1}^{m} \sum_{\ell=1}^{s} \int_0^T dt \int_{\Sigma_o} p_\ell n_\ell b_{j\ell}\phi_j \, d\Sigma. \tag{3.3}$$

We now write this expression as

$$R_g = \sum_{j=1}^{m} \int_0^T dt \int_{\Sigma_o} \xi_j\phi_j \, d\Sigma, \tag{3.4}$$

where

$$\xi_j = \sum_{\ell=1}^{s} p_\ell n_\ell b_{j\ell}. \tag{3.5}$$

If we assume that noxious industrial emission is light and undecomposable, then $\sigma_j = 0$ ($j = 1, 2, \ldots, m$). Then, with allowance made for (2.2), we write

$$R_g = \int_0^T dt \int_{\Sigma_o} \xi\phi \, d\Sigma, \tag{3.6}$$

where

$$\xi = \sum_{j=1}^{m} \gamma_j\xi_j. \tag{3.7}$$

Now we can formulate an adjoint problem with respect to functional R_g:

$$-\frac{\partial\phi^*}{\partial t} - \operatorname{div} \underline{u}\phi^* = \frac{\partial}{\partial z}\nu\frac{\partial\phi^*}{\partial z} + \mu\Delta\phi^* + \xi\delta(z),$$
$$\phi^* = 0 \quad \text{on } \textstyle\sum,$$
$$\frac{\partial\phi^*}{\partial z} = \alpha\phi^* \quad \text{on } \textstyle\sum_o, \tag{3.8}$$
$$\frac{\partial\phi^*}{\partial z} = 0 \quad \text{on } \textstyle\sum_H,$$
$$\phi^*(\underline{r}, T) = \phi^*(\underline{r}, 0).$$

Then on the basis of the general theory we have two equalities:

$$R_g = \int_0^T dt \int_{\Sigma_o} \xi\phi \, d\Sigma, \qquad R_g = Q\int_0^T \phi^*(\underline{r}_o, t)\, dt. \tag{3.9}$$

To solve $\phi^*(\underline{r}, t)$ we construct a graph of function $R(\underline{r}_o)$, which is shown in figure 5.2.

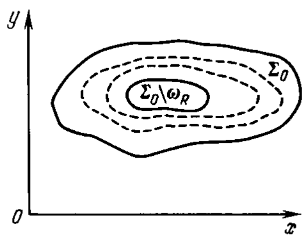


FIGURE 5.2

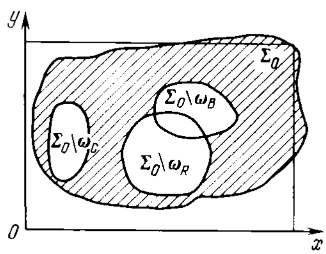


FIGURE 5.3

With the algorithm given we find a domain ω_R where operation of an industrial plant would require lesser depreciation expenditures for restoration of polluted environment than those permitted by sanitary requirements: $R_g \leq B_R$. Thus, in planning the location of an industrial plant that discharges noxious aerosols into the air, we arrive at three criteria.

Pollution of ecologically most important zones must satisfy maximum permissible values stipulated by sanitary requirements. As a result, we find a region $\omega_C \subset \sum_o$.

The losses of biological resources, when polluted, should be minimum. In this case, we find a region $\omega_B \subset \sum_o$.

Depreciation expenditures for restoration of biological resources abated due to environmental pollution. This gives us a region $\omega_R \subset \sum_o$.

The intersection of these regions yields a most suitable area for a construction site. In figure 5.3 this area is hatched. If the intersection of regions does not yield any area, then the limiting economical criteria should be changed.

A case when every component of the aerosol behaves as the entire mixture was also considered. If some aerosol components scatter differently, then all of the problems must be solved for every component j. As a result, we arrive at a more complex, but a simpler problem of intersection of 3j different regions.

5.4. General Economical Criterion

It can happen that the intersection of the regions for which all optimization criteria are fulfilled in the given region $\sum_o$, is empty. It will then be necessary to relax these or other limitations on the functionals being studied, or to increase the dimensions of the region in question. Such changes in the optimization problem are heuristic, in principle, and do not represent a strictly deterministic process.

On the other hand, the optimization criteria formulated in the previous chapters enable us, strictly speaking, to uniquely isolate zones where geographical distribution of industry is inadmissible. Additional information is needed to localize the regions where territorial distribution of industry is economically justified. In this section we shall therefore consider a common economical criterion of total expenditures on restoration of environment polluted with industrial wastes; we shall do this with due regard for mutual optimum location of industrial plants and for ecologically important zones.

The task of mutual optimum location of industrial plants includes consideration of a large number of factors related to economic expenditures on construction in the given site, construction and operation cost of service lines (railways, motor roads, water pipelines, telephone and telegraph service, etc.) under definite conditions, and future development of the region as a whole. Methodologically this problem can be standardized as follows:

- by planning the siting of plants in the region in accord with the established ecological structure (for example, construction of a large integrated plant in a suburb area);

- by forming an ecological structure around industrial installations (for example, by building living accomodations according to the proposed construction of industrial units exploiting mineral resources and, therefore, "connected" with one or another area);

- by simultaneous planning of a new industrial location and location of ecologically important zones.

Let us now formulate the general economic criterion with due consideration for a situation of the first type. We thus direct our attention to expenditures on restoration of environment, which include: expenditures on medical protection of local population, on extra nourishment and on improving its quality, on dispensaries, rest houses, holiday hotels, and hospitals.

Let us denote by a_{jk} the expenditures on restoration of health of the people living in an ecologically important region, marked with k, calculated per person per year and referred to unit concentration of aerosol j. Suppose that N_k is the total population of the given region. Then the amount spent on restoration of health undermined by pollution will equal to

$$c_{jk} = \int_0^T dt \int_{\Omega_k} a_{jk} N_k \phi_j \, d\Sigma . \tag{4.1}$$

Summing up this expression over all ecologically important regions, we obtain

$$R_{pj} = \sum_{k=1}^{n} c_{jk} = \sum_{k=1}^{n} \int_0^T dt \int_{\Omega_k} a_{jk} N_k \phi_j d\Sigma \tag{4.2}$$

or

$$R_{pj} = \int_0^T dt \int_{\Sigma_o} P_p^j \, \phi_j \, d\Sigma , \tag{4.3}$$

where

$$P_p^j = \begin{cases} \sum_{k=1}^{n} a_{jk} N_k , & \underline{r} \in \bigcup_{k=1}^{n} \Omega_k , \\ 0 & \text{outside the domain} \end{cases}$$

The second part of the expenditures is related to the decrease in the biomass of all environmental components (animal kingdom, vegetation cover, etc.) due to the decline in soil productive areas. Denote them by R_{bj}. In compliance with the results of section 5.1 we write

$$R_{bj} = \int_0^T dt \int_{\Sigma_o} P_b^j \phi_j \, d\Sigma , \tag{4.4}$$

where $P_b^j = \sum_{\ell=1}^{s} n_\ell \beta_\ell \, b_{j\ell}$.

The third part is spent on maintaining the productivity of bioresources at a given constant level:

$$R_{gj} = \int_0^T dt \int_{\Sigma_o} P_g^j \phi_j \, d\Sigma, \tag{4.5}$$

where $P_g^j = \sum_{\ell=1}^{s} p_\ell n_\ell b_{j\ell}$.

Then for m different components of toxic impurities we obtain m functionals

$$R = R_{pj} + R_{bj} + R_{gj} \tag{4.6}$$

After adding we get

$$R = \sum_{j=1}^{m} R_j. \tag{4.7}$$

Let us now denote by $c_i(\underline{r})$ the construction cost of an industrial plant, marked with i, at a point $\underline{r}$ of $\sum_o$; by $c_{ik}(\underline{r})$ we denote the construction and operation cost of service lines, calculated per unit of the shortest distance between point $\underline{r}$ of the i-th unit and the k-th protected zone (including average cost of planned transportation of goods and passengers). Let $r_{ik}(\underline{r})$ be the totality of such distances. Now we consider a functional

$$E_{ik}(\underline{r}) = c_i(\underline{r}) + c_{ik}(\underline{r}) r_{ik}(\underline{r}), \tag{4.8}$$

characterizing the construction cost of the i-th unit and of necessary service links with the k-th ecological zone. Summing up (4.8) over all k and taking account of functional (4.7), we find a common functional

$$I_i(\underline{r}_o) = R(\underline{r}_o) + \sum_{k=1}^{n} E_{ik}(\underline{r}_o), \tag{4.9}$$

whose level curves, $I(\underline{r})$ = const, give us a localized domain most suitable for plants siting.

Let us now consider the following model situation. Two settlements are located at points (x_1, y_1) and (x_2, y_2), the first being with double population of the second. Wind blowing parallel to the x-axis predominates in the considered region over a time cycle [0, T]. A point with coordinates (x_2, y_1) is a place where the construction cost of the industrial plant is minimum. As we go farther and farther away from this point the cost increases proportional to the function of type $\Psi(x, y) = 2\text{-}\exp\{-\alpha[(x - x_2)^2 + (y - y_1)^2]\}$. And, finally, in the area $x > (x_1 + x_2)/2$ the cost of service lines exceeds two-fold the cost of communications in $[0, (x_1 + x_2)/2]$.

Value of 01 level 10.0000 Value of 20 level 7.5485

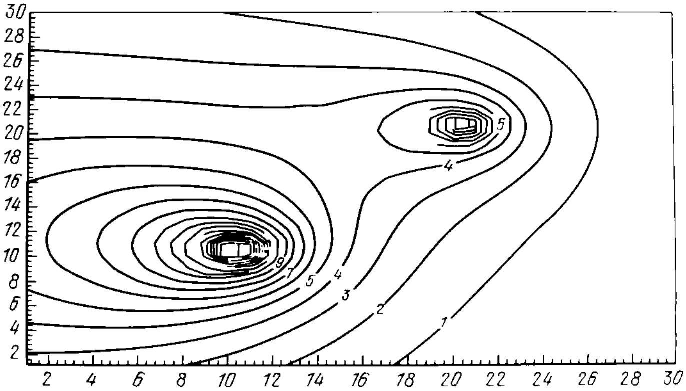


FIGURE 5.4

Value of 01 level 4.5151 Value of 20 level 1.5572

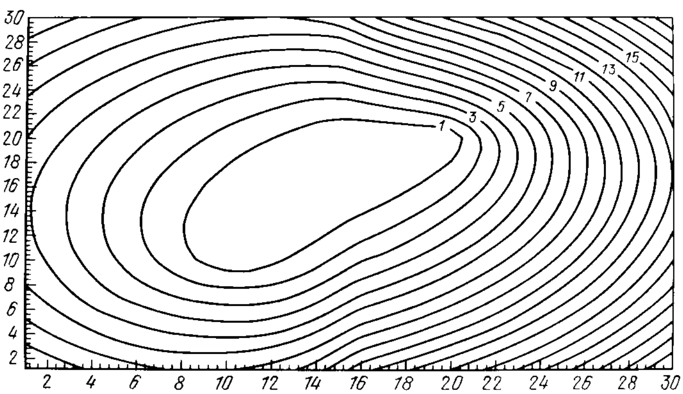


FIGURE 5.5

Figure 5.4 shows isolines of a functional that described only the cost of medical services rendered to the population. The functional shown in figure 5.5 describes the cost of communications. Figure 5.6 gives the construction cost of a factor proper.

Value of 01 level 1.0405 Value of 20 level 1.8102

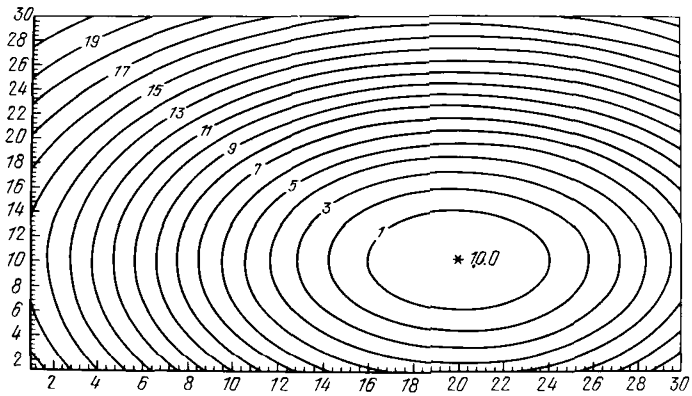


FIGURE 5.6

Isolines of a functional of the type (4.9) are shown in figures 5.7 through 5.10. Different variants conform to prevalence of various types of the considered costs. For example, figure 5.7a shows predominance of the cost of laying communications, that is,

$$I_i(\underline{r}_o) = R(\underline{r}_o) + \sum_{k=1}^{n} (2c_i(\underline{r}_o) + 20c_{ik}(\underline{r}_o)r_{ik}(\underline{r}_o)).$$

whereas figure 5.7b illustrates the surface formed by this functional. Figure 5.8 conforms to a larger share of erection cost of a plant, the cost of laying communications being comparable with the erection cost, that is,

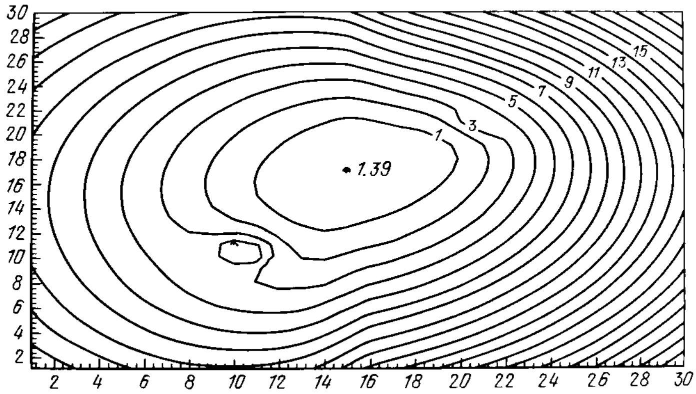
$$I_i(\underline{r}_o) = R(\underline{r}_o) + \sum_{k=1}^{n} (10c_i(\underline{r}_o) + 8c_{ik}(\underline{r}_o)r_{ik}(\underline{r}_o)),$$

The surface corresponding to this functional is represented in figure 5.8b.

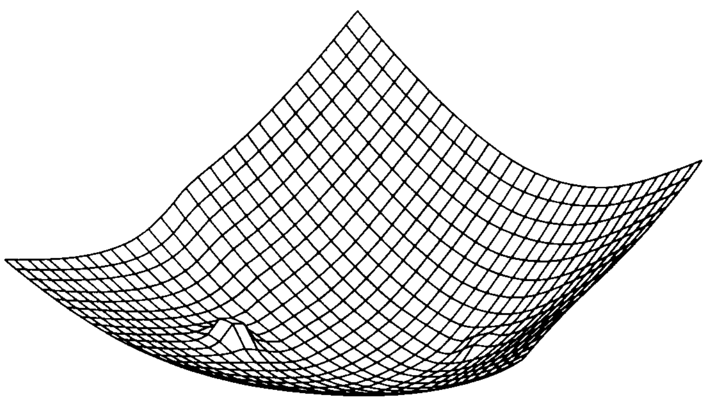
Figure 5.9a illustrates a situation when the cost of communications is almost equal to other costs, that is,

$$I_i(\underline{r}_o) = R(\underline{r}_o) + \sum_{k=1}^{n} (2c_i(\underline{r}_o) + 4c_{ik}(\underline{r}_o)r_{ik}(\underline{r}_o));$$

Value of 01 level 1.5328 Value of 20 level 4.1774



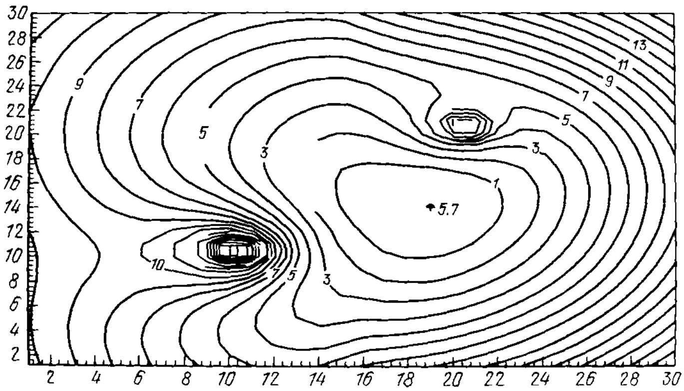
a)



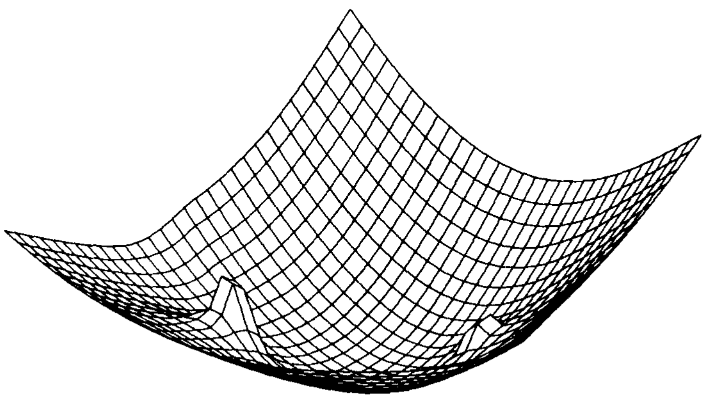
b)

FIGURE 5.7

Value of 01 level 6.0643 Value of 20 level 1.2102



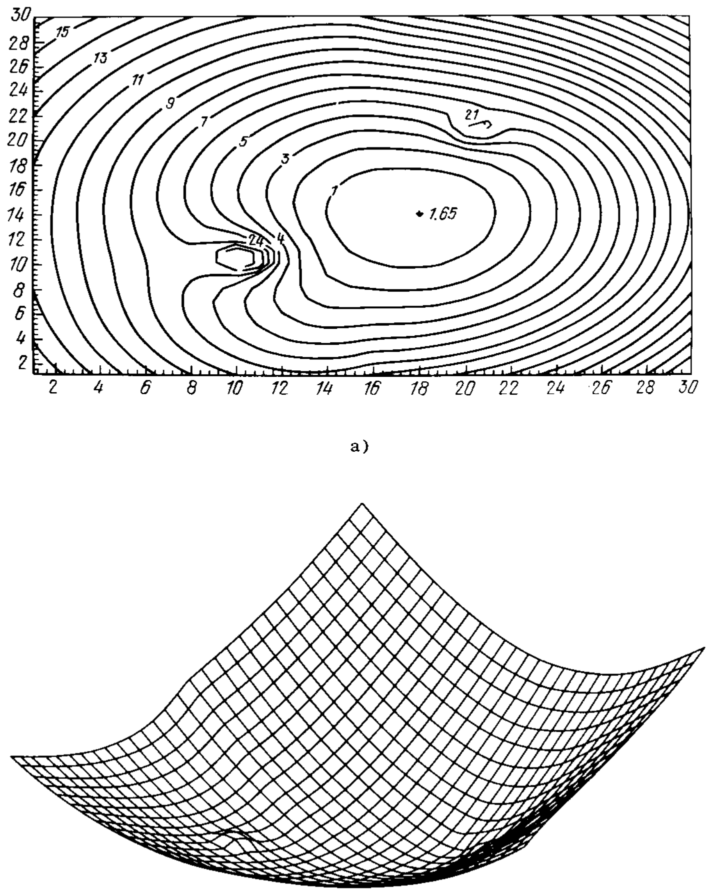
a)



b)

FIGURE 5.8

Value of 01 level 1.7343   Value of 20 level 3.1881

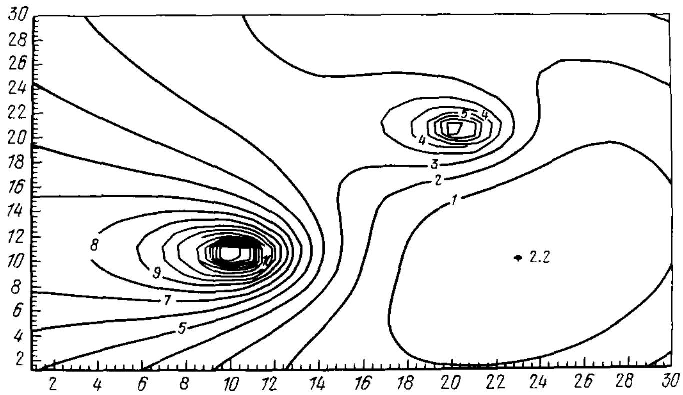


a)

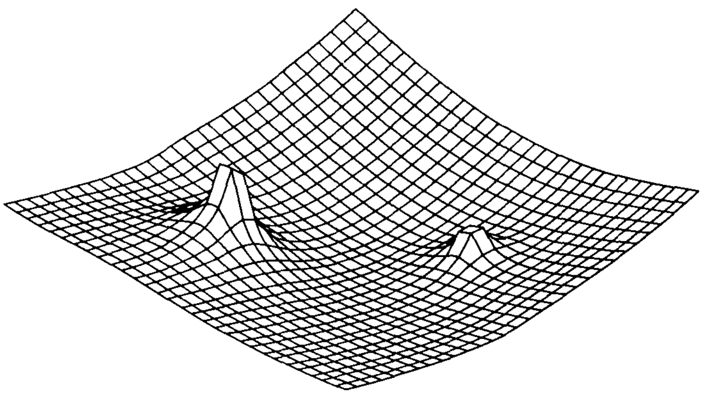
b)

FIGURE 5.9

Value of 01 level 2.5959 Value of 20 level 9.2086



a)



b)

FIGURE 5.10

A corresponding surface is shown in figure 5.9b. Finally, figure 5.10a illustrates a case when all types of costs are equal, and figure 5.10b shows a surface for this case. Areas of industrial plants location, where the total expenditures will be minimum with regard to earlier listed factors, are marked in the figures; therein the total expenditures in the chosen units of measurements are shown for this point.

Chapter 6. MATHEMATICAL PROBLEMS OF OPTIMIZING EMISSIONS FROM OPERATING INDUSTRIAL PLANTS

Protection of environment against industrial pollution is becoming a topical problem of science and engineering. In the previous chapters we have considered an aspect of this problem, which is related to the location of new industrial units (emitting noxious aerosols into the air) with regard to minimum pollution of the neighboring settlements, recreation zones, agricultural lands, and other ecologically important zones. In this chapter we shall consider another aspect of this problem. We shall assume all industrial units in this region to be operating and discharging noxious aerosols into the air. The task resides in determining for every unit a permissible amount of aerosols to be discharged such that their sum will not exceed permissible values stipulated by sanitary requirements. At the same time, total emissions cannot be significantly decreased since this will result in the lowering of economic indices of the industrial units. Thus, we shall talk about such limitations on emissions which will, nevertheless, ensure maximum economic effect at the given limitations.

6.1. Statement of the Problem

Suppose that at $\underline{r}_i$ $(i = 1, 2, \ldots, n)$ points of a given region G with boundary S n industrial units A_i are located and that they discharge every second $Q_i (i = 1, 2, \ldots, n)$ aerosols. For simplicity, we shall assume the composition of these aerosols to be uniform. In region G we shall isolate m ecological zones G_k $(k = 1, 2, \ldots, m)$; the limiting permissible concentration of aerosols emitted in a time interval $[0, T]$, are given for each of these zones. As a result, we arrive at the following mathematical statement of the problem.

Let an equation for diffusion of substances from n industrial units be the following:

$$\frac{\partial \phi}{\partial t} + \operatorname{div} \underline{u}\phi + \sigma\phi = \frac{\partial}{\partial z} \nu \frac{\partial \phi}{\partial z} + \mu\Delta\phi + \sum_{i=1}^{n} Q_i \delta(\underline{r} - \underline{r}_i) \tag{1.1}$$

provided

$$\begin{aligned} \phi &= f_s \quad \text{on} \quad \textstyle\sum, \\ \frac{\partial \phi}{\partial z} &= \alpha\phi \quad \text{on} \quad \textstyle\sum_0, \\ \frac{\partial \phi}{\partial z} &= 0 \quad \text{on} \quad \textstyle\sum_H. \end{aligned} \tag{1.2}$$

Assuming the problem (1.1), (1.2) to be climatically periodic (with a period equal to 1 year), we obtain the initial data

$$\phi(\underline{r}, T) = \phi(\underline{r}, 0) \tag{1.3}$$

Let us consider the functional

$$Y_k = \int_0^T dt \int_{G_k} p_c \phi \, dG, \tag{1.4}$$

which characterizes the safe dose of the aerosol that has settled on Earth's surface (z = 0) within the ecological zone G_k. The problem resides in finding a totality of planned emission of aerosols Q_j, which will ensure average-annual maximum permissible doses of aerosol pollution

$$Y_k \leq c_k, \quad k = 1, 2, \ldots, \ldots, m \tag{1.5}$$

with minimum outlay for technological reconstruction of plants; which will assure a specified volume of output at the given decrease in the emission level.

Of course, in this problem it is necessary to consider a minimizing functional along with the limitations (1.5). As such a functional we take

$$I = \sum_{i=1}^{n} \xi_i(\bar{Q}_i - Q_i), \tag{1.6}$$

in which $\bar{Q}_i$ and Q_i are the initial and the planned emission rates, respectively; coefficient ξ_i determines capital outlay for technology that will ensure the same volume of output on decreasing the emission level (calculated for a unit emission rate). Then the functional I represents total expenses necessary for improving the production processes at all the units A_i as we pass from $\bar{Q}_i$ to Q_i. As a result, we arrive at a problem of finding emissions Q_i in (1.1)-(1.3) such that the following conditions are fulfilled

$$\begin{gathered} I = \sum_{i=1}^{n} \xi_i(\bar{Q}_i - Q_i) = \min \\ Y_k \leq c_k, \quad k = 1, 2, \ldots, m. \end{gathered} \tag{1.7}$$

Problem (1.1)-(1.3), (1.7) can be reduced to a linear programming problem. This can be done in two different ways: with the use of basic equations and by adjoint problems.

6.2. Optimization by Basic Equations

Let us represent the solution to problem (1.1)-(1.3) as superposition of solutions of elementary problems. Suppose that

$$\phi = \sum_{i=1}^{n} Q_i \phi_i(\underline{r}, t) + \phi_S, \tag{2.1}$$

where $\phi_i(\underline{r}, t)$ is the solution of the problem

$$\frac{\partial \phi_i}{\partial t} + u \frac{\partial \phi_i}{\partial x} + v \frac{\partial \phi_i}{\partial y} + w \frac{\partial \phi_i}{\partial z} + \sigma \phi_i = \frac{\partial}{\partial z} \nu \frac{\partial \phi_i}{\partial z} + \mu \Delta \phi_i + \delta(\underline{r} - \underline{r}_i) \tag{2.2}$$

with boundary conditions

$$\begin{aligned} \phi_i &= 0 \quad \text{on } \Sigma, \\ \frac{\partial \phi_i}{\partial z} &= \alpha \phi_i \quad \text{on } \Sigma_o, \\ \frac{\partial \phi_i}{\partial z} &= 0 \quad \text{on } \Sigma_H \end{aligned} \tag{2.3}$$

and the periodicity condition

$$\phi_i(\underline{r}, T) = \phi_i(\underline{r}, 0). \tag{2.4}$$

Along with the problems (2.2)-(2.4), for $i = 1, 2, \ldots, n$, we shall consider one more problem for determining the background of aerosols that come into region G through boundary S:

$$\frac{\partial \phi_S}{\partial t} + \operatorname{div} \underline{u}\phi_S + \sigma \phi_S = \frac{\partial}{\partial z} \nu \frac{\partial \phi_S}{\partial z} + \mu \Delta \phi_S \tag{2.5}$$

given that

$$\begin{aligned} \phi_S &= f \quad \text{on } \Sigma, \\ \frac{\partial \phi_S}{\partial z} &= \alpha \phi_S \quad \text{on } \Sigma_o, \\ \frac{\partial \phi_S}{\partial z} &= 0 \quad \text{on } \Sigma_H, \end{aligned} \tag{2.6}$$

$$\phi_S(\underline{r}, T) = \phi_S(\underline{r}, 0). \tag{2.7}$$

Assume that each of the problems (2.2)-(2.4), for $i = 1, 2, \ldots, n$, and also the problem (2.5)-(2.7) are solved. Then the representation of (2.1) is justified. Now we can make use of (2.1) for computing functionals Y_k. Indeed, substituting (2.1) into (1.4) gives

$$Y_k = \sum_{i=1}^{n} Q_i a_{ik} + b_k, \tag{2.8}$$

where

$$a_{ik} = \int_0^T dt \int_{G_k} p_c \phi_i (\underline{r}, t)\, dG,$$

$$b_k = \int_0^T dt \int_{G_k} p_c \phi_S (\underline{r}, t)\, dG,$$

$$i = 1, 2, \ldots, n; \quad k = 1, 2, \ldots, m.$$

Now a_{ik}, b_k are the known constants. Combining (1.7) and (2.8) we arrive at the problem

$$\sum_{i=1}^{n} \xi_i (\overline{Q}_i - Q_i) = \min,$$
$$\sum_{i=1}^{n} Q_i a_{ik} + b_k \leqq c_k, \quad k = 1, 2, \ldots, m. \tag{2.9}$$

From Q_i we can conveniently change over to $q_i = \overline{Q}_i - Q_i \geqq 0$. Then we arrive at a linear programming problem in finding an optimum set q_i on the strength of the solution of the problem

$$\sum_{i=1}^{n} \xi_i q_i = \min,$$
$$\sum_{i=1}^{n} a_{ik} q_i \geqq R_k, \quad k = 1, 2, \ldots, m, \tag{2.10}$$
$$q_i \geqq 0, \quad i = 1, 2, \ldots, n,$$

where $R_k = \sum_{i=1}^{n} a_{ik}\overline{Q}_i + b_k - c_k$.

It is natural that the number of limitations can be increased at the expense of social and economic requirements resulting from one or another priority considerations.

6.3. Optimization by an Adjoint Problem

An adjoint problem is generated by the Lagrange's identity. In fact, we shall consider the operator

$$L = \frac{\partial}{\partial t} + \operatorname{div}\,(\underline{u}\,\cdot) - \frac{\partial}{\partial z}\,\nu\,\frac{\partial}{\partial z} - \mu\Lambda + \sigma \tag{3.1}$$

on a set of functions $\phi \in \Phi$ continuous together with their first order (with respect to t) and second order (with respect to x, y) derivatives. As to the derivative with respect to z, the flux $\nu\partial\phi/\partial z$ is assumed to be continuous. Further, we suppose that every element of this set satisfies the conditions

$$\begin{aligned} &\phi = 0 && \text{on } \Sigma, \\ &\frac{\partial\phi}{\partial z} = \alpha\phi && \text{on } \Sigma_o, \\ &\frac{\partial\phi}{\partial z} = 0 && \text{on } \Sigma_H, \\ &\phi(\underline{r},\,T) = \phi(\underline{r},\,0). \end{aligned} \tag{3.2}$$

Let us introduce a scalar product

$$(g,\,h) = \int_0^T dt \int_G gh\,dG. \tag{3.3}$$

In the earlier accepted notations, the basic problem (2.2)-(2.4) can now be represented in the operator form

$$L\phi_i = \delta(\underline{r} - \underline{r}_o). \tag{3.4}$$

Let us now consider an adjoint operator L* with the use of the Lagrange's identity

$$(\phi^*,\,L\phi) = (\phi,\,L^*\phi^*), \tag{3.5}$$

Here, ϕ and ϕ^* are assumed to be real. Using a standard technique, we arrive at the definition of the adjoint operator:

$$L^* = -\frac{\partial}{\partial t} - \operatorname{div}\,(\underline{u}\,\cdot) - \frac{\partial}{\partial z}\,\nu\,\frac{\partial}{\partial z} - \mu\Delta + \sigma. \tag{3.6}$$

Every element $\phi^* \in \Phi$, on which operator L* acts, should be a continuous function having first derivative with respect to t, second, with respect to x, y, and a continuous adjoint flux $\nu\partial\phi^*/\partial z$. Besides, ϕ^* should satisfy the following conditions:

$$\begin{aligned} &\phi^* = 0 && \text{on } \Sigma, \\ &\frac{\partial\phi^*}{\partial z} = \alpha\phi^* && \text{on } \Sigma_o, \\ &\frac{\partial\phi^*}{\partial z} = 0 && \text{on } \Sigma_H, \end{aligned} \tag{3.7}$$

$$\phi^*(\underline{r}, T) = \phi^*(\underline{r}, 0).$$

Let us consider an adjoint problem with respect to (3.4)

$$L^*\phi_k^* = p_k \tag{3.8}$$

where p_k is still an undefined function. Multiplying (in scalar product terms) (3.4) by ϕ_k^*, (3.8) by ϕ_i, and subtracting one result from the other, we obtain

$$(\phi_k^*, L\phi_i) - (\phi_i, L^*\phi_k^*) = Q_i \int_0^T \phi_k^*(\underline{r}_i, t)dt - (\phi_i, p_k). \tag{3.9}$$

Since $\phi_i \in \Phi$, $\phi_k^* \in \Phi$, subject to (3.5) the left-hand side of (3.9) vanishes. Then

$$Y_{ik} = (\phi_i, p_k) = Q_i \int_0^T \phi_k^*(\underline{r}_i, t)\ dt; \tag{3.10}$$

As p_k we take

$$p_k(\underline{r}) = \begin{cases} b + a\delta\ (z) & \text{on } G_k, \\ 0 & \text{outside } G_k. \end{cases}$$

As a result, for the functional Y_{ik} we have two equivalent forms generated by equality (3.10) and elementary problems with a unit source Q_i:

$$Y_{ik} = \int_0^T dt \int_\Omega p_k\phi_i\ d\Sigma, \qquad Y_{ik} = Q_i \int_0^T \phi_k^*(\underline{r}_i, t)\ dt. \tag{3.11}$$

Thus, Y_{ik} can be found by solving either a basic or an adjoint problem. Since optimization with basic equations has been considered earlier, we shall focus our attention on the adjoint problem (3.8). Let us write it as

$$-\frac{\partial\phi_k^*}{\partial t} - \operatorname{div} \underline{u}\phi_k^* + \sigma\phi_k^* = \frac{\partial}{\partial z}\nu\frac{\partial\phi_k^*}{\partial z} + \mu\Delta\phi_k^* + p_k(\underline{r}), \tag{3.12}$$

$$\phi_k^* = 0 \qquad \text{on } \Sigma,$$

$$\left.\begin{aligned} \frac{\partial\phi_k^*}{\partial z} &= \alpha\phi_k^* &&\text{on } \Sigma_0, \\ \frac{\partial\phi_k^*}{\partial z} &= 0 &&\text{on } \Sigma_H, \end{aligned}\right. \tag{3.13}$$

$$\phi_k^*(\underline{r}, T) = \phi^*(\underline{r}, 0). \tag{3.14}$$

If the problem (3.12)-(3.14) is solved, then we find the functional Y_{ik} by simple integration. Further steps needed to formulate an optimization problem are now evident. Let us introduce a functional

$$Y_k = \sum_{i=1}^{n} Q_i \int_0^T dt\ \phi_k^*(\underline{r}_i) + \int_0^T dt \int_{G_k} \phi_S\ dG \qquad (3.15)$$

and denote

$$a_{ik}^* = \int_0^T \phi_k^*\ (\underline{r}_i)\ dt, \quad b_k^* = \int_0^T dt \int_{G_k} \phi_S\ dG. \qquad (3.16)$$

Then (3.15) is written as

$$Y_k = \sum_{i=1}^{n} a_{ik}^* Q_i + b_k^*. \qquad (3.17)$$

Thus, similar to the case of a basic problem, we arrive at an optimization problem for the adjoint equations:

$$\sum_{i=1}^{n} \xi_i (\bar{Q}_i - Q_i) = \min,$$
$$\sum_{i=1}^{n} a_{ik}^* Q_i + b_k^* \leqq c_k, \quad k = 1, 2, \dots, m. \qquad (3.18)$$

or, introducing $q_i = \bar{Q}_i - Q_i \geqq 0$ we transform (3.18) into the following:

$$\sum_{i=1}^{n} \xi_i q_i = \min, \qquad (3.19)$$

$$\sum_{i=1}^{n} a_{ik}^* q_i \geqq R_k^*, \quad k = 1, 2, \dots, m,$$
$$q_i \geqq 0, \quad i = 1, 2, \dots, n,$$

where $R_k^* = \sum_{i=1}^{n} a_{ik}\bar{Q} + b_k^* - c_k$. Thus, we have again arrived at a linear programming problem.

In different cases it is convenient to formulate an optimization problem by solving either basic equations or adjoint problems. If the number of industrial plants emitting aerosol is small and the number of ecologically important zones is large, then it is convenient to use basic equations. On the contrary, use is made of adjoint problems.

6.4. Perturbation Theory

The importance of an adjoint problem is by far not exhausted by the possibility of independently stating an optimization problem. In many cases, without solving the problem at large, one can obtain very valuable information about the sensitivity of functionals of Y_k type to the deviation of certain problem parameters from the "normal". Let us consider the simplest case of the perturbation theory by using variations of aerosol emissions. Suppose that an industrial plant discharges $Q_i' = Q_i + \delta Q_i$ aerosols instead of Q_i. Then

$$L\phi_i' = Q_i'\delta(\underline{r} - \underline{r}_i), \tag{4.1}$$

where $\phi_i' = \phi_i + \delta\phi_i$. Let us combine an adjoint problem

$$L^*\phi_k^* = p_k. \tag{4.2}$$

with this problem. Multiplying (4.1) (in scalar product terms) by ϕ_k^* and (4.2) by ϕ_i', and subtracting one result from the other, we obtain

$$(\phi_k^*, L\phi_i') - (\phi_i', L^*\phi_k^*) = Q_i' \int_0^T \phi_k^* dt - \int_0^T dt \int_{G_k} p_k \phi_i' \, dG. \tag{4.3}$$

The left-hand side of this equality vanishes in virtue of the Lagrange's relation. We have

$$(Q_i + \delta Q_i) \int_0^T \phi_k^* dt - \int_0^T dt \int_{G_k} p_k(\phi_i + \delta\phi_i) \, dG = 0. \tag{4.4}$$

Since

$$Q_i \int_0^T \phi_k^* \, dt = \int_0^T dt \int_{G_k} p_k \phi_i \, dG = Y_{ik} \tag{4.5}$$

and

$$\delta Y_{ik} = \int_0^T dt \int_{G_k} p_k \delta\phi_i \, dG,$$

using (4.4), we arrive at a formula of the perturbation theory

$$\delta Y_{ik} = \delta Q_i \int_0^T \phi_k^* \, dt, \quad i = 1, 2, \ldots, n; \quad k = 1, 2, \ldots, m. \tag{4.6}$$

This formula can be obtained also in a simple manner by using (3.15).

After computing $\int_0^T \phi_k^* \, dt$ and constructing isolines $\int_0^T \phi_k^* \, dt = \text{const}$, we can determine the regions where aerosol pollution will be maximum. The factories located in these regions make maximum contribution to aerosol pollution, and therefore the maximum permissible emissions for them should be computed in the first place. This, of course, does not solve the entire optimization problem though it somewhat clarifies its main points.

Finally, we shall consider another important question. Up to now we had assumed the input parameters of basic and adjoint problems to be constant. However, in solving optimization problems the concentration of aerosols over a region G varies and this causes certain changes in the local circulation of the atmosphere. This means that the components of vector $\underline{u}$: $\underline{u}' = \underline{u} + \delta\underline{u}$, the coefficients of exchange turbulence: $\nu' = \nu + \delta\nu$, $\mu' = \mu + \delta\mu$, as well as the parameters: $\alpha' = \alpha + \delta\alpha$, $\beta' = \beta + \delta\beta$ can vary. As a result of perturbations the basic problem takes the form

$$(L + \delta L)\, \phi_i' = (Q + \delta Q)\,\delta(\underline{r} - \underline{r}_i). \tag{4.7}$$

To this equation we add an unperturbed adjoint equation

$$L^* \phi_k^* = p_k. \tag{4.8}$$

Multiplying (4.7) (in scalar product terms) by ϕ_k^*, (4.8) by ϕ_i', subtracting one result from the other, and taking account of the Lagrange's identity, we obtain

$$(\phi_k^*, \delta L \phi_i') = \delta Q_i \int_0^T \phi_k^* \, dt - \delta Y_{ik}; \tag{4.9}$$

Hence,

$$\delta Y_{ik} = \delta Q_i \int_0^T \phi_k^* \, dt - (\phi_k^*, \delta L \phi_i'). \tag{4.10}$$

Assuming the perturbations $\delta\phi_i$ and δL to be small, we arrive at a formula of the theory of minor perturbations, accurate to small terms of second order,

$$\delta Y_{ik} = \delta Q_i \int_0^T \phi_k^* \, dt - (\phi_k^*, \delta L \phi_i). \tag{4.11}$$

Having inserted scalar product in this formula, we get the possibility of estimating the "feedback" of atmospheric processes, which is generated by a change in the aerosol background in G.

The optimization problem considered in this chapter can be extended to other functionals as it was done in chapter 4.

In conclusion we shall say a few words about numerical realization of algorithms. Since a basic and an adjoint problems are linear and periodic in time, they can be solved by the periodicity method (starting from some initial data and continuing until a periodicity occurs). Usually, two- or three-year cycles of calculations are sufficient for this. It is important to note that an adjoint problem should be solved in the opposite direction to time, because, as we have already mentioned, in this case the correctness of the problem will be observed in counting. As to linear programming problems, they are solved by standard procedures. Since $q_i \geqq 0$ and all the coefficients a_{ik}, a^*_{ik} are also positive, the solution to the problem is found on the faces of polyhedrons, which are formed in constructing limitations areas.

Chapter 7. ACTIVE AEROSOL EMISSIONS

The problem of optimum location of industrial plants in the ecologic activity zones has been considered in chapter 6 with regard to their minimum pollution level. In doing so, the aerosol was assumed to be passive, that is, aerosol does not change during its transfer and diffusion into other, may be, more toxic forms. In the same manner, we considered the optimization problem for aerosol emission levels of operating plant, which ensure minimum pollution within the given industrial efficiency limits.

In the present chapter we shall examine a more general statement of the problem: industrial emissions consist of several components of aerosols and part of them forms a chain of consecutively changing chemicals of different toxicity under the impact of atmospheric water vapors, oxygen, nitrogen and other compounds.

7.1. Basic and Adjoint Equations

Suppose that an industrial plant emitting various kinds of aerosol components at a height $z = h$ is located at a point $A(x, y)$ in region G. Call them a_1, a_2, ... They scatter over the given region partially settling on Earth's surface and polluting the environment. During transfer and diffusion, part of such aerosol compounds changes into other forms under the action of chemical reactions that take place in the atmosphere. Thus, the chain of transformations can be represented as: $a_1 \to a_{11} \to a_{12} \to \dots$ and respectively $a_2 \to a_{21} \to a_{22} \to \dots$ Of course, the number of aerosol components and the transformation chain can be large enough, but this does not change the essence of the problem in principle. The task resides in finding an optimum location of the industrial plant in G, taking into account the minimum pollution of all of the ecologically important zones and the given maximum permissible level of pollution.

For the sake of convenience, we consider formalized operator notations. With this in view we shall examine a problem on transfer and diffusion of some aerosol substance ϕ_j $(j = \overline{1, n})$:

$$\frac{\partial \phi_j}{\partial t} + u \frac{\partial \phi_j}{\partial x} + v \frac{\partial \phi_j}{\partial y} + w \frac{\partial \phi_j}{\partial z} + \partial_j \phi_j - \frac{\partial}{\partial z} \nu \frac{\partial \phi_j}{\partial z} - \mu \Delta \phi_j = f_j \quad (1.1)$$

$$u_j = 0 \quad \text{on} \quad \textstyle\sum,$$

$$\frac{\partial \phi_j}{\partial z} = \alpha_j \phi_j \quad \text{on} \quad \textstyle\sum_o, \qquad (1.2)$$

$$\frac{\partial \phi_j}{\partial z} = 0 \quad \text{on} \quad \textstyle\sum_H; \qquad (1.3)$$

$$\phi_j\ (\underline{r}, T) = \phi_j\ (\underline{r}, 0). \qquad (1.4)$$

Let us now introduce a linear operator

$$A = \frac{\partial}{\partial t} + \text{div}\ (\underline{u}\cdot) - \frac{\partial}{\partial z} \nu \frac{\partial}{\partial z} - \mu\Delta \qquad (1.5)$$

and a space of functions Φ, whose elements satisfy certain smoothness conditions, as well as the boundary conditions (1.2) and the initial data (1.3). Problem (1.1)-(1.3) can now be formally represented as

$$A\phi_{jo} + \sigma_{jo}\phi_{jo} = f_j. \qquad (1.6)$$

As mentioned earlier, ϕ_j is not a passive substance. On the contrary, after going into the atmosphere it undergoes the following changes: $\phi_j = \phi_{jo} \rightarrow \phi_{j1} \rightarrow \rightarrow \phi_{j2} \rightarrow \ldots$ This implies that m new equations should be added to (1.6):

$$\begin{aligned}
A\phi_{j1} + \sigma_{j1}\phi_{j1} - \sigma_{jo}\phi_{jo} &= 0,\\
A\phi_{j2} + \sigma_{j2}\phi_{j2} - \sigma_{j1}\phi_{j1} &= 0,\\
\cdots\cdots\cdots\cdots\cdots\cdots & \qquad (1.7)\\
A\phi_{j,m-1} + \sigma_{j,m-1}\phi_{j,m-1} - \sigma_{j,m-2}\phi_{j,m-2} &= 0,\\
A\phi_{jm} - \sigma_{j,m-1}\phi_{j,m-1} &= 0.
\end{aligned}$$

For simplicity, here and further we have dropped index j at m. A term of the form $\sigma\phi$ is absent in the last equation, because the chain of transformations of substance ϕ is assumed to be finite, and, therefore, ϕ_{jm} is an undercomposed mixture.

To solve (1.6), (1.7) it is necessary that the smoothness conditions and relationships, similar to (1.2), (1.3), should be fulfilled:

$$\begin{aligned} \phi_{j\ell} &= 0 \quad \text{on } \Sigma, \\ \frac{\partial \phi_{j\ell}}{\partial z} &= \alpha_{j\ell}\phi_{j\ell} \quad \text{on } \Sigma_o, \\ \frac{\partial \phi_{j\ell}}{\partial z} &= 0 \quad \text{on } \Sigma_H, \\ \phi_{j\ell}(\underline{r}, T) &= \phi_{j\ell}(\underline{r}, 0), \ \ell = \overline{0, m}. \end{aligned} \tag{1.8}$$

Let us consider a space of vectors

$$\underline{\phi}_j = \begin{bmatrix} \phi_{jo} \\ \phi_{j1} \\ \vdots \\ \phi_{jm} \end{bmatrix}, \quad \underline{f}_j = \begin{bmatrix} f_j \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

and the matrix

$$L_j = \begin{bmatrix} A + \sigma_{jo} & & 0 \\ -\sigma_{jo} & \ddots & A + \sigma_{j,m-1} \\ 0 & \ddots & -\sigma_{j,m-1} \quad A \end{bmatrix}.$$

For the migration and transformation of $\underline{\phi}_j$ aerosols into new components, problem (1.6), (1.7) can now be represented in the vector-matrix form:

$$L_j \underline{\phi}_j = \underline{f}_j \tag{1.9}$$

Let us now introduce a Hilbert space of vector-function with a scalar product

$$(\underline{g}, \underline{h}) = \sum_{\ell=0}^{m} \int_0^T dt \int_G g_\ell h_\ell \, dG$$

and consider an adjoint problem

$$L_j^* \underline{\phi}_j^* = \underline{p}_j, \tag{1.10}$$

$$\underline{\phi}_j^* = \begin{vmatrix} \phi_{jo}^* \\ \phi_{j1}^* \\ \vdots \\ \phi_{jm} \end{vmatrix}, \quad \underline{p}_j = \begin{vmatrix} p_{jo} \\ p_{j1} \\ \vdots \\ p_{jm} \end{vmatrix}, \tag{1.11}$$

where $\underline{p}_j$ is still an undefined vector-function. We find operator L_j^* by the Lagrange's identity

$$(\underline{\phi}_j^*, L_j\underline{\phi}_j) = (\underline{\phi}_j, L_j^*\underline{\phi}_j^*). \tag{1.12}$$

Using the definition of scalar product and integrating the left-hand relationship by parts, we arrive at L_j^*:

$$L_j^* = \begin{vmatrix} A^* + \sigma_{jo} & -\sigma_{jo} & & 0 \\ & A^* + \sigma_{j1} & \ddots & \\ & & \ddots & \\ & & A^*+\sigma_{j,m-1} & -\sigma_{j,m-1} \\ 0 & & & A^* \end{vmatrix},$$

where operator A* appears as

$$A^* = -\frac{\partial}{\partial t} - \mathrm{div}\,(\underline{u}\cdot) - \frac{\partial}{\partial z}\nu\frac{\partial}{\partial z} - \mu\Delta.$$

The space of adjoint functions Φ^* contains elements of necessary smoothness which satisfy the following conditions for their components:

$$\begin{aligned} \phi^*_{j\ell} &= 0 \qquad \text{on } \textstyle\sum, \\ \frac{\partial\phi^*_{j\ell}}{\partial z} &= \alpha_{j\ell}\phi^*_{j\ell} \qquad \text{on } \textstyle\sum_o, \\ \frac{\partial\phi^*_{j\ell}}{\partial z} &= 0 \qquad \text{on } \textstyle\sum_H, \\ \phi^*_{j\ell}(\underline{r},T) &= \phi^*_{j\ell}(\underline{r},0), \quad \ell = \overline{0,m}. \end{aligned} \tag{1.13}$$

Further, we write (1.10) in the componentwise form

$$\begin{aligned} A^*\phi^*_{jo} + \sigma_{jo}\phi^*_{jo} - \sigma_{jo}\phi^*_{j1} &= p_{jo}, \\ A^*\phi^*_{j1} + \sigma_{j1}\phi^*_{j1} - \sigma_{j1}\phi^*_{j2} &= p_{j1}, \\ \cdots\cdots\cdots\cdots\cdots \\ A^*\phi^*_{jm} &= p_{jm}. \end{aligned} \tag{1.14}$$

Now we go over the determination of vector-function $\underline{p}_j$. To this end, we first assume that the aerosol source with the j-th component f_j is a delta function of the coordinates, i.e.

$$f_j = Q_j\,\delta(\underline{r} - \underline{r}_o) \tag{1.15}$$

where Q_j is the rate at which aerosols are emitted into air. Multiplying (1.9) in scalar product terms by $\underline{\phi}^*_j$, (1.10) by $\underline{\phi}_j$, and subtracting one result from the other, gives

$$(\underline{\phi}^*_j, L_j\underline{\phi}_j) - (\underline{\phi}_j, L^*_j\underline{\phi}^*_j) = (\underline{\phi}_j,\underline{f}_j) - (\underline{p}_j,\underline{\phi}_j). \tag{1.16}$$

By the Lagrange's identity the left-hand side vanishes and we get

$$(\underline{\phi}_j^*,\ \underline{f}_j) = (\underline{p}_j,\ \underline{\phi}_j) \tag{1.17}$$

Now we choose $\underline{p}_j$ in the following fashion. Suppose that safe pollution with aerosol component $\phi_{j\ell}$ settled on area G_k over a year is equal to

$$\xi_{j\ell} \int_0^T dt \int_{G_k} \phi_{j\ell}\, dG,$$

where $\xi_{j\ell}$ is a coefficient which characterizes toxicity of this component. Total toxicity of all the components marked with j will then equal

$$Y_j = \sum_{\ell=0}^{m} \xi_{j\ell} \int_0^T dt \int_{G_k} \phi_{j\ell}\, dG. \tag{1.18}$$

Let us take this functional as initial functional and demand $(\underline{p}_j,\ \underline{\phi}_j)$ to agree with Y_j. For this it suffices to assume that

$$p_{j\ell} = \begin{cases} \xi_{i\ell}, & \text{if } \underline{r} \in G_k, \\ 0 & \text{outside } G_k. \end{cases}$$

For the chosen value of $\underline{p}_j$ the right-hand side in (1.17) will equal to Y_j and the left-hand side will, therefore, be equal to

$$Y_j = (\underline{\phi}_j^*,\ \underline{f}_j) = \int_0 dt \int_G Q_j \phi_{jo}^*\ \delta(\underline{r} - \underline{r}_o) dG,$$

or, more simply,

$$Y_j = Q_j \int_0^T \phi_{jo}^*(\underline{r}_o,\ t)\ dt. \tag{1.19}$$

Thus, to determine the extent to which region G_k is polluted with all components of the chain $\phi_{jo} \to \phi_{j1} \to \phi_{j2} \to \dots$, it is necessary to solve the adjoint problem (1.4) in the reverse order:

$$\begin{aligned} &A^*\phi_{jm}^* = p_{jm}, \\ &A^*\phi_{j,m-1}^* + \sigma_{j,m-1}\phi_{j,m-1}^* - \sigma_j\phi_{jm}^* = p_{j,m-1}, \\ &\dots\dots\dots\dots\dots\dots\dots\dots \\ &A^*\phi_{jo}^* + \sigma_{jo}\phi_{jo}^* - \sigma_{jo}\phi_{j1}^* = p_{jo}, \end{aligned} \tag{1.20}$$

For this we use boundary conditions and initial data in the form (1.13) during count down.

Now we go over to complete determination of pollution due to all aerosol components $j = \overline{1, m}$. In this case the functionals (1.18) and (1.19) will change to the following:

$$Y^k = \sum_j \sum_\ell \xi_{j\ell} \int_0^T dt \int_{G_k} \phi_{j\ell}\, dG, \tag{1.21}$$

$$Y^k = Q \sum_j \eta_j \int_0^T \phi^*_{jo}(\underline{r}_o, t)\, dt. \tag{1.22}$$

Here, Q denotes the emission rate of all aerosols and η_j represents a fraction of every component $(j = \overline{1, n})$.

7.2. Influence Function

Formula (1.22) has particular significance in choosing the construction site for a new plant with the given structure of aerosols and the total emission rate Q. As a matter of fact, we can *a priori* compute the function $\Psi^*_k(\underline{r})$

$$\Psi^*_k(\underline{r}) = \sum_j \eta_j \int_0^T \phi^*_{jo}(\underline{r}, t)\, dt. \tag{2.1}$$

after solving an adjoint problem in relation to the pollution of region G_k. Note that the right-hand side of (2.1) depends on G_k because the values of $p_{j\ell}$ were taken to be different from zero for this ecologically important region. Using the notations of (1.21), we write the functional representing total dose of pollution in the region G_k as

$$Y^k = Q\, \Psi^*_k\, (\underline{r}_o) \tag{2.2}$$

We call Ψ^*_k the *influence function* of an industrial plant emitting aerosol at a point $\underline{r}_o \in G$, that is the function affecting the average yearly safe dose for the region G_k.

If we have several protection zones, say G_k, the adjoint problem will then have to be solved for as many times; every time a new function Ψ^*_k $(k = 1, 2, \ldots)$ is obtained. Thereafter, the problem of choosing the best site for an industrial plant is solved by clear exhaustion of functions Ψ^*_k for every point of G. In consequence, we can find a point where the minimax condition is fulfilled

$$\max_k \Psi^*_k(\underline{r}) = \min_{\underline{r} \in G} \tag{2.3}$$

7.3. Two-dimensional Approximation

We shall now consider in detail the problem formulated in section 7.1.; the domain of the function ϕ is assumed to be two-dimensional. For definiteness assume that the chain of aerosol ϕ transformations consists of three links. Thus, we arrive at the following problem:

$$\frac{\partial\phi_1}{\partial t} + u\frac{\partial\phi_1}{\partial x} + v\frac{\partial\phi_1}{\partial y} + \sigma_1\phi_1 - \mu\Delta\phi_1 = f,$$

$$\frac{\partial\phi_2}{\partial t} + u\frac{\partial\phi_2}{\partial x} + v\frac{\partial\phi_2}{\partial y} + \sigma_2\phi_2 - \sigma_1\phi_1 - \mu\Delta\phi_2 = 0, \tag{3.1}$$

$$\frac{\partial\phi_3}{\partial t} + u\frac{\partial\phi_3}{\partial x} + v\frac{\partial\phi_3}{\partial y} - \sigma_2\phi_2 - \mu\Delta\phi_3 = 0;$$

$$\phi_j = 0 \qquad \text{on } \textstyle\sum; \tag{3.2}$$

$$\phi_j(\underline{r}, T) = \phi_j(\underline{r}, 0). \tag{3.3}$$

The set of Eqs.(3.1) describes a very particular case of scattering a mixture that does not interfere with atmospheric components. Summing up the set of equations and calling $\phi = \phi_1 + \phi_2 + \phi_3$ we in fact arrive at the following equation

$$\frac{\partial\phi}{\partial t} + u\frac{\partial\phi}{\partial x} + v\frac{\partial\phi}{\partial y} - \mu\Delta\phi = f, \tag{3.4}$$

which corresponds to the case of a passive substance. Suppose that the initial substance reacts during its transformation with the ambient air and the change in mass per unit of time for every subsequent component of the chain is proportional to the amount of substance that has changed into the new state. In addition, we shall assume the substance ϕ_3 to be decomposable. This implies that the first three substances (more important in one or other respect), say the substances may prove hazardous for humane health, are chosen from the chain of transformations $\phi_1 \to \phi_2 \to \ldots \to \phi_n$. The set of Eqs.(3.1) is then written as

$$\frac{\partial\phi_1}{\partial t} + u\frac{\partial\phi_1}{\partial x} + v\frac{\partial\phi_1}{\partial y} + \sigma_1\phi_1 - \mu\Delta\phi_1 = f,$$

$$\frac{\partial\phi_2}{\partial t} + u\frac{\partial\phi_2}{\partial x} + v\frac{\partial\phi_2}{\partial y} + \sigma_2\phi_2 - \bar{\sigma}_1\phi_1 - \mu\Delta\phi_2 = 0, \tag{3.5}$$

$$\frac{\partial\phi_3}{\partial t} + u\frac{\partial\phi_3}{\partial x} + v\frac{\partial\phi_3}{\partial y} + \sigma_3\phi_3 - \bar{\sigma}_2\phi_2 - \mu\Delta\phi_3 = 0,$$

where $\bar{\sigma}_i = \sigma_i + S_i$ and S_i is the quantitative characteristic of variation in the substance mass as a result of its interaction with atmospheric components.

For determining a functional of the type (1.21) from the solution of the problem (3.5), (3.2), (3.3) we shall use mathematical methods described in chapter 1, and formulate a statistical model for the processes in question. For this, we shall assume the adaptation time τ for the types of circulations to be much less than the characteristics time Δt for a circulation of the given type. Then for every interval Δt we obtain a set of stationary equations

$$u \frac{\partial \phi_1}{\partial x} + v \frac{\partial \phi_1}{\partial y} + \sigma_1 \phi_1 - \mu \Delta \phi_1 = Q\delta(\underline{r} - \underline{r}_o),$$

$$u \frac{\partial \phi_2}{\partial x} + v \frac{\partial \phi_2}{\partial y} + \sigma_2 \phi_2 - \mu \Delta \phi_2 = \bar{\sigma}_1 \phi_1, \tag{3.6}$$

$$u \frac{\partial \phi_3}{\partial x} + v \frac{\partial \phi_3}{\partial y} + \sigma_3 \phi_3 - \mu \Delta \phi_3 = \bar{\sigma}_2 \phi_2.$$

Let us introduce a notation

$$L = u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} - \mu \Delta \tag{3.7}$$

and write (3.6) in the formalized form

$$L\phi_1 + \sigma_1 \phi_1 = f,$$

$$L\phi_2 + \sigma_2 \phi_2 = \bar{\sigma}_1 \phi_1 \tag{3.8}$$

$$L\phi_3 + \sigma_3 \phi_3 = \bar{\sigma}_2 \phi_2$$

where $f = Q\delta(\underline{r} - \underline{r}_o)$.

When no σ_i are equal among themselves, (3.8) can be reduced to a sequence of equations formally not linked with each other. In fact, multiplying the first two equations by indeterminate factors α and β and summing up these equations yields

$$L\,(\alpha\phi_1 + \beta\phi_2) + (\sigma_1\alpha - \bar{\sigma}_1\beta)\phi_1 + \sigma_2\beta\phi_2 = \alpha f. \tag{3.9}$$

We now pick arbitrary factors α and β such that the equality is fulfilled

$$\sigma_2(\alpha\phi_1 + \beta\phi_2) = (\sigma_1\alpha - \bar{\sigma}_1\beta)\phi_1 + \sigma_2\beta\phi_2. \tag{3.10}$$

This requirement is satisfied, for example, by

$$\alpha = \bar{\sigma}_1, \quad \beta = \sigma_1 - \sigma_2. \tag{3.11}$$

Then (3.9) takes the form

$$L(\alpha\phi_1 + \beta\phi_2) + \sigma_2(\alpha\phi_1 + \beta\phi_2) = \alpha f. \tag{3.12}$$

Multiplying the set of equations by arbitrary factors α, β, and γ gives

$$L(\alpha\phi_1 + \beta\phi_2 + \gamma\phi_3) + \sigma_3(\alpha\phi_1 + \beta\phi_2 + \gamma\phi_3) = \alpha f, \tag{3.13}$$

where $\alpha = \bar{\sigma}_1$, $\beta = \sigma_1 - \sigma_3$, $\gamma = (\sigma_1 - \sigma_3)(\sigma_2 - \sigma_3)/\bar{\sigma}_2$ or $\alpha = \bar{\sigma}_1\bar{\sigma}_2/(\sigma_1 - \sigma_3)$, $\beta = \bar{\sigma}_2$, $\gamma = \sigma_2 - \sigma_3$.

We introduce the following notations:

$$\begin{gathered}
\Phi_1 = \phi_1, \quad \Phi_2 = \bar{\sigma}_1\phi_1 + (\sigma_1 - \sigma_2)\phi_2, \\
\Phi_3 = \bar{\sigma}_1\phi_1 + (\sigma_1 - \sigma_3)\phi_2 + \frac{(\sigma_1 - \sigma_3)(\sigma_2 - \sigma_3)}{\bar{\sigma}_2}\phi_3, \\
F_1 = Q\delta(\underline{r} - \underline{r}_o), \quad F_2 = \bar{\sigma}_1 Q\delta(\underline{r} - \underline{r}_o), \\
F_3 = \sigma_1 Q\delta(\underline{r} - \underline{r}_o).
\end{gathered} \tag{3.14}$$

The set of Eqs.(3.6) now takes the form

$$\begin{aligned}
L\Phi_1 + \sigma_1\Phi_1 &= F_1, \\
L\Phi_2 + \sigma_2\Phi_2 &= F_2, \\
L\Phi_3 + \sigma_3\Phi_3 &= F_3.
\end{aligned} \tag{3.15}$$

All the equations have a similar structure and can be solved in succession by one and the same method. Having determined Φ_1, Φ_2, and Φ_3, functions ϕ_1, ϕ_2, ϕ_3 are found by formulae (3.14).

Let us now consider a very important case when wind of constant direction predominates in every type of circulation, that is u = const, v = const. We shall find solution to every equation of the system(3.15)

$$u\frac{\partial\Phi}{\partial x} + v\frac{\partial\Phi}{\partial y} + \sigma\Phi - \mu\Delta\Phi = Q\delta(\underline{r} - \underline{r}_o) \tag{3.16}$$

in the following form

$$\Phi = \phi \exp\{(\underline{u}, \underline{r} - \underline{r}_o)/(2\mu)\}, \tag{3.17}$$

where $(\underline{u}, \underline{r}) = ux + vy$. Substituting (3.17) into (3.16) we get an equation in ϕ:

$$-\mu\Delta\phi + \beta\phi = Q\delta(\underline{r} - \underline{r}_o), \tag{3.18}$$

where $\beta = \sigma + (u^2 + v^2)/(4\mu)$. The solution to Eq.(3.18) in plane (x, y) is obtained by

$$\phi = \frac{Q}{2\pi\mu} K_o\left(\sqrt{\frac{\beta}{\mu}}\,|\underline{r} - \underline{r}_o|\right), \tag{3.19}$$

where K_o is the McDonald function of the form

$$K_o(x) = \int_0^\infty e^{-x\,\mathrm{ch}\,y}\,dy, \quad x > 0. \tag{3.20}$$

With consideration for (3.19) we obtain the solution to (3.16):

$$\Phi = \frac{Q}{2\pi\mu}\exp\{(\underline{u}, \underline{r} - \underline{r}_o)/(2\mu)\}\, K_o\left(\sqrt{\frac{\beta}{\mu}}\,|\underline{r} - \underline{r}_o|\right) \tag{3.21}$$

Let us now estimate the characteristic dimensions of the region G, for which (3.21) gives an approximate solution to a boundary problem. With this in mind we shall introduce for every function Φ_i a value ε_i and assume that condition of the type (3.2) is fulfilled, provided

$$\Phi_i \leqq \varepsilon_i \tag{3.22}$$

The selection of ε_i is dictated by the instrumental errors of measuring the level of aerosol concentration, its background concentration, and also by that minimum level for which the effect of a given type of mixture can be neglected.

Taking *a priori* the values $|\underline{r} - \underline{r}_o|$ such that the asymptotic formula holds

$$K_o(x) \sim \sqrt{\frac{\pi}{2x}}\, e^{-x},$$

and using the inequality $(\underline{u}, \underline{r} - \underline{r}_o) \leq |\underline{u}|\,|\underline{r} - \underline{r}_o|$, we find that

$$\Phi \leq \frac{Q}{2\pi\mu}\exp\left(\frac{|\underline{u}|\,|\underline{r}-\underline{r}_o|}{2\mu}\right) - \exp\left(-\frac{|\underline{u}|\,|\underline{r}-\underline{r}_o|}{2\mu}\right)\sqrt{\frac{2\pi\mu}{|\underline{r}-\underline{r}_o|\,(4\sigma\mu+u^2+v^2)}}, \tag{3.23}$$

Hence, we arrive at the following relation

$$|\underline{r} - \underline{r}_o| \sim \max_i \left(\frac{Q^2}{\varepsilon_i^2}\,\frac{1}{2\pi\mu(4\mu\sigma_i+u^2+v^2)}\right), \tag{3.24}$$

Fulfilment of this relation for the chosen domain of definition G guarantees a solution to the problem (3.6), (3.2) with a given degree of accuracy.

Formulae (3.21) and (3.14) yield a solution to the problem (3.1)-(3.3) from the statistical model of (3.6), (3.2):

$$\phi_1 = \frac{Q}{2\pi\mu}\exp\left(\frac{\underline{u},\ \underline{r} - \underline{r}_o}{2\mu}\right) K_o\left(\sqrt{\frac{\beta_1}{\mu}}\,|\underline{r} - \underline{r}_o|\right),$$

$$\phi_2 = \frac{\bar{\sigma}_1 Q\,\exp\{(\underline{u},\underline{r} - \underline{r}_o)/(2\mu)\}}{2\pi\mu\,(\sigma_1-\sigma_2)}\left\{K_o\left(\sqrt{\frac{\beta_1}{\mu}}\,|\underline{r} - \underline{r}_o|\right) - K_o\left(\sqrt{\frac{\beta_2}{\mu}}\,|\underline{r} - \underline{r}_o|\right)\right\}, \tag{3.25}$$

$$\phi_3 = \frac{\sigma_1\sigma_2 Q \exp\{(\underline{u},\underline{r}-\underline{r}_o)/(2\mu)\}}{(\sigma_1-\sigma_3)(\sigma_2-\sigma_3)\ 2\pi\mu} \left[K_o\left(\sqrt{\frac{\beta_3}{\mu}}\,|\underline{r}-\underline{r}_o|\right) - \right.$$

$$\left. - \left(1 + \frac{\sigma_1-\sigma_3}{\sigma_1-\sigma_2}\right) K\left(\sqrt{\frac{\beta_1}{\mu}}\,|\underline{r}-\underline{r}_o|\right) + \frac{\sigma_1-\sigma_3}{\sigma_1-\sigma_2}\, K_o\left(\sqrt{\frac{\beta_2}{\mu}}\,|\underline{r}-\underline{r}_o|\right)\right],$$

where $\beta_i = \sigma_i + (u^2 + v^2)/(4\mu)$ $(i = 1, 2, 3)$.

When n - the number of considered time intervals with different types of circulations - is more than or equal to two, the solution to the problem is found by formula of chapter 1:

$$\overline{\phi}_i = \frac{1}{T}\sum_{k=1}^{n} \phi_i^k\,\Delta t_k, \quad i = 1, 2, 3. \tag{3.26}$$

Here k is the circulation type number.

In conclusion, it may be noted that the solution of every equation of (3.15), when $u = u(x, y)$, $v = v(x, y)$, is found numerically by the methods described in the previous chapters.

Chapter 8. MODELLING THE LOCATION OF POLLUTION SOURCES IN WATER BODIES AND COASTAL SEAS

The rapid development of industry calls for the determination of optimum conditions of locating new industrial plants and for technological restrictions on run-offs that pollute water bodies (seas, lakes, bays, etc.) so that the pollution of water areas, including the chosen coastal areas, will be minimum. Mathematically this is reduced to a minimax problem.

In this chapter, we have examined different ways of solving the problem of determining the location of a hydrosol pollution source. For this, the information on flow velocity field and turbulent diffusion coefficients is assumed to be known. Meteorological and practical aspects of using this information will be considered in the following chapters.

8.1. Basic Equations

Consider a limited region $\overline{G}$ in some water body. For simplicity, we shall assume this region to be cylindrical with a lateral surface $\overline{\Sigma}$, bases Σ_o, Σ_H, and constant depth H. We shall suppose that the lateral surface $\overline{\Sigma}$ is a combination of the solid (coastal contour) $\overline{\Sigma}_1$ and liquid $\overline{\Sigma}_2$ boundaries:

$$\overline{\Sigma} = \overline{\Sigma}_1 \cup \overline{\Sigma}_2 \tag{1.1}$$

Let us take the hydrosol diffusion equation in the form

$$\frac{\partial\phi}{\partial t} + u\frac{\partial\phi}{\partial x} + v\frac{\partial\phi}{\partial y} + w\frac{\partial\phi}{\partial z} + \sigma\phi - \frac{\partial}{\partial z}\nu\frac{\partial\phi}{\partial z} - \mu\Delta\phi = f, \tag{1.2}$$

where ϕ denotes the concentration of the polluting hydrosol, $f = Q\delta(\underline{r} - \underline{r}_o)$, $\underline{r}_o = (x_o, y_o, z_o)$ are the coordinates of the conjectural run-off; u, v, w are the components of the flow velocity vector $\underline{u}$ which satisfies the continuity equation

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0. \tag{1.3}$$

As to the flow velocity vector, we shall assume in addition that

$$u_n = 0 \quad \text{when} \quad \underline{r} \in \bar{\sum}_1 \cup \sum_o \cup \sum_H, \tag{1.4}$$

where u_n is the projection of vector u on the outer normal to the surface $\bar{\sum} \cup \sum_o \cup \sum_H$.

The boundary and initial conditions, which have different physical meanings and lead to correct statement of the problem, have been discussed in the previous chapters. Here we shall consider a mixed problem

$$\frac{\partial \phi}{\partial n} = 0 \qquad \text{on } \bar{\sum} \cup \sum_o \cup \sum_H, \tag{1.5}$$

$$\phi\Big|_{t=o} = 0, \tag{1.6}$$

where n is the normal to the boundary of the region G.

To solve the problem of locating the sources of industrial run-offs in the water body area, we shall consider a functional

$$J_k = \int_0^T dt \int_{\bar{G}} p_k(\underline{r})\phi(\underline{r}, t)\, dG, \tag{1.7}$$

where

$$p_k(\underline{r}) = \begin{cases} \dfrac{1}{TS_k} & \text{when } \underline{r} \in G_k, \\ 0 & \text{outside } G_k. \end{cases}$$

Here, S_k is a measure of the region G_k which has to be protected against pollution (for example, a measure of the region in the immediate neighborhood of a settlement, recreation zone, etc.).

Functional (1.7) represents the average concentration of the polluting impurity in time T. In case of accumulatable impurities the current value of the functional

$$J_{1k} = T \int_{\bar{G}} p_k(\underline{r})\phi(\underline{r}, t)\, dG$$

for a stationary source may exceed the average value. To take a correct decision on the possible locating a pollution source in a particular region of water area it is necessary to study a functional of the type

$$J_{1k} = \left[T \int_G p_k(\underline{r})\phi(\underline{r}, t)\, dG \right]_{t=T}. \tag{1.8}$$

Let us consider limitations imposed by sanitary requirements, that is, we shall demand that the point $\underline{r}_o$ lies in the region ω_k and the following condition is fulfilled for all points of the region

$$J_k(\underline{r}) \leq C_k, \tag{1.9}$$

where C_k is a constant related to sanitary requirements for the ecological region G_k. Thus, the problem is reduced to integrating Eq.(1.2) with conditions (1.5), (1.6) and a restriction of the type (1.9).

8.2. Adjoint Equations

We shall suppose that the earlier formulated problem permits sufficiently smooth solutions to be obtained from the space ϕ with a scalar product of the type

$$(\phi, \phi^*) = \int_0^T dt \int_G \phi\phi^* dG. \tag{2.1}$$

Taking the earlier described procedure of solving problems of the given type as the base, the problem of determining the polluting hydrosol disposal site with regard to restriction (1.9) can be solved by dual representation of the functional (1.7):

$$J_k = Q \int_0^T \phi^*(\underline{r}_o, t)\, dt. \tag{2.2}$$

Here ϕ^* represents the solution of the adjoint problem

$$L^*\phi^* = p_k \tag{2.3}$$

where L^* is an operator adjoint from the viewpoint of the Lagrange's identity to the operator of problem (1.2), (1.5), (1.6), and

$$\phi^*(T) = 0 \tag{2.4}$$

and the problem (2.3), (2.4) is solved in the decreasing direction of t. Definite form of operator L^* is obtained from the relation

$$(L\phi - f,\ \phi^*) = \int_0^T dt \int_G \phi^*\left(\frac{\partial\phi}{\partial t} + \mathrm{div}\,\phi\underline{u} + \sigma\phi - \mu\Delta\phi - \frac{\partial}{\partial z}\nu\frac{\partial\phi}{\partial z} - f\right) dG =$$

$$= \int_0^T dt \int_G \phi\left(-\frac{\partial\phi^*}{\partial t} - \mathrm{div}\,\phi^*\underline{u} + \sigma\phi^* - \mu\Delta\phi^* - \frac{\partial}{\partial z}\nu\frac{\partial\phi^*}{\partial z} - p_k\right) dG + \tag{2.5}$$

$$+ \int_0^T dt \int_\Gamma \phi\left(\phi^* u_n + \bar{\mu}\frac{\partial\phi^*}{\partial n}\right) d\Gamma = (L^*\phi^* - p_k,\ \phi) = 0,$$

where

$$\Gamma = \bar{\sum} \cup \sum_0 \cup \sum_H, \quad \bar{\mu} = \begin{cases} \mu, & \underline{r} \in \sum, \\ \nu & \underline{r} \in \sum_0, \text{ or } \sum_H. \end{cases}$$

In deducing (2.5) we used the continuity equation

$$\mathrm{div}\ \underline{u} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

and conditions (1.5), (1.6), (2.4). Now we transform (2.5) using the identities

$$\mathrm{div}\ \alpha\underline{u} = \underline{u}\nabla\alpha + \alpha\,\mathrm{div}\ \underline{u} = \underline{u}\nabla\ \alpha, \tag{2.6}$$

$$\alpha\underline{u}\nabla\beta = \alpha\sqrt{\beta}\ \underline{u}\ \nabla\sqrt{\beta} + \mathrm{div}\ \alpha\beta\underline{u} - \sqrt{\beta}\ \underline{u}\nabla(\alpha\sqrt{\beta}), \tag{2.7}$$

where

$$\underline{u}\nabla\alpha = u\frac{\partial\alpha}{\partial x} + v\frac{\partial\alpha}{\partial y} + w\frac{\partial\alpha}{\partial z},$$

which hold true when the continuity equation is satisfied and $\beta \geq 0$. Choosing functions ϕ^* from the subset of non-negative functions of the set Φ, we obtain

$$(L^*\phi^* - p_k, \phi) = \int_0^T dt \int_G \Big(-\phi\frac{\partial\phi^*}{\partial t} + \sqrt{\phi^*}\ \underline{u}\nabla(\phi\sqrt{\phi^*}) -$$
$$- (\phi\sqrt{\phi^*})\underline{u}\nabla\sqrt{\phi^*} + \mu\nabla\phi\nabla\phi^* + \nu\frac{\partial\phi}{\partial z}\frac{\partial\phi^*}{\partial z} - \phi p_k\Big)\ dG = 0. \tag{2.8}$$

Note that at ϕ = constant (2.8) changes into the balance relation without any additional transformations

$$\int_G \phi^*\ dG\Big|_{\bar{t}=T-t} = \int_0^T dt \int_G p_k\ dG. \tag{2.9}$$

Now imparting the meaning of trial function to ϕ in (2.8), we shall take the given identity as definition of a generalized solution to the adjoint problem.

For constructing an effective computational algorithm of the solution of (2.8) we shall use the idea of the method of imaginary regions. With this in view we shall introduce a rectangular region

$$D = \{X_1 \leq x \leq X_2, \quad Y_1 \leq y \leq Y_2\}, \tag{2.10}$$

where $X_1 = \inf(x)$, $X_2 = \sup(x)$, $Y_1 = \inf(y)$, $Y_2 = \sup(y)$, $x, y \in \bar{\bar{G}}$, and the region

$$G = D \cdot [0, H]. \tag{2.11}$$

As above, we shall assume that the boundary $\sum$ of region G consists of solid $\sum_1$ and liquid $\sum_2$ boundaries. We shall extend functions ϕ, ϕ^*, $\underline{u}$, and μ to the whole region G as follows:

$$\underline{u} = \begin{cases} \underline{u}, & \underline{r} \in \bar{G} \\ 0, & \underline{r} \in G \setminus \bar{G}; \end{cases} \qquad \mu = \begin{cases} \mu, & \underline{r} \in \bar{G}, \\ 0, & \underline{r} \in G \setminus \bar{G}; \end{cases}$$
$$\int_0^T dt \int_{G \setminus \bar{G}} \phi \frac{\partial \phi^*}{\partial t} \, dG = 0. \tag{2.12}$$

Then the integral identity (2.8) takes the form

$$(L^*\phi^* - p, \phi) = \int_0^T dt \int_G \left(- \phi \frac{\partial \phi^*}{\partial t} + \sqrt{\phi^*}\, \underline{u}\nabla(\phi\sqrt{\phi^*}) - \right.$$
$$\left. - (\phi\sqrt{\phi^*})\, \underline{u}\nabla\sqrt{\phi^*} + \mu\nabla\phi\nabla\phi^* + \nu \frac{\partial \phi}{\partial z} \frac{\partial \phi^*}{\partial z} - p\phi\right) dG = 0. \tag{2.13}$$

For simplicity, here and further we have dropped index k at function p. This, i.e. (2.13), is an initial identity for constructing a numerical algorithm for the problem solution.

8.3. Finite-Difference Approximations

Let us now proceed to the construction of finite-difference approximations of (2.3). In range G we shall determine a network region as direct product of regular one-dimensional nets:

$$G^h = G^h_x \cdot G^h_y \cdot G^h_z, \tag{3.1}$$

where

$$G^h_x = \{x_i \in [X_1, X_2] \,|\, x_i = X_1 + i\delta x, \quad i = \overline{0, N}, \; \delta x = \frac{X_2 - X_1}{N}\},$$

$$G_y^h = \{y_j \in [Y_1, Y_2] \mid y_j = Y_1 + i\delta y, \quad j = \overline{0, M}, \quad \delta y = \frac{Y_2 - Y_1}{M}\},$$

$$G_z^h = \{z_k \in [0, H] \mid z_k = k\delta z, \quad k = \overline{0, K}, \quad \delta z = \frac{H}{K}\}.$$

We shall now consider a space of network functions defined on the net G^h:

$$\Phi^h = \{\underline{\phi} = \{\phi_{ijk}\} \mid \phi_{ijk} = \phi(t, x_i, y_j, z_k), \quad i = \overline{0, N}, \quad j = \overline{0, M}, \quad k = \overline{0, K}\}. \tag{3.2}$$

Scalar product is determined by the relation

$$(\underline{\phi}, \underline{\phi}^*) = \sum_{i=0}^{N} \sum_{j=0}^{M} \sum_{k=0}^{K} \phi_{ijk}\phi^*_{ijk}\delta x_i \delta y_j \delta z_k, \tag{3.3}$$

where

$$\delta x_i = \begin{cases} \delta x/2, & i = 0, N, \\ \delta x, & i = \overline{1, N-1} \end{cases} \qquad \delta y_j = \begin{cases} \delta y/2, & j = 0, M, \\ \delta y, & j = \overline{1, M-1} \end{cases}$$

$$\delta z_k = \begin{cases} \delta z/2, & k = 0, K, \\ \delta z, & k = \overline{1, K-1}. \end{cases}$$

Using identity (2.13) as the base, we shall construct finite-difference schemes to solve (2.3). Suppose that the difference operators Λ_x, Λ_y, Λ_z are given. They approximate differential operators $\partial/\partial x$, $\partial/\partial y$, $\partial/\partial z$ at the nodes of the network region G^h with due regard to the relation $\partial\phi^*/\partial n = 0$, $\underline{r} \in \Sigma \cup \Sigma_o \cup \Sigma_H$ which is natural for the functional (2.5). Considering the fact that the adjoint problem is solved in the decreasing direction of t we introduce a network on $[0, T]$ as follows:

$$G_t^h = \{t_\ell \in [0, T] \mid t_\ell = T - \tau\ell, \quad \ell = \overline{0, L}, \quad \tau = T/L\}. \tag{3.4}$$

Let us consider an expression of the type (2.13) in an elementary time interval $[t_\ell, t_{\ell+1}]$. Using the difference analogies of differential operators and considering the form of the scalar product (3.3), we obtain

$$(L^*\phi^* - p, \phi) \cong (L^*\underline{\phi}^* - \underline{Pe}, \underline{\phi})^h = (\underline{\phi}^{\ell+1/14}, (\underline{\phi}^*)^{\ell+1/7} - (\underline{\phi}^*)^{\ell} - \tau\underline{Pe}) +$$

$$+ \left(\underline{\phi}^{\ell+3/14}, \frac{\Omega^{\ell+2/7} + \Omega^{\ell+1/7}}{2} (2(\underline{\omega}^{\ell+2/7} - \underline{\omega}^{\ell+1/7}) + \tau(\Lambda_x^*U - U\Lambda_x^*) \cdot \right.$$

$$\left. \cdot \frac{\underline{\omega}^{\ell+2/7} + \underline{\omega}^{\ell+1/7}}{2}\right)\Bigg) + \left(\underline{\phi}^{\ell+5/14}, \frac{\Omega^{\ell+3/7} + \Omega^{\ell+2/7}}{2} (2(\underline{\omega}^{\ell+3/7} - \underline{\omega}^{\ell+2/7}) + \right.$$

$$+ \tau(\Lambda_y^* V - V\Lambda_y^*) \frac{\underline{\omega}^{\ell+3/7} + \underline{\omega}^{\ell+2/7}}{2} \Big) \Big\} + \Big(\underline{\phi}^{\ell+7/14}, \frac{\Omega^{\ell+4/7} + \Omega^{\ell+3/7}}{2} \cdot \tag{3.5}$$

$$\cdot (2(\underline{\omega}^{\ell+4/7} - \underline{\omega}^{\ell+3/7}) + \tau(\Lambda_z^* W - W\Lambda_z^*) \frac{\underline{\omega}^{\ell+4/7} + \underline{\omega}^{\ell+3/7}}{2} \Big) \Big\} +$$

$$+ (\underline{\phi}^{\ell+9/14}, (\underline{\phi}^*)^{\ell+5/7} - (\underline{\phi}^*)^{\ell+4/7} + \tau\Lambda_x^* A\Lambda_x (\underline{\phi}^*)^{\ell+5/7}) + (\underline{\phi}^{\ell+11/14},$$

$$(\underline{\phi}^*)^{\ell+6/7} - (\underline{\phi}^*)^{\ell+5/7} + \tau\Lambda_y^* A\Lambda_y (\underline{\phi}^*)^{\ell+6/7}) + (\underline{\phi}^{\ell+13/14}, (\underline{\phi}^*)^{\ell+1} -$$

$$- (\underline{\phi}^*)^{\ell+6/7} + \tau\Lambda_z^* \bar{A}\Lambda_z (\underline{\phi}^*)^{\ell+1}),$$

where U, V, W, A, $\bar{A}$, P, $\Omega^{\ell+r}$ are block-diagonal matrices on whose diagonals are located the values u_{ijk}, v_{ijk}, w_{ijk}, μ_{ijk}, ν_{ijk}, p_{ijk}, $\omega_{ijk}^{\ell+r}$, with respect to the order defined by the structure of vectors from the space Φ^h; $\underline{e}$ is a unit vector; $\omega_{ijk} = \sqrt{\phi_{ijk}^*}$; $\underline{\phi}^{\ell+r} = \underline{\phi}|_{t=t_{\ell+rT}}$; Λ_x^*, Λ_y^*, Λ_z^* are the operators adjoint towards Λ_x, Λ_y, Λ_z in (3.3); $\Lambda^* = R^{-1}\Lambda^T R$; R is a block-diagonal matrix of the type $R = \mathrm{diag}\,\{1/2, 1, \ldots, 1, 1/2\}$; index T denotes the transposition operation.

We take the relation

$$(L^*\underline{\phi}^* - P\underline{e}, \underline{\phi})^h = 0 \tag{3.6}$$

as a definition of the generalized solution to the difference analog of problem (2.3, (2.4). For $\underline{\phi} = \underline{e}$, (3.6) changes into the following equality without any additional transformations

$$(L^*\underline{\phi}^* - P\underline{e}, \underline{e})^h = \sum_{i,j,k} ((\phi_{ijk}^*)^{\ell+1} - (\phi_{ijk}^*)^{\ell} - \tau(P\underline{e})_{ijk})\delta x_i \delta y_i \delta z_k = 0 \tag{3.7}$$

This equality is the difference analog of balance of first moments of the differential problem.

The finite-difference scheme for the numerical solution to problem (2.3) is determined by choosing $\{\underline{\phi}^{\ell+r}\}$ functions in the form

$$\underline{\phi}(\alpha) = \{0, \ldots, 0, \underline{\phi}^{\ell+\alpha/14}, 0, \ldots, 0\}, \ \underline{\phi}^{\ell+\alpha/14} = \underline{e}, \qquad \alpha = 1, 3, 5, \ldots, 13. \tag{3.8}$$

Substituting (3.8) into (3.5) we obtain a difference scheme

$$\underline{\phi}^{\ell+1/7} = \underline{\phi}^{\ell} + \tau P\underline{e}, \tag{3.9a}$$

$$(E + \frac{\tau}{4}\bar{\Lambda}_x)\underline{\omega}^{\ell+2/7} = (E - \frac{\tau}{4}\bar{\Lambda}_x)\underline{\omega}^{\ell+1/7}, \tag{3.9b}$$

$$(E + \frac{\tau}{4}\bar{\Lambda}_y)\underline{\omega}^{\ell+3/7} = (E - \frac{\tau}{4}\bar{\Lambda}_y)\underline{\omega}^{\ell+2/7}, \tag{3.9c}$$

$$(E + \frac{\tau}{4}\bar{\Lambda}_z)\underline{\omega}^{\ell+4/7} = (E - \frac{\tau}{4}\bar{\Lambda}_z)\underline{\omega}^{\ell+3/7}, \tag{3.9d}$$

$$(E + \tau\Lambda_x^h)\underline{\phi}^{\ell+5/7} = \underline{\phi}^{\ell+4/7}, \tag{3.9e}$$

$$(E + \tau\Lambda_y^h)\ \underline{\phi}^{\ell+6/7} = \underline{\phi}^{\ell+5/7}, \tag{3.9f}$$

$$(E + \tau\Lambda_z^h)\ \underline{\phi}^{\ell+1} = \underline{\phi}^{\ell+6/7}, \tag{3.9g}$$

where

$$\bar{\Lambda}_x = R^{-1}\Lambda_x^T RU - U\Lambda_x, \quad \bar{\Lambda}_y = R^{-1}\Lambda_y^T RV - V\Lambda_y, \quad \bar{\Lambda}_z = R^{-1}\Lambda_z^T RW - W\Lambda_z,$$

$$\Delta_x^h = R^{-1}\Lambda_x^T RA\Lambda_x, \quad \Delta_y^h = R^{-1}\Lambda_y^T RA\Lambda_y, \quad \Delta_z^h = R^{-1}\Lambda_z^T R\bar{A}\Lambda_z, \quad \phi_{ijk}^o = 0,$$

$$\omega_{ijk}^{\ell+1/7} = \sqrt{\phi_{ijk}^{\ell+1/7}}, \quad \phi_{ijk}^{\ell+4/7} = (\omega_{ijk}^{\ell+4/7})^2, \quad i = \overline{0,\ N}, \quad j = \overline{0,\ M},$$

$$k = \overline{0,\ K}.$$

For abbreviation, here and further we have dropped asterisk at function $\underline{\phi}$.

Note that bicyclic splitting schemes considered in chapter 2 are obtained upon symmetric approximation of the functional (2.13) in respect of point $t_{\ell+1/2}$. Such schemes lead, as mentioned earlier, to approximation of the second order time variable. For positive semi-definiteness P, the scheme (3.9) does not take function $\underline{\phi}$ out of the class of the positive functions. In this case, (3.7) is a testimony to the stability of the difference scheme (3.9). The operators Λ_x, Λ_y, Λ_z approximating the differential operators in region G are chosen very arbitrarily. We determine them so as to ensure simple and effective realization of the network (3.9). For (3.9b)-(3.9d) we choose these operators from a class conforming to approximation on a three-point pattern:

$$\left(\frac{\partial\phi}{\partial x}\right)_i \sim \frac{\phi_{i+1} - \phi_{i-1}}{2\delta x}$$

and for (3.9e)-(3.9g), from a class conforming to a two-point pattern:

$$\left(\frac{\partial\phi}{\partial x}\right)_i \sim \frac{\phi_{i+1} - \phi_i}{\delta x} .$$

Such a selection ensures a second order approximation in space variables for (2.3). In this case, the operators in (3.9) represent block-three-diagonal matrices and are reverted by the run method. The step τ is chosen in such a way as to ensure the sufficient condition for run stability.

In conclusion, it may be mentioned that the general form of the scheme and the structure of the algorithm remain unaltered when any other network region in G is chosen.

8.4. Finite Element Method

Here we shall describe another method of solving (1.2) which is a basic equation for finding optimum location of a run-off source in the water body. In this section we have applied the ideas used in chapter 3 for solving motion equations by the method of finite elements in combination with the splitting method. In doing so, we succeed in combining approximation advantages of the finite elements method with simple realization of the splitting method.

First, as before, we shall reduce the advective terms of (1.2) to the anti-symmetric form by isolating the barotropic component of speed. Suppose that

$$u = \overline{u} + u', \qquad v = \overline{v} + v', \qquad w = w' \tag{4.1}$$

where

$$\overline{u} = \frac{1}{H}\int_0^H u\, dz, \qquad \overline{v} = \frac{1}{H}\int_0^H v\, dz.$$

Then the velocity components $\overline{u}$, $\overline{v}$, u', v', w' will satisfy the continuity equations

$$\frac{\partial \overline{u}}{\partial x} + \frac{\partial \overline{v}}{\partial y} = 0, \tag{4.2}$$

$$\frac{\partial u'}{\partial x} + \frac{\partial v'}{\partial y} + \frac{\partial w}{\partial z} = 0. \tag{4.3}$$

Equation (4.2) enables a flow function to be introduced by the relations

$$u = -\frac{\partial \psi}{\partial y}, \qquad v = \frac{\partial \psi}{\partial x}. \tag{4.4}$$

For a closed basin the flow function ca be found from the solution of the boundary problem

$$\begin{aligned} \Delta\psi &= \mathrm{rot}\,\overline{u}, \\ \psi &= 0 \quad \text{on } \Gamma. \end{aligned} \tag{4.5}$$

Integrating over vertical from z to H and using the fact that $w_H = 0$, we find w from (4.3)

$$w = \frac{\partial}{\partial x}\int_z^H u\, dz + \frac{\partial}{\partial y}\int_z^H v\, dz. \tag{4.6}$$

Introducing notations

$$\tilde{u} = \int_z^H u\,dz, \qquad \tilde{v} = \int_z^H v\,dz \tag{4.7}$$

and substituting (4.6), (4.4), (4.7) into (1.2), we obtain

$$\frac{\partial\phi}{\partial t} - \frac{\partial}{\partial x}\psi\frac{\partial\phi}{\partial y} + \frac{\partial}{\partial y}\psi\frac{\partial\phi}{\partial x} - \frac{\partial}{\partial z}\tilde{u}\frac{\partial\phi}{\partial x} + \frac{\partial}{\partial y}\tilde{u}\frac{\partial\phi}{\partial z} - \frac{\partial}{\partial z}\tilde{v}\frac{\partial\phi}{\partial y} + \frac{\partial}{\partial y}\tilde{v}\frac{\partial\phi}{\partial z} - $$
$$- \mu\Delta\phi - \frac{\partial}{\partial z}\nu\frac{\partial}{\partial z} + \sigma\phi = f, \tag{4.8}$$

In further discussion we shall assume the basin to be closed. Then the following relations hold for the coefficients that appear in (4.8):

$$\psi|\Gamma = 0; \tag{4.9}$$

$$\tilde{u}|_{z=H} = 0, \quad \tilde{v}|_{z=H} = 0, \quad \tilde{u}|_{z=0} = 0, \quad \tilde{v}|_{z=0} = 0; \tag{4.10}$$

$$\tilde{u}_n|_\Sigma = 0. \tag{4.11}$$

Also we shall recall that the following expressions were considered as boundary conditions for (1.2):

$$\left.\frac{\partial\phi}{\partial n}\right|_{\Sigma} = 0; \tag{4.12}$$

$$\left.\frac{\partial\phi}{\partial z}\right|_{z=0} = 0; \tag{4.13}$$

$$\left.\frac{\partial\phi}{\partial z}\right|_{z=H} = 0. \tag{4.14}$$

If the conditions (4.9)-(4.11) are satisfied, the boundary conditions (4.12)-(4.14) are natural in the variation sense for the space operator appearing in (4.8), and this enables us to construct the projection-difference approximations of the equation.

Let us now consider the space operator that appears in (4.8). As in the case of motion equations, it may be presented as a sum of three plane operators:

$$A = A_{xy} + A_{xz} + A_{yz} \tag{4.15}$$

where

$$A_{xy} = -\frac{\partial}{\partial z}\frac{\mu}{2}\frac{\partial}{\partial x} - \frac{\partial}{\partial x}\psi\frac{\partial}{\partial y} + \frac{\partial}{\partial y}\psi\frac{\partial}{\partial x} - \frac{\partial}{\partial y}\frac{\mu}{2}\frac{\partial}{\partial y} + \frac{\sigma}{3},$$

$$A_{xz} = -\frac{\partial}{\partial x}\frac{\mu}{2}\frac{\partial}{\partial x} - \frac{\partial}{\partial z}\tilde{u}\frac{\partial}{\partial x} + \frac{\partial}{\partial x}\tilde{u}\frac{\partial}{\partial z} - \frac{\partial}{\partial z}\frac{\nu}{2}\frac{\partial}{\partial z} + \frac{\sigma}{3}, \tag{4.16}$$

$$A_{yz} = -\frac{\partial}{\partial y}\frac{\mu}{2}\frac{\partial}{\partial y} - \frac{\partial}{\partial z}\tilde{v}\frac{\partial}{\partial y} + \frac{\partial}{\partial y}\tilde{v}\frac{\partial}{\partial z} - \frac{\partial}{\partial z}\frac{\nu}{2}\frac{\partial}{\partial z} + \frac{\sigma}{3}.$$

Let us now study the properties of the operators A_{xy}, A_{yz}, A_{xz}, and prove that they are positively defined in $\bar{G}$. We shall consider, for example, operator A_{xy} and construct an energy functional (A_{xy}, ϕ, ϕ) for it. Then

$$(A_{xy}\phi,\phi) = \int_G \left(-\frac{\partial}{\partial x}\frac{\mu}{2}\frac{\partial\phi}{\partial x} - \frac{\partial}{\partial x}\psi\frac{\partial\phi}{\partial y} + \frac{\partial}{\partial y}\psi\frac{\partial\phi}{\partial x} - \frac{\partial}{\partial y}\frac{\mu}{2}\frac{\partial\phi}{\partial y}\right)\phi\, dG =$$

$$= \int_\Sigma \left(-\frac{\mu}{2}\frac{\partial\phi}{\partial x}\cos(n,\ x) - \psi\frac{\partial\phi}{\partial y}\cos\ (n,\ y) + \psi\frac{\partial\phi}{\partial x}\cos(n,\ y) - \right. \tag{4.17}$$

$$\left. - \frac{\mu}{2}\frac{\partial\phi}{\partial y}\cos(n,\ y)\right)\phi\, d\Sigma + \int_{\bar{G}}\left(\frac{\mu}{2}\left(\frac{\partial\phi}{\partial x}\right)^2 + \frac{\mu}{2}\left(\frac{\partial\phi}{\partial y}\right)^2 + \frac{\sigma\phi^2}{3}\right) dG,$$

where (n, x) denotes the angle between x-axis and the direction of the outer normal. Taking account of the condition $\psi|_{\bar{\Sigma}} = 0$ in the boundary integral, we arrive at the following expression

$$(A_{xy}\phi,\phi) = \int_{\bar{\Sigma}} -\frac{\mu}{2}\frac{\partial\phi}{\partial n}\, d\Sigma + \int_{\bar{G}}\left(\frac{\mu}{2}\left(\frac{\partial\phi}{\partial x}\right)^2 + \frac{\mu}{2}\left(\frac{\partial\phi}{\partial y}\right)^2 + \frac{\sigma\phi^2}{3}\right) dG, \tag{4.18}$$

Considering condition (4.12) we have

$$(A_{xy}\phi,\ \phi) = \int_G \left(\frac{\mu}{2}\left(\frac{\partial\phi}{\partial x}\right)^2 + \frac{\mu}{2}\left(\frac{\partial\phi}{\partial y}\right)^2 + \frac{\sigma\phi^2}{3}\right) dG, \tag{4.19}$$

This proves the positive definiteness of operator A. When $\sigma = 0$ the operator A_{xy} is positively semi-definite. In a similar manner the positive definiteness of operators A_{xz}, A_{yz} is proved. This property has a dominant role in constructing the splitting network and in approximation by the finite elements method. Dividing the integration interval [0, T]: $t_\ell \leqq t \leqq t_{\ell+1}$, $t_{\ell+1} - t_\ell = \tau$, we write a weak approximation scheme on $t_{\ell-1} \leqq t \leqq t_{\ell+1}$ for Eq.(1.2):

on the interval $t_{\ell-1} \leqq t \leqq t_\ell$:

$$\begin{aligned} &\frac{\partial\phi_1}{\partial t} + A_{xy}\phi_1 = f, \quad \phi_1(t_{\ell-1}) = \phi(t_{\ell-1}), \\ &\frac{\partial\phi_2}{\partial t} + A_{xz}\phi_2 = 0, \quad \phi_2(t_{\ell-1}) = \phi_1(t_\ell), \\ &\frac{\partial\phi_3}{\partial t} + A_{yz}\phi_3 = 0, \quad \phi_3(t_{\ell-1}) = \phi_2(t_\ell); \end{aligned} \tag{4.20}$$

on the interval $t_\ell \leqq t \leqq t_{\ell+1}$:

$$\frac{\partial\phi_4}{\partial t} + A_{yz}\phi_4 = 0, \quad \phi_4(t_\ell) = \phi_3(t_\ell),$$

$$\frac{\partial\phi_5}{\partial t} + A_{xz}\phi_5 = 0, \quad \phi_5(t_\ell) = \phi_4(t_{\ell+1}), \tag{4.20'}$$

$$\frac{\partial\phi_6}{\partial t} + A_{xy}\phi_6 = f, \quad \phi_6(t_\ell) = \phi_5(t_{\ell+1}).$$

At every step of splitting the boundary conditions for operators A_{xy}, A_{yz}, A_{yz} are selected so that they are natural in the variation sense for a corresponding operator. The boundary conditions in this case are so splitted that their sum will yield initial boundary conditions.

Further we shall consider the sections $\sum_i$, $\sum_j$, $\sum_k$ of the region G:

$$\sum_i = \{\underline{r} \in G \,|\, x = X_1 + i\delta x, \quad i = \overline{0,\ N}\},$$

$$\sum_j = \{\underline{r} \in G \,|\, y = Y_1 + j\delta y, \quad j = \overline{0,\ M}\},$$

$$\sum_k = \{\underline{r} \in G \,|\, z = k\delta z, \quad k = \overline{0,\ K}\}.$$

Denote the boundaries of the sections $\sum_i$, $\sum_j$, $\sum_k$ by Γ_i, Γ_j, Γ_k. The sections are parallel to the coordinate planes and divide G with steps $\delta x, \delta y$, δz in the direction of the corresponding coordinate. In every section $\sum_i$, $\sum_j$, $\sum_k$ we can determine network regions $\sum_i^h$, $\sum_j^h$, $\sum_k^h$ which consist of G^h points belonging to these sections. Call the network boundaries Γ_i^h, Γ_j^h, Γ_k^h. In the next step of construction Eqs. (4.20) will be considered only on these sections. Thus, we get a set $(N + 1)\ (M + 1)\ (K + 1)$ of plane parabolic equations on the sections of G. Now if we approximate every problem with network equations on corresponding networks $\sum_i^h$, $\sum_j^h$, $\sum_k^h$ in such a manner that the property of positive semi-definiteness of space network operators is retained in these approximations, then the scheme obtained from (4.20) will be convergent.

Let us denote by Λ_{xyi}, Λ_{xzj}, Λ_{xzk} the network operators which approximate the operators A_{xy}, A_{xz}, A_{yz} on the sections $\sum_i$, $\sum_j$, $\sum_k$, respectively. Equations (4.20), after their quantization by space variables will take the form:

on the interval $t_{\ell-1} \leqq t \leqq t_\ell$:

$$\frac{\partial\underline{\phi}_{1k}}{\partial t} + \Lambda_{xyk}\,\underline{\phi}_{1k} = \underline{F}_k, \quad \underline{\phi}_{1k}(t_{\ell-1}) = \underline{\phi}_k(t_\ell) \quad \text{on } \sum_k^h,$$

$$\frac{\partial\underline{\phi}_{2j}}{\partial t} + \Lambda_{xzj}\,\underline{\phi}_{2j} = 0, \quad \underline{\phi}_{2j}(t_{\ell-1}) = \underline{\phi}_{1j}(t_\ell) \quad \text{on } \sum_j^h, \tag{4.21}$$

$$\frac{\partial\underline{\phi}_{3i}}{\partial t} + \Lambda_{yzi}\,\underline{\phi}_{3i} = F_i, \quad \underline{\phi}_{3i}(t_{\ell-1}) = \underline{\phi}_{2i}(t_\ell) \quad \text{on } \sum_i^h.$$

on the interval $t_\ell \leq t \leq t_{\ell+1}$:

$$\frac{\partial \phi_{4i}}{\partial t} + \Lambda_{yzi}\, \phi_{4i} = 0, \quad \phi_{4i}(t_\ell) = \phi_{3i}(t_\ell) \quad \text{on} \quad \textstyle\sum_i^h,$$

$$\frac{\partial \phi_{5j}}{\partial t} + \Lambda_{xzj}\, \phi_{5j} = 0, \quad \phi_{5j}(t_\ell) = \phi_{4j}(t_{\ell+1}) \quad \text{on} \quad \textstyle\sum_j^h, \tag{4.21}$$

$$\frac{\partial \phi_{6k}}{\partial t} + \Lambda_{xyk}\, \phi_{6k} = F_k, \quad \phi_{6k}(t_\ell) = \phi_{5k}(t_{\ell+1}) \quad \text{on} \quad \textstyle\sum_k^h.$$

Now we shall determine the type of approximation of operators appearing in (4.21) and the method of solving every problem. As a quantization method we shall use the method of finite elements described in section 3.3 of chapter 3 for solving equations of motion.

Let us now consider in detail an approximation and the method of solving only one of the Eqs.(4.20). Let it be an equation containing operator A_{xy}. All other splitting steps are realized similarly, as the type of operators and their properties are completely analogous.

Thus, we shall describe an approximation of plane equations of the type (4.20) by the finite elements method, as it has been done for equations of motion in chapter 3. In this case, the equations contain diffusion terms demanding formulation of boundary conditions. The equations take the form

$$\frac{\partial \phi}{\partial t} + A\phi = f,$$

$$A = -\mu \frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial x}\psi\frac{\partial}{\partial y} + \frac{\partial}{\partial y}\psi\frac{\partial}{\partial x} - \mu\frac{\partial^2}{\partial y^2} + \sigma. \tag{4.22}$$

We choose the boundary and initial conditions as follows:

$$\left.\frac{\partial \phi}{\partial n}\right|_\Gamma = 0; \tag{4.23}$$

$$\phi\big|_{t=0} = 0. \tag{4.24}$$

In the integration range D we now introduce the network D^h formed by the intersection of straightlines $x_i = X_1 + i\delta x$, $y_j = t_j\delta y$. As before, we triangulate the network cells with positive direction diagonals. Suppose that region $\tilde{D}$ with boundary $\tilde{\Gamma}$ has the least union of triangles, which is contained in D. At every point (x_i, y_i) of the network D^h we determine the functions $\omega_{ij}(x, y)$ continuous in D, linear on every triangle, and satisfying the relations

$$\omega_{ij}(x_m, y_n) = \begin{cases} 1, & i = m \text{ and } j = n, \\ 0, & i \neq m \text{ or } j \neq n. \end{cases}$$

We shall find an approximate solution in the form of a linear combination of functions ω_{ij}:

$$\bar{\phi}(x, y, t) = \sum_{i,j} \phi_{ij}(t)\, \omega_{ij}, \quad (x_i, y_j) \in \tilde{D} \cup \tilde{\Gamma}. \tag{4.25}$$

Then the equations for finding coefficients $\phi_{ij}(t)$, when a quadrature formula is used to approximate an evolutionary term, can be written as

$$\frac{\partial \phi_{ij}}{\partial t} \int_D \omega_{ij}\, dD + \int_D \left(\mu \frac{\partial \bar{\phi}}{\partial x} \frac{\partial \omega_{ij}}{\partial x} + \mu \frac{\partial \bar{\phi}}{\partial y} \frac{\partial \omega_{ij}}{\partial y} + \psi \frac{\partial \bar{\phi}}{\partial y} \frac{\partial \omega_{ij}}{\partial x} - \right.$$

$$\left. - \psi \frac{\partial \bar{\phi}}{\partial x} \frac{\partial \omega_{ij}}{\partial y} + \sigma \bar{\phi} \omega_{ij} \right) dD = \int_D f \omega_{ij}\, dD. \tag{4.26}$$

The mathematical aspects of obtaining Eqs.(4.26) are not detailed since they are discussed in the monographs on the method of finite elements.

Computing (4.26) with the use of table 3.1 (section 3.3) and grouping like terms, we find a system of differential equations

$$\kappa \frac{\partial \underline{\phi}}{\partial t} + \Lambda \underline{\phi} = \underline{F}, \qquad \underline{\phi}\big|_{t=0} = \underline{\phi}^{o}, \tag{4.27}$$

where κ is the diagonal matrix operator:

$$[\kappa \underline{\phi}]_{ij} = \phi_{ij} \int_D \omega_{ij}\, dD,$$

Λ is the matrix operator which can be represented as

$$\begin{aligned}
[\Lambda \underline{\phi}]_{ij} = {} & \alpha^{ij}_{i+1,j} \phi_{i+1,j} - (\alpha^{ij}_{i+1,j} + \alpha^{ij}_{i-1,j}) \phi_{ij} + \alpha^{ij}_{i-1,j} \phi_{i-1,j} + \\
& + \gamma^{ij}_{i+1,j} \phi_{i+1,j} + (\gamma^{ij}_{i+1,j} + \gamma^{ij}_{i-1,j}) \phi_{ij} + \gamma^{ij}_{i-1,j} \phi_{i-1,j} + \\
& + \alpha^{ij}_{i,j+1} \phi_{i,j+1} - (\alpha^{ij}_{i,j+1} + \alpha^{ij}_{i,j-1}) \phi_{ij} + \alpha^{ij}_{i,j-1} \phi_{i,j-1} + \\
& + \gamma^{ij}_{i,j+1} \phi_{i,j+1} + (\gamma^{ij}_{i,j+1} + \gamma^{ij}_{i,j-1}) \phi_{ij} + \gamma^{ij}_{i,j-1} \phi_{i,j-1} + \\
& + \alpha^{ij}_{i+1,j+1} \phi_{i+1,j+1} - (\alpha^{ij}_{i+1,j+1} + \alpha^{ij}_{i-1,j-1}) \phi_{ij} + \\
& + \alpha^{ij}_{i-1,j-1} \phi_{i-1,j-1} + \gamma^{ij}_{i+1,j+1} \phi_{i+1,j+1} + (\gamma^{ij}_{i+1,j+1} + \\
& + \gamma^{ij}_{i-1,j-1}) \phi_{ij} + \gamma^{ij}_{i-1,j-1} \phi_{i-1,j-1} + \beta^{ij}_{i+1,j} \phi_{i+1,j} + \\
& + \beta^{ij}_{i-1,j} \phi_{i-1,j} + \beta^{ij}_{i,j+1} \phi_{i,j+1} + \beta^{ij}_{i,j-1} \phi_{i,j-1} + \beta^{ij}_{i+1,j+1} \phi_{i+1,j+1} + \\
& + \beta^{ij}_{i-1,j-1} \phi_{i-1,j-1},
\end{aligned} \tag{4.28}$$

where

$$\alpha^{ij}_{i,j-1} = -\frac{\mu}{\delta y^2}(B^5_{ij} + B^6_{ij}),\quad \beta^{ij}_{i,j-1} = \frac{1}{\delta x\delta y}(\psi^5_{ij} - \psi^6_{ij}),$$

$$\alpha^{ij}_{i,j+1} = -\frac{\mu}{\delta y^2}(B^2_{ij} + B^3_{ij}),\quad \beta^{ij}_{i,j+1} = \frac{1}{\delta x\delta y}(\psi^2_{ij} - \psi^3_{ij}),$$

$$\alpha^{ij}_{i-1,j} = -\frac{\mu}{\delta x^2}(B^3_{ij} + B^4_{ij}),\quad \beta^{ij}_{i-1,j} = \frac{1}{\delta x\delta y}(\psi^3_{ij} - \psi^4_{ij}),$$

$$\alpha^{ij}_{i+1,j} = -\frac{\mu}{\delta x^2}(B^6_{ij} + B^1_{ij}),\quad \beta^{ij}_{i+1,j} = \frac{1}{\delta x\delta y}(\psi^6_{ij} - \psi^1_{ij}),$$

$$\alpha^{ij}_{i-1,j-1} = -\frac{\mu}{\delta y^2}(B^1_{ij} + B^2_{ij}),\quad \beta^{ij}_{i-1,j-1} = \frac{1}{\delta x\delta y}(\psi^1_{ij} - \psi^2_{ij}),$$

$$\alpha^{ij}_{i+1,j+1} = -\frac{\mu}{\delta y^2}(B^4_{ij} + B^5_{ij}),\quad \beta^{ij}_{i+1,j+1} = \frac{1}{\delta x\delta y}(\psi^4_{ij} - \psi^5_{ij}),$$

$$\gamma^{ij}_{i,j-1} = \sigma\int_D \omega_{i,j-1}\omega_{ij}\,dD,\quad \gamma^{ij}_{i,j+1} = \sigma\int_D \omega_{i,j+1}\omega_{ij}\,dD, \tag{4.29}$$

$$\gamma^{ij}_{i-1,j} = \sigma\int_D \omega_{i-1,j}\omega_{ij}\,dD,\quad \gamma^{ij}_{i+1,j} = \sigma\int_D \omega_{i+1,j}\omega_{ij}\,dD,$$

$$\gamma^{ij}_{i+1,j+1} = \sigma\int_D \omega_{i+1,j+1}\omega_{ij}\,dD,\quad \gamma^{ij}_{i-1,j-1} = \sigma\int_D \omega_{i-1,j-1}\omega_{ij}\,dD,$$

$$B^k_{ij} = \int_{T^k_{ij}\cap D} dD,\qquad \psi^k_{ij} = \int_{T^k_{ij}\cap D}\psi\,dD.$$

The set of Eqs.(4.27) approximates the second order differential problem (4.22) with respect to the step of the network. On the strength of (4.28), operator appearing in (4.27) can be represented, as in the case of network operator in section 3.3, as a sum of one-dimensional operators:

$$\Lambda = \Lambda_1 + \Lambda_2 + \Lambda_3, \tag{4.30}$$

where

$$[\Lambda_1\underline{\phi}]_{ij} = \alpha^{ij}_{i,j+1}\phi_{i,j+1} - (\alpha^{ij}_{i,j+1} + \alpha^{ij}_{i,j-1})\phi_{ij} + \alpha^{ij}_{i,j-1}\phi_{i,j-1} +$$

$$+ \gamma^{ij}_{i,j+1}\phi_{i,j+1} + (\gamma^{ij}_{i,j+1} + \gamma^{ij}_{i,j-1})\phi_{ij} + \gamma^{ij}_{i,j-1}\phi_{i,j-1} +$$

$$+ \beta^{ij}_{i,j+1}\phi_{i,j+1} + \beta^{ij}_{i,j-1}\phi_{i,j-1},$$

$$[\Lambda_2\underline{\phi}]_{ij} = \alpha^{ij}_{i+1,j}\phi_{i+1,j} - (\alpha^{ij}_{i+1,j} + \alpha^{ij}_{i-1,j})\phi_{ij} + \alpha^{ij}_{i-1,j}\phi_{i-1,j} +$$

$$+ \gamma^{ij}_{i+1,j}\phi_{i+1,j} + (\gamma^{ij}_{i+1,j} + \gamma^{ij}_{i-1,j})\phi_{ij} + \gamma^{ij}_{i-1,j}\phi_{i-1,j} +$$

$$+ \beta^{ij}_{i+1,j}\phi_{i+1,j} + \beta^{ij}_{i-1,j}\phi_{i-1,j}, \tag{4.31}$$

$$[\Lambda_3\underline{\phi}]_{ij} = \alpha^{ij}_{i+1,j+1}\phi_{i+1,j+1} - (\alpha^{ij}_{i+1,j+1} + \alpha^{ij}_{i-1,j-1})\phi_{ij} +$$

$$+ \alpha^{ij}_{i-1,j-1}\phi_{i-1,j-1} + \gamma^{ij}_{i+1,j+1}\phi_{i+1,j+1} + (\gamma^{ij}_{i+1,j+1} + \gamma^{ij}_{i-1,j-1})\phi_{ij} +$$

$$+ \gamma^{ij}_{i-1,j-1}\phi_{i-1,j-1} + \beta^{ij}_{i+1,j+1}\phi_{i+1,j+1} + \beta^{ij}_{i-1,j-1}\phi_{i-1,j-1}.$$

Analysing the type of coefficients α, β, γ given by relations (4.29) one may note that the following relations are satisfied for them:

$$\alpha^{ij}_{i\pm1,j} = \alpha^{i\pm1,j}_{ij}, \quad \alpha^{ij}_{i,j\pm1} = \alpha^{i,j\pm1}_{ij}; \tag{4.32}$$

$$\beta^{ij}_{i\pm1,j} = -\beta^{i\pm1,j}_{ij}, \quad \beta^{ij}_{i,j\pm1} = -\beta^{i,j\pm1}_{ij},$$

$$\beta^{ij}_{i\pm1,j\pm1} = -\beta^{i\pm1,j\pm1}_{ij}; \tag{4.33}$$

$$\gamma^{ij}_{i\pm1,j} = \gamma^{i\pm1,j}_{ij}, \quad \gamma^{ij}_{i,j\pm1} = \gamma^{i,j\pm1}_{ij},$$

$$\gamma^{ij}_{i\pm1,j\pm1} = \gamma^{i\pm1,\, j\pm1}_{ij}. \tag{4.34}$$

Using (4.32)-(4.34) it can be shown that the operators Λ_1, Λ_2, Λ_3 have positive semi-definiteness in the space of network functions, that is,

$$(\Lambda_1\underline{\phi}, \underline{\phi}) \geqq 0, \quad (\Lambda_2\underline{\phi}, \underline{\phi}) \geqq 0, \quad (\Lambda_3\underline{\phi}, \underline{\phi}) \geqq 0. \tag{4.35}$$

This enables the splitting method to be used for solving (4.27), which (the splitting method) will be absolutely stable. Making use of the bicyclic splitting plan, we finally obtain

$$\kappa\,(\underline{\phi}^{\ell-2/3} - \underline{\phi}^{\ell-1}) + \frac{\tau}{2}\;\Lambda_1\,(\underline{\phi}^{\ell-2/3} + \underline{\phi}^{\ell-1}) = \underline{F},$$

$$\kappa\,(\underline{\phi}^{\ell-1/3} - \underline{\phi}^{\ell-2/3}) + \frac{\tau}{2}\;\Lambda_2\,(\underline{\phi}^{\ell-1/3} + \underline{\phi}^{\ell-2/3}) = 0,$$

$$\kappa\,(\underline{\phi}^{\ell} - \underline{\phi}^{\ell-1/3}) + \frac{\tau}{2}\;\Lambda_3\,(\underline{\phi}^{\ell} + \underline{\phi}^{\ell-1/3}) = 0,$$

$$\kappa\,(\underline{\phi}^{\ell+1/3} - \underline{\phi}^{\ell}) + \frac{\tau}{2}\,\Lambda_3\,(\underline{\phi}^{\ell+1/3} + \underline{\phi}^{\ell}) = 0, \tag{4.36}$$

$$\kappa\,(\underline{\phi}^{\ell+2/3} - \underline{\phi}^{\ell+1/3}) + \frac{\tau}{2}\,\Lambda_2\,(\underline{\phi}^{\ell+2/3} + \underline{\phi}^{\ell+1/3}) = 0,$$

$$\kappa\,(\underline{\phi}^{\ell+1} - \underline{\phi}^{\ell+2/3}) + \frac{\tau}{2}\,\Lambda_1\,(\underline{\phi}^{\ell+1} + \underline{\phi}^{\ell+2/3}) = F.$$

This is realized by performing operations in three directions,including the diagonal direction of the network triangulation.

Figures 8.1 through 8.4 represent isolines of difference analogues of functionals (1.7), (1.8) parametrically dependent on the coordinates $\underline{r}_o$. Figure 8.1 shows the field of isolines of the functional (1.7), calculated by (3.9), in the plane II-type "channel" with the inflow in its right branch being constant in time. For these very conditions the isolines of the functional (1.8) are shown in figure 8.2. Figures 8.3 and 8.4 illustrate the case of a closed two-dimensional reservoir in which the liquid circulates in the clockwise direction with a constant in time velocity. For this case, the isolines of functionals (1.7) and (1.8) are shown in figures 8.3 and 8.4, respectively. The last two figures have been obtained by the method of finite elements. The triangulation for this method is shown in figure 8.5.

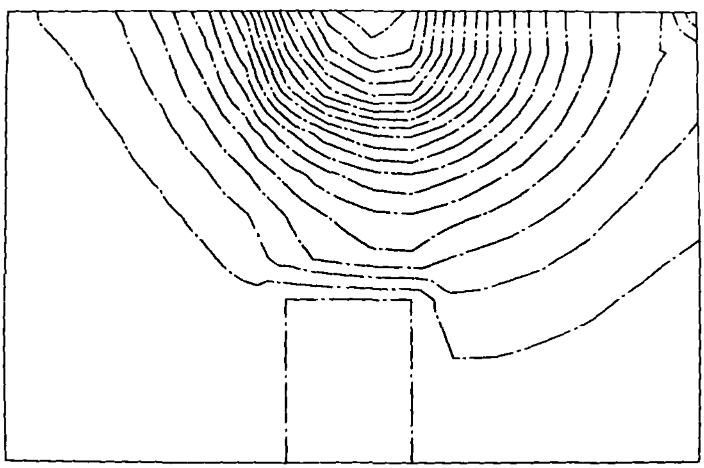


FIGURE 8.1

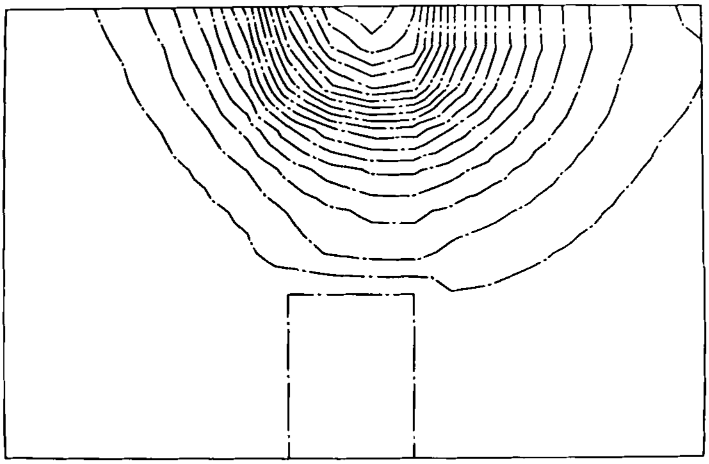


FIGURE 8.2

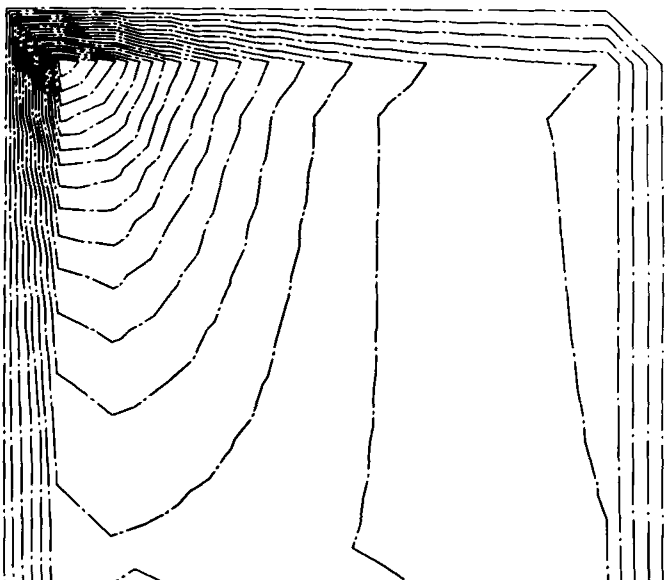


FIGURE 8.3

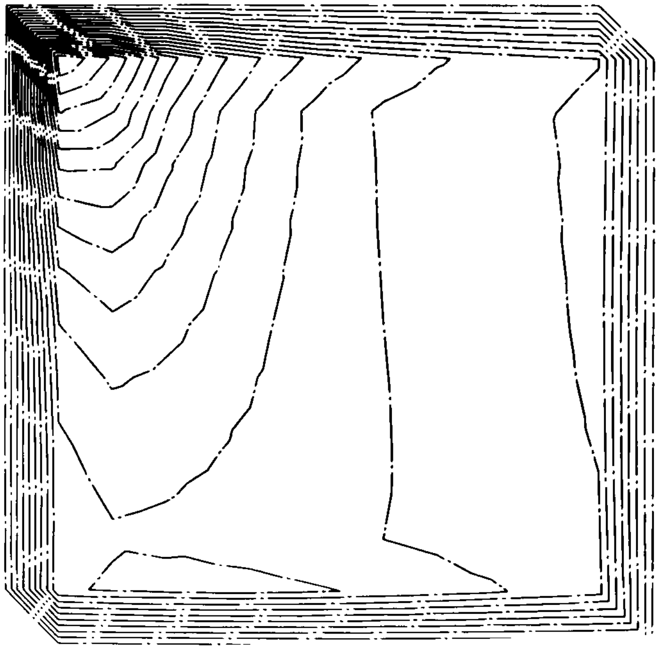


FIGURE 8.4

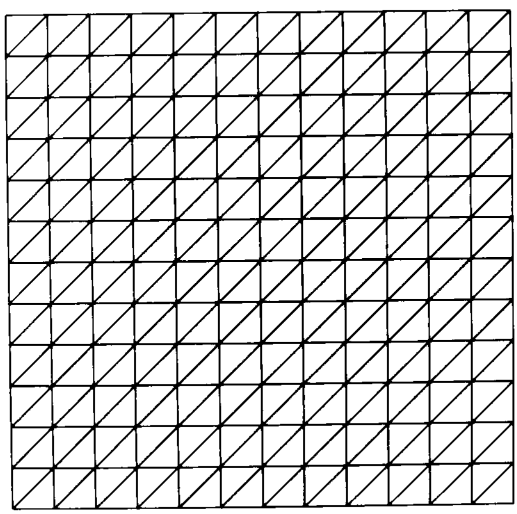


FIGURE 8.5

Lines show equal values of the functional $J_k(\underline{r}_o)$ because the pollution sources located at the points of one and the same line $J_k(\underline{r}_o)$ = const have similar effect on the region G_k. As the industrial waste sources are moved farther away from the region G_k, their pollution effect decreases. Suppose that in the range of determination of solution we have found a surface on which J_k = const = $= C_k$. It implies that within the range $J_k(\underline{r}_o) > C_k$, and outside the range bounded by the given line, $J_k(\underline{r}_o) \leq C_k$. Hence, the sanitary requirements for emissions will be observed with regard to pollution of the water body area G_k.

Now we suppose that there are n ecologically protected zones $D_k(k = \overline{1, n})$, each having its own sanitary requirements. We shall solve n adjoint problems of the type (2.3), (2.4) and obtain n functionals J_k. For every functional we shall have a situation similar to that shown in figures 8.1 through 8.4. The intersection of all the regions ω_k will yield the desired region (if it exists) for which all of the conditions $J_k(\underline{r}_o) \leq C_k(k = \overline{1, n})$ are satisfied. This means that the location of the industrial waste sources in such a zone will simultaneously provide a normal ecological situation in all the water areas $G_1, \ldots, G_n$. If such a zone does not exist, particular requirements must be placed on the production process and the amount of emissions Q should be decreased to a level until the region becomes non-empty.

Let us now consider a problem of finding such a point $\underline{r}_o$ for hydrosols discharge at which the maximum value of J_k for all ecological zones G_k will be minimum. For this we introduce normalized functionals

$$B_k(\underline{r}_o) = \frac{1}{C_k} J_k(\underline{r}_o), \quad k = \overline{1, n},$$

for which the restriction holds

$$B_k(\underline{r}_o) \leq 1.$$

Exact equalities

$$B_k(\underline{r}_o) = 1$$

will hold true and sanitary requirements for the surface be met.

Further, we shall compute $B_k(\underline{r}_o)$ at all the points of the domain of permissible values meeting sanitary requirements for all D_k and find a maximum value for each of them, that is, we shall perform explicit exhaustion of all $B_k(\underline{r}_o)$. Going over from one point $\underline{r}_o$ to another we shall perform explicit exhausion at all the points. As a result, we shall find a point $M(\underline{r}_o)$ at which the maximum component $B_k(\underline{r}_o)$ has a minimum value, and this will be the solution of the minimax problem, that is

$$\max_k B_k(\underline{r}_o) = \min_{\underline{r}_o}, \quad \underline{r}_o \in \sum\nolimits_o, \quad k = 1, 2, \ldots, n.$$

Note that here the minimax problem is solved by the explicit exhaustion method. In this resides the remarkable property of adjoint problems which permit of the most simple realization of the minimax problem. If we had not made use of the adjoint problems, then for solving a minimax problem we had to solve a vast number of problems with different locations of the industrial waste sources. Such a methodology would have hardly provided the required accuracy even with the use of most advanced computers.

Appendix. MESOMETEOROLOGICAL AND MESOOCEANIC PROCESSES

1. Mesometeorological problem of determining local atmospheric circulations

With the growing scale of man's economic activities energy production increases, and so do the amount of heat and impurities discharged into atmosphere. Discharged impurities undergo various transformations and spread over large distances, polluting environment. Environmental pollution with harmful substances depends not only on the technological parameters but also on such meteorological factors as wind velocity, atmospheric stratification, terrain orography, characteristics of the underlying surface, turbulence field and the like. Accordingly, greater emphasis should be placed on the study of meteorological factors of environmental pollution and on the development of appropriate mathematical models.

In most cases the main bulk of contaminants is discharged into the lower atmospheric layers. Then, under the influence of local circulations brought about by large-scale movement due to thermal and orographic inhomogeneity of underlying surface, impurities are lifted to the boundary layer. Hence, construction of mathematical models requires simultaneous solution of atmosphere dynamics and impurity transfer problems. Here we give some examples on the solution of problems of atmosphere dynamics.

We begin with a model for the dynamics of the boundary layer. Accordingly, we consider the system of equations used in mesometeorological problems. The equations are written in left-hand Cartesian system of coordinates x, y, z (x-axis is directed eastward, y - northward, z - vertically upward). For the initial data we take the equation of motion:

$$\frac{du}{dt} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \ell v + \tilde{\Delta} u,$$

$$\frac{dv}{dt} = -\frac{1}{\rho}\frac{\partial p}{\partial y} - \ell u + \tilde{\Delta} v, \tag{1.1}$$

$$\frac{dw}{dt} = -\frac{1}{\rho}\frac{\partial p}{\partial z} - g + \tilde{\Delta} w;$$

the equation of continuity

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} + \frac{1}{\rho}\frac{d\rho}{dt} = 0; \tag{1.2}$$

the equation of state

$$p = \rho RT; \tag{1.3}$$

and the equation of heat influx

$$\frac{d\theta}{dt} = \frac{L_w}{c_p}\Phi + Q_r + \tilde{\Delta}\theta, \tag{1.4}$$

where

$$\theta = T\left(\frac{1000}{p}\right)^{AR/c_p}. \tag{1.5}$$

The operators $d\phi/dt$ and $\tilde{\Delta}p$ are:

$$\frac{d}{dt} = \frac{\partial}{\partial t} + u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y} + w\frac{\partial}{\partial z} = \frac{\partial}{\partial t} + \underline{u}\ \mathrm{grad}, \tag{1.6}$$

$$\tilde{\Lambda} = \frac{\partial}{\partial x}\mu\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\mu\frac{\partial}{\partial y} + \frac{\partial}{\partial z}\nu\frac{\partial}{\partial z}. \tag{1.7}$$

Here, t is time; u, v, w are the components of the wind velocity vector along x, y, z, respectively; T is temperature; θ is potential temperature; p is pressure; ρ is density; R is the universal gas constant; L_w is the latent heat of evaporation; Φ is the rate of liquid phase formation; c_p is specific heat capacity of air at constant pressure; Q_r is the radiative component of heat flow; μ, ν are the horizontal and vertical turbulent exchange coefficients, respectively; A is thermal equivalence of work; g is the acceleration due to gravity.

We do not use Eqs.(1.1)-(1.7) in solving mesometeorological problems as, besides the latter, this system also describes large-scale meteorological processes, acoustic waves, etc. On the other hand, all terms in the equations are not of the same order of magnitude; therefore, in solving specific mesometeorological problems the system can be simplified by neglecting small terms. By way of example, consider linearization of nonlinear terms of the type $\frac{1}{\rho}$ grad p. For this purpose, introduce a new function

$$\pi = \frac{c_p\Theta_o}{A}\left(\frac{p}{1000}\right)^{AR/c_p} = \frac{c_p\Theta_o}{A\Theta}T, \tag{1.8}$$

where Θ_o is the mean potential temperature. Using the equation of state, definitions of potential temperature and function π, we obtain

$$-\frac{1}{\rho}\,\text{grad}\ p = -\frac{\theta}{\Theta_o}\,\text{grad}\ \pi. \tag{1.9}$$

Since we are interested in mesoprocesses in which horizontal scales considerably exceed the vertical ones, the terms containing w in the third equation of motion (1.1) is small compared with the other two terms. In this case, the third equation in (1.1) is considerably simplified and we obtain the equation of statics

$$\frac{\partial \pi}{\partial z} = \lambda\theta. \tag{1.10}$$

After these simplifications and since in (1.9) $\theta/\Theta_o = (\Theta + \theta')/\Theta_o \cong 1$ as $\theta'/\Theta_o \ll 1$, the system (1.1) can be expressed as

$$\begin{aligned}
\frac{du}{dt} &= -\frac{\partial \pi}{\partial x} + \ell v + \tilde{\Delta} u,\\
\frac{dv}{dt} &= -\frac{\partial \pi}{\partial y} - \ell u + \tilde{\Delta} v,\\
\frac{\partial \pi}{\partial z} &= \lambda\theta.
\end{aligned} \tag{1.11}$$

Assuming the space-time variations of ρ to be small we write the equation of continuity (1.2) as

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0. \tag{1.12}$$

For the sake of simplicity, we can also neglect the influence of radiative heat flow into the atmospheric boundary layer.

In nature meso- and large-scale processes always interact. But the influence of large-scale circulation on mesoscale one is the most important in the mesometeorological theory.

To obtain a consistent system of boundary layer equations, we represent the meteorological fields as

$$\begin{aligned}
u = U + u', \quad v = V + v', \quad w = W + w', \quad \theta = \Theta + \theta',\\
\pi = \Pi + \pi', \quad p = P + p',
\end{aligned} \tag{1.13}$$

where capital letters denote background large-scale components of meteorological fields, and letters with prime denote deviations. Substituting (1.13) into (1.10)-(1.12), and neglecting small quantities which arise on the assumption that

$$p' \ll P, \quad \theta' \ll \Theta, \quad \pi' \ll \Pi, \quad |\Theta - \Theta_o| \ll \Theta_o, \tag{1.14}$$

and taking into account appropriate equations for background fields, we obtain the required system of mesometeorology equations. There are different ways of defining background fields. To construct the perturbation equations, it is necessary that the background fields satisfy the initial system to small terms.

Let us now consider a spatial nonstationary numerical model of an atmospheric boundary layer over orographically and thermally inhomogeneous surface based on a system of perturbation equations. We formally divide the atmosphere into two layers: the constant-flux layer and upper layer. The constant-flux layer is expressed in a parametrized form. We supplement the initial system with an equation for specific humidity:

$$\frac{\partial u'}{\partial t} + \operatorname{div} \underline{u}u' = -\frac{\partial \pi'}{\partial x} + \ell v' + \lambda\delta_x\theta' + \frac{\partial}{\partial z}\nu_u\frac{\partial u'}{\partial z} + \Delta u'; \tag{1.15}$$

$$\frac{\partial v'}{\partial t} + \operatorname{div} \underline{u}v' = -\frac{\partial \pi'}{\partial y} - \ell u' + \lambda\delta_y\theta' + \frac{\partial}{\partial z}\nu_u\frac{\partial v'}{\partial z} + \Delta v'; \tag{1.16}$$

$$\frac{\partial \pi'}{\partial z} = \lambda\theta'; \tag{1.17}$$

$$\frac{\partial \theta'}{\partial t} + \operatorname{div} \underline{u}\theta' + Sw' = -u'(S\delta_x + \boldsymbol{\theta}_x) - v'(S\delta_y + \boldsymbol{\theta}_y) + \frac{\partial}{\partial z}\nu_\theta\frac{\partial \theta'}{\partial z} + \Delta\theta + \frac{L_w}{c_p}\Phi + Q_r; \tag{1.18}$$

$$\frac{\partial u'}{\partial x} + \frac{\partial v'}{\partial y} + \frac{\partial w'}{\partial z} = 0, \qquad q = Q + q'; \tag{1.19}$$

$$\frac{\partial q'}{\partial t} + \operatorname{div} \underline{u}q' = -\frac{\partial Q}{\partial z}(w' + u'\delta_x + v'\delta_y) - uQ_x - vQ_y + \frac{\partial}{\partial z}\nu_\theta\frac{\partial q'}{\partial z} + \Delta q' - \Phi; \tag{1.20}$$

$$u = U + u', \quad v = V + v', \quad w = W + w', \quad \theta = \boldsymbol{\Theta} + \theta', \quad \pi = \Pi + \pi'; \tag{1.21}$$

here

$$\Delta = \frac{\partial}{\partial x}\mu_1\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\mu_2\frac{\partial}{\partial y};$$

x, y, z are curvilinear coordinates mutually orthogonal along the relief, $z = z_i - \delta(x, y)z_i$ is the height above the sea level; the equation $z_i = \delta(x, y)$ describes the relief; $\underline{u}$ is the wind vector; λ, S are convection and stratification parameters; μ_1, μ_2 are horizontal turbulence coefficients; ν_u, ν_θ are vertical turbulence coefficients for momentum and heat; q is the specific humidity; u', v', w', θ', q', π' are deviations from the respective background values; $\boldsymbol{\theta}_x$, $\boldsymbol{\theta}_y$ and Q_x, Q_y are horizontal gradients of the background potential temperature and the background specific humidity. To describe the constant-flux layer structure, we employ the Monin-Obukhov similarity theory and *Businger* empirical functions. To approximate the elevation profiles of meteorological fields in the constant-flux layer under strong instability, we use the "$\frac{1}{3}$ - law" and under str-ng stability - linear law. Then, the constant-flux layer model can be expressed by the following equations:

$$\kappa z \frac{\partial|\underline{u}|}{\partial z} = u_*\phi_u(\xi), \quad z\frac{\partial p}{\partial z} = p_*\phi_\theta(\xi), \quad P = \theta,\ q; \tag{1.22}$$

$$\kappa|\underline{u}| = u_*f_u(\xi,\ \xi_u), \ p - p_o = p_*f_\theta(\xi,\ \xi_o), \ \xi = z/L; \tag{1.23}$$

$$\nu_i = \frac{u_*\kappa z}{\phi_i(\xi)}, \quad (\nu_i)_h = \frac{u_*\kappa h}{\phi_i(\xi_h)}, \quad i = u,\ \theta,$$

$$\xi_h = \frac{h}{L}, \quad L = \frac{u_*^2}{\lambda\kappa^2\theta_*}; \tag{1.24}$$

$$H_o = \rho c_p\left(\nu_\theta\frac{\partial\theta}{\partial z}\right)_o = \rho c_p c_u c_v\ |\underline{u}|_h\ (\theta_h - \theta_o); \tag{1.25}$$

$$c_u = \frac{\kappa}{f_u(\xi_h,\xi_u)}, \quad c_\theta = \frac{\kappa}{f_\theta(\xi_h,\xi_o)}, \quad \xi_u = \frac{\xi_h}{H}, \quad \xi_o = \frac{\xi_h}{HZ}, \ H = \frac{h}{z_u},$$

$$Z = \frac{z_u}{z_\theta}; \tag{1.26}$$

$$f_u(\xi,\ \xi_u) = \int_{\xi_u}^{\xi}\frac{\phi_u(\xi)}{\xi}d\xi, \quad f_\theta(\xi,\ \xi_o) = \int_{\xi_o}^{\xi}\frac{\phi_\theta(\xi)}{\xi}d\xi; \tag{1.27}$$

here, $|\underline{u}| = (u^2 + v^2)^{\frac{1}{2}}$ is the modulus of the velocity vector; u_* is friction rate; θ_*, q_* are the scales of potential temperature and specific humidity; h is the constant-flux layer height; κ is the *Karman* constant; z_u, z_v are roughness parameters for wind and temperature (indices 0 and h denote meteorological fields at z = 0 and z = h, respectively); H_o is the heat flux; c_u, c_θ are friction and heat transfer coefficients, respectively; ϕ_i, f_i are continuous universal functions.

Numerically, the problem (1.15)-(1.21) is solved as follows. The constant-flux layer is included into the model in such a manner that we have only to vary the way of assigning the conditions for z=h, leaving the algorithm unchanged.For this purpose, we transform the Eqs.(1.22)-(1.27) so that they yield the respective conditions for z = h.

Finally, the boundary conditions for the system (1.15)-(1.21) take the following form:

$$u' = 0, \quad v' = 0, \quad q' = 0, \quad \theta' = 0 \quad \text{for } t = 0; \tag{1.28}$$

$$\frac{\partial u'}{\partial x} = 0, \quad \frac{\partial v'}{\partial x} = 0, \quad \frac{\partial \theta'}{\partial x} = 0, \quad \frac{\partial q'}{\partial x} = 0 \quad \text{for } x = \pm X; \tag{1.29}$$

$$\frac{\partial u'}{\partial y} = 0, \quad \frac{\partial v'}{\partial y} = 0, \quad \frac{\partial \theta'}{\partial y} = 0, \quad \frac{\partial q'}{\partial y} = 0 \quad \text{for } y = \pm Y \tag{1.30}$$

$$u' = 0, \quad v' = 0, \quad \theta' = 0, \quad q' = 0, \quad w' = 0 \quad \text{for } z = H; \tag{1.31}$$

$$w = 0, \quad h\frac{\partial \underline{u}}{\partial z} = a_u \underline{u}, \quad h\frac{\partial p}{\partial z} = a_\theta (p - p_o) \quad \text{for } z = h; \tag{1.32}$$

here $\underline{u} = (u, v)$; $\varepsilon_i = \phi_i(\xi_h)/f_i(\xi_h, \xi_o)$, $i = u, \theta$; H is the conventional height of atmospheric boundary layer; X, Y are lateral boundaries of the domain under consideration.

Conditions (1.29), (1.30) provide a way for completing the problem. They express the requirement for the disturbance to be smooth in the vicinity of the domain boundary to a greater extent, than the physical meaning of the simulated processes. Therefore, along with (1.29), (1.30) we consider the conditions that allow the processes occurring within the domain D to tend to the background flow mode. These conditions can be written as follows:

$$\begin{gathered} u = U_\phi, \quad v = V_\phi, \quad \theta = \Theta_\phi, \\ q = Q_\phi, \quad x = \pm X, \quad y = \pm Y. \end{gathered} \tag{1.33}$$

Over water, the functions θ_o, and q_o are supposed to be given

$$\theta_o = f_o(t), \qquad q_o = 0{,}622 E_o(\theta_o)/p, \tag{1.34}$$

where E_o is the resilience of water vapor saturation at temperature θ_o; p is atmospheric pressure; $f_o(t)$ is water surface temperature assumed to be a known function of the horizontal coordinates and time. Land temperature is found from the heat balance equation, and the function q_o is computed by formula

$$q_o = 0{,}622\,\eta_o E_o(\theta_o)/p, \tag{1.35}$$

where η_o is relative humidity assumed to be a known function of x, y, t. The heat balance condition at the atmosphere-soil interface is of the form

$$G_S - \rho c_p \left(\nu_\theta \frac{\partial \theta}{\partial z}\right)_o - a_\Gamma \rho L_w \left(\nu_\theta \frac{\partial q}{\partial z}\right)_o = I_o(1 - A_S) + I_S - F_S, \tag{1.36}$$

where $G_S = \lambda_S (\partial T/\partial z)_S$ is heat transfer through soil surface (subscript S shows that the values are taken for z = 0); $\lambda_S = c_S \rho_S K_S$; ρ_S, c_S, K_S, T are density, specific heat, temperature conductivity coefficient and absolute soil temperature;

ρ is atmospheric density; I_o is solar short-wave radiation, A_S is the subsurface albedo; F_S is the effective long-wave radiation; a_r is a dimensionless coefficient which accounts for different amount of heat spent on evaporation (condensation) at different points of the underlying surface due to surface non-uniformity; I_S (x, y, t) is a function which describes the flow of heat released during energy production and consumption.

The models of hydrometeorological regime over industrial regions do not take account of artificial heat flows. This is still an open question. Heat can be released into atmosphere either in real or latent form, hence there are different ways of parametrization of heat release. In particular, artificial heat flow can be accounted for by adding it to the radiative heat flow.

Under calm conditions, the temperature drop between the levels $z = 0$ and $z = z_\theta$ may be quite high. Hence, in solving (1.36), semi-empirical parametrization is used for viscous sublayer:

$$\theta - \theta_o = 0{,}0962\theta_*(u_* z_\theta/\nu)^{0{,}45}, \tag{1.37}$$

where ν is the climatic viscosity factor.

The soil temperature distribution is described by the equation

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial \xi} K_S \frac{\partial T}{\partial \xi}, \tag{1.38}$$

where $K_S = K_S(x, y, z)$ is the soil temperature conductivity coefficient which is considered to be given.

Equation (1.36) is the boundary condition for (1.38) for $z = 0$. We give the second boundary condition for (1.38) at a small depth H_Π and assume that diurnal temperature fluctuation decay, i.e.

$$T = T_\Pi \quad \text{at} \quad z = -H_\Pi. \tag{1.39}$$

To determine the heat flow into soil as a function of T_S, we approximate G_S as follows:

$$G_S = \lambda_S(T_S - T_1)/\Delta\xi_1, \tag{1.40}$$

where $\Delta\xi_1$ is the grid step with respect to depth, T_1 is soil temperature at the first level.

To solve (1.38), let us construct its finite-difference analogue and employ the triangle factorization technique. Omitting the untermediate formulas, we represent solution in the form

$$T_1 = \beta_1 T_S + z_1, \tag{1.41}$$

where β_1 and z_1 are parameters triangle factorization technique. Substituting

(1.41) into (1.40) we obtain

$$G_S = \frac{\lambda_S(1-\beta_1)T_S - \lambda_S z_1}{\Delta\xi_1}. \tag{1.42}$$

By virtue of (1.37), (1.42) we can write the solution of (1.36) as

$$\theta_o = \frac{\bar{\theta}_o + cF\theta_h}{1 + cF}, \tag{1.43}$$

where

$$F = \left(A + L_w + 4\left(\frac{F_S}{T_S}\right)^{j-1} - \lambda_S(\beta_1 - 1)\right)^{-1},$$

$$A = \rho c_u c_\theta |\underline{u}|_h, \quad \mu = \eta_o\left(\frac{dE_o(\theta_o)}{d\theta_o}\right)^{j-1},$$

$$c = Ac_p + \left(4\left(\frac{F_S}{T_S}\right)^{j-1} - \frac{\lambda_S\theta_o^{j-1}(\beta-1)}{\Delta\xi_1}\right)\frac{0{,}0962\ c_\theta(c_u|\underline{u}|_h z_\theta/\nu)^{0{,}45}}{\kappa},$$

$$\bar{\theta}_o = \theta_o^{j-1} + F[I_o(1 - A_S) - F_S^{j-1} + \lambda_S\theta_S^{j-1}(1 - \beta_1)/\Delta\xi_1 + \lambda_S z_1/\Delta\xi_1] +$$

$$+ I_S + a_\Gamma AFL_w(q_h - q_o^{j-1}) + a_\Gamma A\mu F(\theta_o - \theta_S)^{j-1}.$$

Knowing θ_o from (1.37), we can determine θ_S. To calculate the near-ground characteristics the following empirical formulas are used.

Albrecht formula:

$$I_o = a_o \sin h_c - b_o\sqrt{\sin h_c},$$

$$I_o \geqq 0; \ \sin h_c = \sin\phi \sin\psi - \cos\alpha \cos\psi \cos\Omega; \tag{1.44}$$

$$\Omega = (t - 12)\ \pi/12;$$

h_c is sun's zenith angle; ϕ is the latitude; Ω is sun's hour angle; ψ is sun's declination; a_o = 2 cal/(sq·cm·min); b_o = 0.3 cal/(sq · cm·min); (t is reckoned by local time in hours, starting from midnight);

Brent formula:

$$F_S = \sigma f_c T_o(a_e - b_e\sqrt{e}), \tag{1.45}$$

where σ is the Stefan-Boltzmann constant; f_c is soil albedo; a_e, b_e are empirical constants; e is water vapor resilience; and the Charnok formula for determining roughness parameter over water:

$$z_o = 0{,}035\ u_*^2/g. \tag{1.46}$$

It must be noted that the *Albrecht formula* is suitable for calculating solar radiation flux for a flat terrain. It is well known that the ground temperature and aggregate evaporation of wet surface depend on the active surface insolation. Consequently, the differences in insolation of slopes, depending on their exposition, may, under rough terrain, lead to significant mesometeorological contrasts. Therefore, we write the formula for calculating solar radiation from slope surface as

$$S_h = S_o \cos \alpha, \tag{1.47}$$

where $\cos \alpha = \sin h_c \cos \alpha_r + \cos \psi_a (\sin \phi \cos \psi \cos \Omega - \sin \psi \cos \psi_a \cos \psi) \sin \alpha_r + \sin \psi \cos \psi \sin \Omega \sin \alpha_r$; S_o is the solar constant; α_r is angle of incidence of sun rays on surface; ψ_a is azimuth of the projection of normal on horizontal surface reckoned from the meridian plane (ψ_a is positive in reckoning from the south clockwise). The functions α_r and ψ_a are calculated as follows:

$$\alpha_\Gamma = \operatorname{arctg} [(\delta_x^2 + \delta_y^2)^{\frac{1}{2}}], \quad \psi_a = \operatorname{arctg} (\delta_x/\delta_y) + k\pi. \tag{1.48}$$

The value of the parameter k varies depending on the orientation of the slope.

By analogy with (1.44), we write a formula for S_r—the total radiation flow to the slope:

$$S_\Gamma = a_o \cos \alpha - b_o \sqrt{\cos \alpha}. \tag{1.49}$$

It can easily be seen that for $\alpha_\Gamma = 0$, formulas (1.44) and (1.49) coincide. Exact calculation of diffuse radiation is more difficult due to anisotropy. Diffuse radiation flux from different sections of the heavenly dome depends on the Sun position.

Figure A.1 illustrates diurnal variation of S_Γ, calculated by (1.49) and that of the total heat S_Σ received by the slope since sunrise. The following values are used for parameters:

$$\phi = 42.5°, \quad \psi = 11°, \quad \alpha_\Gamma = 10°, \quad a_o = 2 \text{ cal/(sq·cm·min)},$$

$$b_o = 0.3 \text{ cal/(sq·cm·min)}.$$

It is clear from the figure that the southern slope receives much more heat than the northern one. For $\alpha_\Gamma = 0$, the curves fuse into one curve. For a specific region with complex terrain, the values of a_o and b_o must be found experimentally.

The systems (1.15)-(1.20) and (1.28)-(1.32) are not closed as the vertical turbulence exchange coefficients ν_h and ν_θ are unknown. To determine them, consider the turbulent energy equation

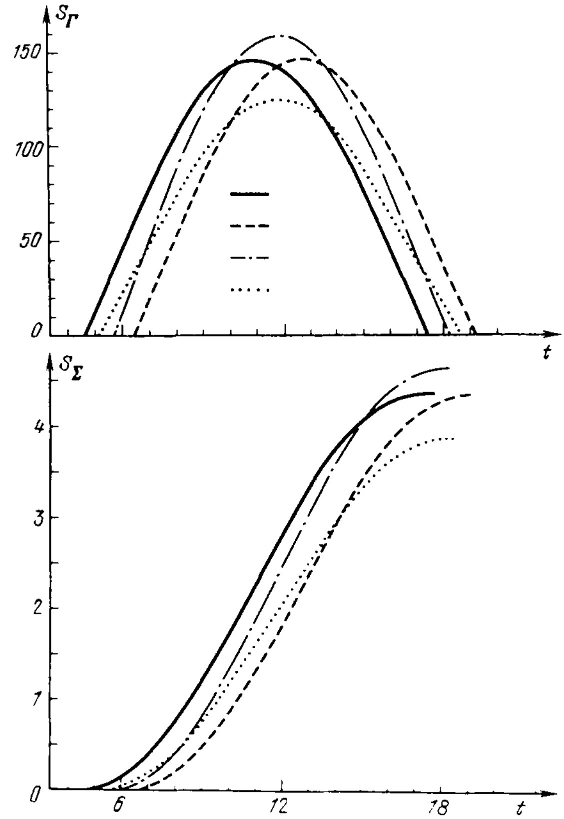


FIGURE A.1

$$\frac{\partial b}{\partial t} + \underline{u} \text{ grad } b = \nu_u \left\{ \left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2 - \alpha_\Gamma \lambda \frac{\partial \theta'}{\partial z} - \alpha_\Gamma \lambda S \right\} + \\ + \alpha_b \frac{\partial}{\partial z} \nu_u \frac{\partial bcb^2}{\partial z \nu_u} , \tag{1.50}$$

where $\alpha_\Gamma = \nu_\theta/\nu_u = \phi_u(\xi)/\phi_\theta(\xi)$; α_b and c are dimensionless universal constants. To determine the turbulence characteristics, we use the Kolmogorov approximate similarity hypothesis which implies that the turbulent exchange coefficients ν_u and the rate of turbulent energy dissipation into heat ε are uniquely expressed in terms of turbulence kinetic energy b and turbulence scale ℓ:

$$\nu_u = c\ell b^{\frac{1}{2}}, \quad \varepsilon = cb^2/\nu_\theta . \tag{1.51}$$

The turbulence scale is computed by the Karman generalized formula for displacement path:

$$\ell = -\kappa\psi \frac{\partial\psi}{\partial z}, \quad \psi = \frac{b^{\frac{1}{2}}}{\ell} . \tag{1.52}$$

Let us now formulate the boundary conditions for the system (1.50)-(1.52). As is known, meteorological fields near the underlying surface can have steep gradients, and to describe them the numerical models need high vertical resolution. Hence, direct inclusion of (1.50)-(1.52) into spatial models it rather difficult due to limited computer capabilities. Therefore, we use (1.22)-(1.27) and (1.51), (1.52) to derive parametrization formula for the function b in the near-ground atmospheric layer.

First, consider parametrization of the mean kinetic energy of turbulent fluctuations $b_u^2 = (\overline{u'u'} + \overline{v'v'} + \overline{w'w'})/2$ (u', v', w' - fluctuations of wind velocity components; bar above denotes averaging; $b_u = -\sqrt{b}$) in the near-ground atmospheric layer. The value of b_u^2 for $z = h$ can serve as a boundary condition for the equation of turbulence energy in the domain above the ground layer. Express the system (1.51), (1.52) to the form

$$\frac{\partial b_u}{\partial z} - f_u b_u + g_u b_u^2 = 0, \tag{1.53}$$

where

$$f_u = \frac{1}{2\nu_u} \frac{\partial \nu_u}{\partial z}, \quad g_u = \frac{\kappa c}{2\nu_u} . \tag{1.54}$$

If f_u and g_u are known functions of height, then we find b_u from (1.53), taking no energy flow at roughness level as the boundary condition, i.e.

$$\frac{\partial b_u^2}{\partial z} = 2b_u \left(\frac{\partial b_u}{\partial z}\right) = 0 \quad \text{for } z = z_o$$

Assuming that $b_u \neq 0$ for $z = z_o$ and using (1.53), we finally obtain

$$b_u = f_u/g_u \qquad \text{for } \quad z = z_o \tag{1.55}$$

It is apparent from (1.24) and (1.53), (1.54) that the functions f_u, g_u and b_u parametrically depend on u_* and L. To make further presentation convenient, we pass to dimensionless variables

$$\tilde{b} = \frac{cb_u}{u_*}, \quad \nu = \frac{\nu_u}{\kappa u_* L} = \frac{\xi}{\phi(\xi)} ,$$

$$f = Lf_u = \frac{1}{2} \frac{\partial \ln\nu}{\partial\xi} = \frac{1}{2\xi} - \frac{1}{2} \frac{\partial \ln\phi(\xi)}{\partial\xi} , \tag{1.56}$$

$$g = \frac{u_*L}{c} \qquad g_u = \frac{1}{2\nu} = \frac{\phi(\xi)}{2\xi}$$

and rewrite (1.53)-(1.55) as

$$\frac{\partial\tilde{b}}{\partial z} - \tilde{b}f + g\tilde{b}^2 = 0, \tag{1.57}$$

where $b = f/g$ for $\xi = \xi_o$ $(\xi_o = z_o/L)$.

On substituting $y = \tilde{b}^{-1}$ into (1.57), the latter is reduced to a first-order linear differential equation whose solution is

$$y = \tilde{b}(\xi, \xi_o)^{-1} = \exp\left[-\int_{\xi_o}^{\xi} f(\xi)\, d\xi \left(\frac{g(\xi_o)}{f(\xi_o)} + \int_{\xi_o}^{\xi} g(\xi') \exp \cdot \right.\right.$$
$$\left.\left. \cdot \left[\int_{\xi_o}^{\xi'} f(\xi'')\, d\xi''\right] d\xi'\right)\right]. \tag{1.58}$$

Substituting (1.56) into (1.58) and putting $z = h$, we obtain

$$\tilde{b}(\xi_h, \xi_o)^{-1} = \Phi(\xi_h, \xi_o) + \sqrt{\frac{\phi(\xi_h)}{4|\xi_h|}} \int_{|\xi_o|}^{|\xi_h|} \sqrt{\frac{\phi(\xi)}{|\xi|}}\, d|\xi|, \tag{1.59}$$

where

$$\Phi(\xi, \xi_o) = \frac{\sqrt{\phi(\xi)\phi(\xi_o)^3}}{\sqrt{\frac{\xi}{\xi_o}}\, \phi(\xi_o) - \xi_o\left[\frac{\partial\phi(\xi)}{\partial\xi}\right]_{\xi=\xi_o}}, \tag{1.60}$$

$\xi_h = h/L$, $\xi_o = \xi_h/H$, $H = h/z_o$.

In deriving (1.59) we have taken that the function ϕ is always positive and ξ changes its sign, depending on stratification. Note that ξ_o is no longer an independent variable, hence, the functions actually depend on ξ_h and H, though ξ_o is still retained.

Specific expressions for $\phi(\xi)$, found from experimental data and asymptotic laws of the similarity theory, as well as the functions $\Phi(\xi, \xi_o)$ determined from (1.60) are listed in table A.1 where

$$\begin{aligned} \eta(x) &= (1 - \gamma x)^{-1/4}, \quad & \xi(x) &= \eta(\xi')(\xi'/x)^{1/3}, \\ \delta(x) &= (1 + \beta x)^{1/2}, \quad & \sigma(x) &= [(1/\xi'' + \beta)x]^{1/2}, \end{aligned} \tag{1.61}$$

and ν, ξ', ξ'', β are empirical constants.

TABLE A.1

Functions	Instability		Stability	
	strong	weak	stong	weak
$\phi(\xi)$	$\xi''H \leq \xi \leq \xi''$	$\xi' \leq \xi \leq 0$	$0 \leq \xi \leq \xi''$	$\xi'' \leq \xi \leq \xi'H$
	$\xi(\xi)$	$\eta(\xi)$	$\delta^2(\xi)$	$\sigma^2(\xi)$
$\sqrt{\frac{\xi}{\xi_o}}\,\Phi(\xi,\ \xi_o)$	$\frac{4\sqrt{\xi(\xi)\eta(\xi_o)}}{5-\eta^4(\xi_o)}$	$\frac{4\sqrt{\eta(\xi)\eta(\xi_o)}}{5-\eta^4(\xi_o)}$	$\delta(\xi)\delta^3(\xi_o)$	$\sigma(\xi)\delta^3(\xi_o)$

Since ξ_h varies in the interval $H\xi' \leq \xi_h \leq \xi''$, then from $\xi_o = \xi_h/H$ it follows that $\xi' \leq \xi_o \leq \xi''$. Therefore, the expression for $\Phi(\xi,\xi_o)$ contains only $\eta(\xi_o)$ and $\delta(\xi_o)$. Substituting $\phi(\xi)$ and $\Phi(\xi,\ \xi_o)$ from table A.1 into (1.59) we obtain the expressions for $\tilde{b}(\xi_h,\ \xi_o)$ in different ranges of ξ_h. Thus, for stable stratification in the interval $0 \leq \xi_h \leq \xi''$, we have

$$\tilde{b}(\xi_h,\ \xi_o)^{-1} = \Phi(\xi_h,\xi_o) + \frac{\delta(\xi_h)}{2} - \frac{\delta(\xi_h)\delta(\xi_o)}{\sqrt{4H}} + \frac{\delta(\xi_h)}{\sqrt{4\beta\xi_h}}\,[A(\xi_h) - A(\xi_o)], \quad (1.62)$$

where $A(x) = \ln[\sqrt{\beta x} + \delta(x)]$. It is easy to demonstrate that

$$\lim_{x\to 0} \frac{\delta(x)}{\sqrt{\beta x}}\,[\,A(x) - A\,\frac{x}{H}\,] = 1 - \frac{1}{\sqrt{H}}\,.$$

Then from table A.1 and (1.22)-(1.24), (1.56), (1.57), (1.62), as $\xi_h \to 0$ it follows that $b = 1$ ($b_u = u_*/c$), $\ell = \varkappa z$, corresponding to neutral stratification.

In a similar manner, the strong stability range $\xi'' \leq \xi_n \leq \xi''$ we obtain

$$\tilde{b}(\xi_h,\ \xi_o)^{-1} = \Phi(\xi_h,\ \xi_o) + \frac{\delta(\xi'')\xi_h}{2\xi''} - \frac{\delta(\xi'')\delta(\xi_o)\xi_h^{1/2}}{\sqrt{4\xi''H}} + \\ + \frac{\delta(\xi'')}{\sqrt{4\beta\xi''}}\,[A(\xi'') - A(\xi_o)], \quad (1.63)$$

which, for $\xi_h = \xi''$ coincides with (1.62).

Under stable stratification, solution in the interval $\xi' \leq \xi_h \leq 0$ can be represented as

$$b(\xi_h,\ \xi_o)^{-1} = \Phi(\xi_h,\ \xi_o) + \sqrt{\frac{\eta(\xi_h)}{-4\xi_h}}\,[I(-\xi_h) - I(-\xi_o)], \quad (1.64)$$

where

$$I(x) = \int_0^x \sqrt{\frac{\eta(-t)}{t}}\, dt, \quad 0 \leq x \leq |\xi'|, \; |\xi| = -\xi.$$

The integrals I(x) are calculated approximately.

In the strong instability range, we have

$$\tilde{b}(\xi_h, \xi_o)^{-1} = \Phi(\xi_h, \xi_o) + \sqrt{\frac{\xi(\xi_h)}{-4\xi_h}} \left[\int_{|\xi_o|}^{|\xi'|} \sqrt{\frac{\eta(-\xi)}{|\xi|}}\, d|\xi| + \right.$$

$$\left. + \int_{|\xi|}^{|\xi_h|} \sqrt{\frac{-\xi(|\xi|)}{|\xi|}}\, d|\xi| \right] = \Phi(\xi_h, \xi_o) + \tag{1.65}$$

$$+ \sqrt{\frac{\xi(\xi_h)}{-4\xi_h}} [\tilde{c} - I - (\xi_o)] + \frac{3\xi(\xi_h)}{2} - \frac{3\xi(\xi_h)}{2} \left(\frac{\xi'}{\xi_h}\right)^{1/3},$$

where $\tilde{c} = I(-\xi') \cong 3.955$.

Thus, for different stratifications we obtain boundary conditions for the functions b_u at the upper boundary of the near-ground layer (z = h). This approach is useful in solving the turbulent energy equation in a space model with grids of rather rough vertical resolution. Using (1.62)-(1.65), we can write the boundary condition for the problem (1.50)-(1.52) as

$$b = 0 \quad \text{for} \quad t = 0; \tag{1.66}$$

$$b = \tilde{b}_u^2(\xi_h, \xi_o) \quad \text{for} \quad z = h; \tag{1.67}$$

$$\frac{\partial b}{\partial z} = 0 \quad \text{for} \quad z = H; \tag{1.68}$$

$$\frac{\partial b}{\partial x} = 0 \quad \text{for} \quad z = \pm X; \tag{1.69}$$

$$\frac{\partial b}{\partial y} = 0 \quad \text{for} \quad y = \pm Y. \tag{1.70}$$

Note that boundary condition (1.68) holds for a stable stratified atmosphere. For unstable stratification this condition takes a different form.

We solve system (1.15)-(1.21), (1.28)-(1.32) by splitting with respect to physical processes. We shall represent the solution on time step $t^i \leq t < t^{j+1}$ as a sequence of two more simple problems:

1. Transport of matter along trajectories and turbulent exchange (regardless of humidity):

$$\frac{\partial u'}{\partial t} + \operatorname{div} \underline{u}u - \Delta u' - \frac{\partial}{\partial z} \nu_u \frac{\partial u'}{\partial z} - \lambda \delta_x \theta' = 0; \tag{1.71}$$

$$\frac{\partial v'}{\partial t} + \text{div}\ \underline{u}v' - \Delta u - \frac{\partial}{\partial z}\nu_u \frac{\partial v}{\partial z} - \lambda\delta_y \theta' = 0; \qquad (1.72)$$

$$\frac{\partial \theta'}{\partial t} + \text{div}\ \underline{u}\theta' - \Delta\theta' - \frac{\partial}{\partial z}\nu_\theta \frac{\partial \theta'}{\partial z} + u'(S\delta_x + \theta_x) + v'(S\delta_y + \theta_y) = 0. \quad (1.73)$$

System (1.71)-(1.73) is solved under the following boundary conditions:

$$\frac{\partial u'}{\partial x} = 0, \quad \frac{\partial v'}{\partial x} = 0, \quad \frac{\partial \theta'}{\partial x} = 0, \quad x = \pm X; \qquad (1.74)$$

$$\frac{\partial u'}{\partial y} = 0, \quad \frac{\partial v'}{\partial y} = 0, \quad \frac{\partial \theta'}{\partial y} = 0, \quad y = \pm Y; \qquad (1.75)$$

$$u' = 0, \quad v' = 0, \quad \theta' = 0, \quad w' = 0, \quad z = H; \qquad (1.76)$$

$$h\frac{\partial u}{\partial z} = a_u u, \quad h\frac{\partial v}{\partial z} = a_v v, \quad h\frac{\partial \theta'}{\partial z} = a_\theta(\theta - \theta_o), \quad z = h. \ (1.77)$$

2. Matching of mesometeorological fields:

$$\frac{\partial u'}{\partial t} - \ell v' = -\frac{\partial \pi'}{\partial x}; \qquad (1.78)$$

$$\frac{\partial v'}{\partial t} + \ell u' = -\frac{\partial \pi'}{\partial y}; \qquad (1.79)$$

$$\frac{\partial \theta'}{\partial t} + Sw' = 0; \qquad (1.80)$$

$$\frac{\partial \pi'}{\partial z} = \lambda\theta'; \qquad (1.81)$$

$$\frac{\partial u'}{\partial x} + \frac{\partial v'}{\partial y} + \frac{\partial w'}{\partial z} = 0 \qquad (1.82)$$

under the boundary conditions

$$\frac{\partial u'}{\partial x} = 0, \quad \frac{\partial v'}{\partial x} = 0 \quad \text{for} \quad x = \pm X; \qquad (1.83)$$

$$\frac{\partial v'}{\partial y} = 0, \quad \frac{\partial v'}{\partial y} = 0 \quad \text{for} \quad y = \pm Y; \qquad (1.84)$$

$$w = 0 \quad \text{for} \quad z = h; \qquad (1.85)$$

$$\theta' = 0, \quad w' = 0 \quad \text{for} \quad z = H. \qquad (1.86)$$

Solution of the problem (1.71)-(1.77) for $t = t_{j+1}$ is the initial condition for the problem (1.78)-(1.86) for $t = t_j$.

Omitting intermediate transformations, write the finite-difference analogue of system (1.71)-(1.73) in the form

$$\frac{\partial \underline{\phi}}{\partial t} + (\Lambda_1^h + \Lambda_2^h + \Lambda_3^h)\underline{\phi} = F, \qquad (1.87)$$

where

$$\Lambda_1^h = \begin{vmatrix} A_1 & 0 & -\lambda B_1 \\ 0 & A_1 & -\lambda B_2 \\ SB_1 & SB_2 & A_1 \end{vmatrix} \quad \Lambda_2^h = \begin{vmatrix} A_2 & 0 & 0 \\ 0 & A_2 & 0 \\ 0 & 0 & A_2 \end{vmatrix},$$

$$\Lambda_3^h = \begin{vmatrix} A_3 & 0 & 0 \\ 0 & A_3 & 0 \\ 0 & 0 & A_3 \end{vmatrix};$$

$$(A_1\Psi)_{ijk} = \frac{u_{i+1/2,jk}\Psi_{i+1,jk} - u_{i-1/2,jk}\Psi_{i-1,jk}}{2\delta_i} -$$

$$- \frac{1}{\delta_i}\left(\mu_{1,i+1/2}\frac{\Psi_{i+1,jk} - \Psi_{ijk}}{\Delta x_{i+1}} - \mu_{1,i-1/2}\frac{\Psi_{ijk} - \Psi_{i-1,jk}}{\Delta x_i}\right),$$

$$(A_2\Psi)_{ijk} = \frac{v_{i,j+1/2,k}\Psi_{i,j+1,k} - v_{i,j-1/2,k}\Psi_{i,j-1,k}}{2r_j} -$$

$$- \frac{1}{r_j}\left(\mu_{2,j+1/2}\frac{\Psi_{i,j+1,k} - \Psi_{ijk}}{\Delta y_{j+1}} - \mu_{2,j-1/2}\frac{\Psi_{ijk} - \Psi_{i,j-1,k}}{\Delta y_j}\right),$$

$$(A_3\Psi)_{ijk} = \frac{w_{ij,k+1/2}\Psi_{ij,k+1} - w_{ij,k-1/2}\Psi_{ij,k-1}}{2d_k} -$$

$$- \frac{1}{d_k}\left(\tilde{\nu}_{ij,k+1/2}\frac{\Psi_{ij,k+1} - \Psi_{ijk}}{\Delta z_{k+1}} - \tilde{\nu}_{ij,k-1/2}\frac{\Psi_{ijk} - \Psi_{ij,k-1}}{\Delta z_k}\right);$$

$$\tilde{\nu} = \nu_u, \quad \mu = \nu_\theta, \quad \delta_i = \frac{\Delta x_i + \Delta x_{i+1}}{2};$$

$$r_j = \frac{\Delta y_j + \Delta y_{j+1}}{2}, \quad d_k = \frac{\Delta z_k + \Delta z_{k+1}}{2};$$

$$B_1 = \text{diag}\,\{\delta_x(x_i)\}, \quad B_2 = \text{diag}\,\{\delta_y(y_i)\}; \quad \phi = (u, v, \theta', q').$$

To approximate the problem (1.87) with respect to time, we use the scheme of component-wise splitting

$$\frac{\phi^{n+i/3} - \phi^{n+(i-1)/3}}{\Delta t/2} + \Lambda_i^h \frac{\phi^{n+i/3} + \phi^{n+(i-1)/3}}{2} = 0, \tag{1.88}$$

$$i = 1, 2, 3,$$

$$\frac{\phi^{n+i/3} - \phi^{n+(i-1)/3}}{\Delta t/2} + \Lambda_{7-i}^h \frac{\phi^{n+i/3} + \phi^{n+(i-1)/3}}{2} = 0, \tag{1.89}$$

$$i = 4,\ 5,\ 6,$$

where Δt is time step. The stability of numerical scheme is guaranteed by the condition

$$(\Lambda_{\alpha}^{h}\underline{\phi},\ \underline{\phi}) \geqq 0, \quad \alpha = 1,\ 2,\ 3, \tag{1.90}$$

where $\underline{\phi} \in \tilde{\Phi}$ is an arbitrary vector-function in the domain of definition of operator the Λ_{α}^{h} satisfying the homogeneous boundary conditions.

Let us now consider the problem (1.78)-(1.86). By virtue of the approximation we have chosen the energy balance of its discrete analogues is guaranteed and they are consistent with the approximation of continuity equations used at the transport step

$$\frac{u^{j+1}_{i+1/2,jk} - u^{j+k}_{i-1/2,jk}}{\delta_i} + \frac{v^{j+1}_{i,j+1/2,k} - v^{j+1}_{i,j-1/2,k}}{r_j} + \\ + \frac{w^{j+1}_{ij,k+1/2} - w^{j+1}_{ij,k-1/2}}{d_k} = 0. \tag{1.91}$$

Since $S \neq 0$, from (1.80) we find

$$w = -\frac{1}{S}\frac{\partial\theta'}{\partial t}. \tag{1.92}$$

Regarding the difference analogues (1.78), (1,79) as a system of linear algebraic equations in u^{j+1} and v^{j+1}, we obtain

$$u^{j+1} = \frac{1}{1+(\ell\Delta t)^2}\left[u^{j+1/2} + \ell\Delta t v^{j+1/2} - \ell\Delta t^2\frac{\partial\pi'}{\partial y} - \Delta t\frac{\partial\pi'}{\partial x}\right]; \tag{1.93}$$

$$v^{j+1} = \frac{1}{1+(\ell\Delta t)^2}\left[v^{j+1/2} - \ell\Delta t u^{j+1/2} + \ell\Delta t^2\frac{\partial\pi'}{\partial x} - \Delta t\frac{\partial\pi'}{\partial y}\right]. \tag{1.94}$$

Here, just like in (1.87), it is more convenient to use differential expressions instead of finite-difference ones for space variables. Substituting (1.92), (1.93) and (1.94) into continuity equation (1.91), we obtain an equation for the function $\underline{\pi}'$:

$$(L_1 + L_2 + L_3)\,\underline{\pi}' = \underline{F}, \tag{1.95}$$

where

$$(L_1\underline{\pi}')_{ijk} = -\frac{a}{\delta_i}\left(\frac{\pi'_{i+1,jk} - \pi'_{ijk}}{\Delta x_{i+1}} - \frac{\pi'_{ijk} - \pi'_{i-1,jk}}{\Delta x_i}\right),$$

$$(L_2\underline{\pi}')_{ijk} = -\frac{a}{r_j}\left(\frac{\pi'_{i,j+1,k} - \pi'_{ijk}}{\Delta y_{j+1}} - \frac{\pi'_{ijk} - \pi'_{i,j-1,k}}{\Delta y_j}\right),$$

$$(L_3\underline{\pi}')_{ijk} = -\frac{b}{d_k}\left(\frac{\pi'_{ij,k+1} - \pi'_{ijk}}{\Delta z_{k+1}} - \frac{\pi'_{ujk} - \pi_{ij,k-1}}{\Delta z_k}\right),$$

$$a = \frac{1}{1+(\ell\Delta t)^2}, \quad b = \frac{1}{S\lambda\Delta t}.$$

The vector $\underline{F}$ depends on $u^{j+1/2}_{ijk}$, $v^{j+1/2}_{ijk}$, $\theta^{j+1/2}_{ijk}$ and nonuniformity of boundary conditions.

Direct verification shows that

$$(L_\alpha\underline{\pi}', \underline{\pi}') \geqq 0, \quad (L_\alpha\underline{\pi}', \underline{e}) = 0, \quad (\underline{F}, \underline{e}) = 0, \quad \alpha = 1,2,3, \tag{1.96}$$

where the scalar product is defined in the grid function space by the expression

$$(\underline{\pi}', \underline{\pi}') = \sum_{ijk} \pi'_{1ijk}\, \pi'_{2ijk}\, \delta_i r_j d_k, \tag{1.97}$$

and $\underline{e}$ is a unit vector.

To solve (1.95) we use separation of variables in the discrete case. For the algorithm to be efficient with respect to the number of computational steps, the spectral problems, arising in the course of variable separation, must be solved for two matrices of lower order. If the operator of matrices L_2 and L_3 satisfy this condition, then the following spectral problems are solved:

$$L_2\omega = \lambda\omega; \tag{1.98}$$

$$L_3\Omega = \tilde{\lambda}\Omega. \tag{1.99}$$

As the operators L_2 and L_3 are self-conjugate in the function space with the scalar product (1.97), these problems determine the complete orthonormal systems of eigenfunctions $\{\omega_q\}$ and $\{\Omega_\eta\}$ and the sequences of non-negative eigenvalues $\{\lambda_q\}$ and $\{\tilde{\lambda}_\eta\}$ ($q = \overline{1, K}$, $ = \overline{1, J}$), respectively. Representing vectors $\underline{F}$ and $\underline{\pi}'$ in (1.95) as Fourier series in $\{\omega_q\}$ and $\{\Omega_\eta\}$:

$$F_i = \sum_{q=1}^{K}\sum_{\eta=1}^{J} F_{iq\eta}\,\omega_q\,\Omega_\eta; \tag{1.100}$$

$$\pi'_i = \sum_{q=1}^{K}\sum_{\eta=1}^{J} \pi'_{iq\eta}\,\omega_q\,\Omega_\eta, \tag{1.101}$$

where $F_{iq\eta}$ and $\pi'_{iq\eta}$ are Fourier coefficients, we obtain the system of equations

$$(L_1\pi'_{q\eta})_i + \lambda_q\pi'_{iq\eta} + \tilde{\lambda}_\eta\pi'_{iq\eta} = Q_{iq\eta},$$

$$i = \overline{1, I}, \quad q = \overline{1, K}, \quad \eta = \overline{1, J}. \tag{1.102}$$

This system for each pair q and η is solved by the finite-difference technique in x. After determining π', we find u^{j+1} and v^{j+1} from (1.93) and (1.94), θ'^{j+1} from the equation of statics, and w^{j+1} - from the continuity equation.

Let us give an example of computation in this model. Computation involves five steps and is so carried that starting from a relatively simple problem, additional factors are gradually introduced in the model. This procedure reveals the influence of different factors on processes taking place in the boundary layer.

In the calculations we have taken the following values for the input parameters: $X = Y = 85$ km, $h = 50$ m, $H = 2050$ m, $\Delta x = \Delta y = 10$ km {$\Delta z = 100$ m if $z \leqq 300$ m; $\Delta z = 150$ m if $300 \text{ m} \leqq z \leqq 750$ m; $\Delta z = 200$ m if $750 \text{ m} < z \leqq 2150$ m, $\lambda = 0.035$ m/(sec grad), $\ell = 10^{-4}s^{-1}$, $\mu_1 = \mu_2 = 10^4$ sq m/s, $S = 3\ 10^{-3}$ deg/m, $z_o = 0.01$ m, $\kappa = 0.35$, $\rho = 1300$ g/cu m, $P = 1000$ mb, $C_p = 0.24$ cal/(g deg), $L_w = 530$ cal/g, $A = 0.3$, $\rho_S c_S = 44\ 10^4$ cal/(cu m deg), $k_S = 3\ 10$ sq m/s, $g = 9.8$ m/s^2, $f_c = 0.9$, $a_e = 0.56$, $b_e = 0.08$, $I_s = 0$ (in version 2, $a_e = 0.2$, $b_e = 09$m $\phi = 42.5°$, $\psi = 11°$,

$$f(t) = 300 + \cos\left(\frac{\pi}{12}(t - 22)\right).$$

The turbulence coefficients in the range $h \leqq z \leqq H$ were taken as linear functions decreasing with height from $(v_i)_h$ to zero. The relative humidity (in per cent) on the soil surface was given in the form $\eta_o = 59 - 22 \cos \alpha - 11 \sin \alpha - 3 \cos 2\alpha - 4 \sin \alpha$, $\alpha = \pi(t - 4)/12$; background fields of temperature and specific humidity were taken as follows: $\theta = \bar{\theta} + Sz_1$, $\theta_x = \theta_y = 0$, $Q = \bar{Q} \exp \cdot$ $\cdot(-\beta z_1)$, $Q_x = Q_y = 0$, $\partial Q/\partial z = -\beta Q$ where $\theta = 300$ K, $\bar{Q} = 12$ g/km, $\beta = 6 \cdot 10^{-5}$ m. In calculations, it was assumed that $\bar{T} = \theta_o$, $Q_r = 0$, $W = 0$, $\Phi = 0$.

Let us consider the mesometeorological process developing in the absence of background wind over a circular island of 30 km radius, regardless of humidity processes in atmosphere and in soil. From sunrise, the island starts to warm up, and a temperature gradient appears between land and sea promoting breeze circulation which reaches its peak at 14 hrs (15 hrs 40 min)*. Maximum wind speed modulus, 9 m/s (7 m/s) is reached at an altitude of 100 m at a distance of 20 km away from the center of the island. Ascending currents, which are of an order of magnitude higher than the descending ones, reach their maximum 29 cm/s (20 cm/s) over the center of the island at an altitude of 600 m. The power of the sea breeze is 1400 m (1200 m); at higher altitudes antibreeze occurs with a maximum speed of 2.6 m/s (2 m/s) at an altitude of 1700 m (1500 m). In the evening the sea breeze subsides and land breeze develops. It is weaker than the sea breeze. The power of the land breeze is 600 m, at a higher position a strong antibreeze takes place with a speed of 0.5 m/s.

*Brackets contain the values for the second version.

In contrast to the first, the second version takes account of humidity which markedly changes breeze circulation development over the island. Changes occur due to diurnal ground temperature variation during these mesoprocesses. Figure A.2 illustrates the calculated time variation of components of heat balance and ground temperature with (figure A.2a) and without (figure A.2b) humidity at the center of the island. During daytime, when a major part of heat is spend on evaporation, wet soil warms up slower than dry soil. As a consequence, compared to the first version, turbulent heat flow into atmosphere decreases and a local circulation develops less intensively.

At night, there are no turbulent flows of heat and moisture, only two components G_o and F remain in the heat balance. Since a_3 and b_3 in the Brent formula were so selected that the radiation balances in versions 1 and 2 were approximately the same, it is clear why at night the processes with and without humidity are practically identical.

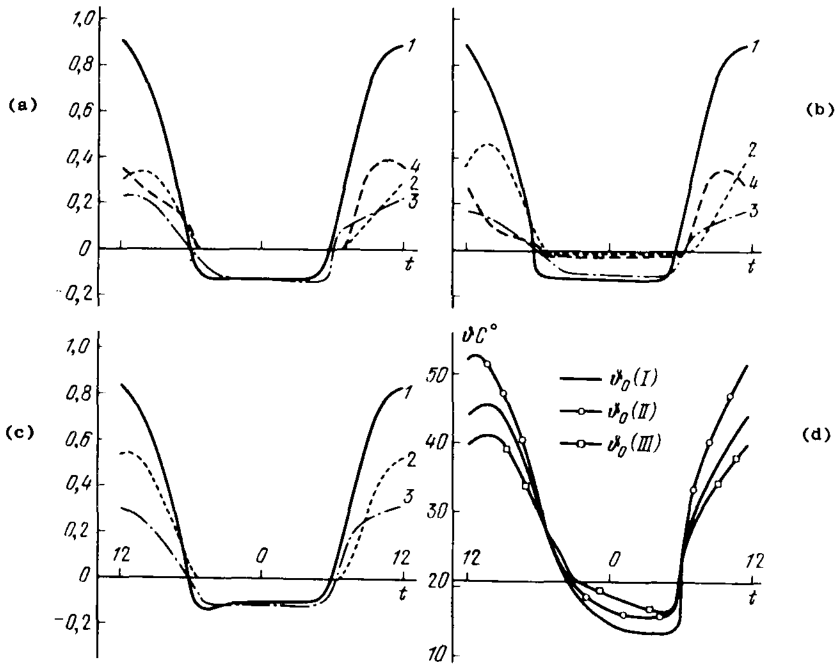


FIGURE A.2

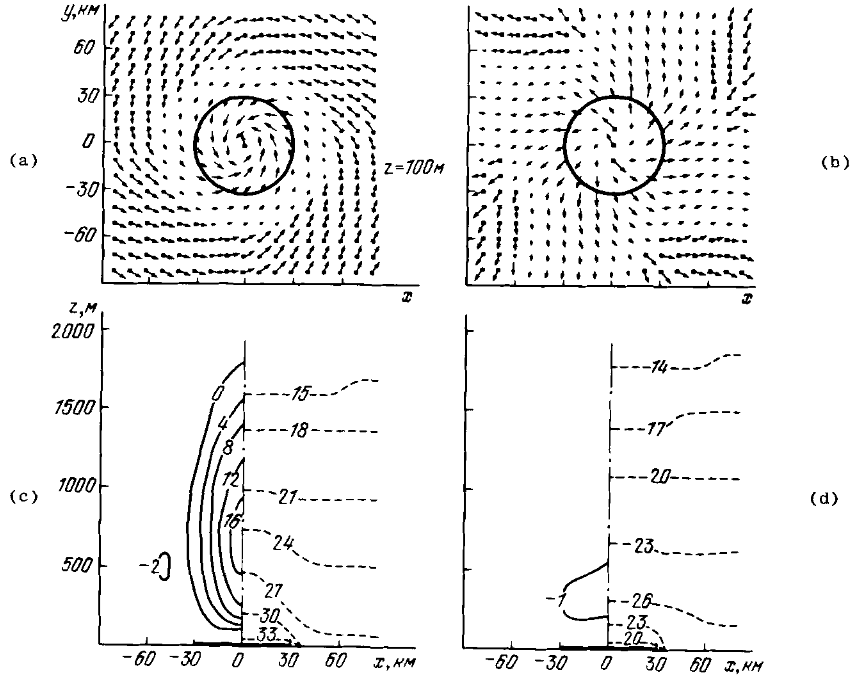


FIGURE A.3

Figure A.3 shows results calculated for 16 hrs (left half) and midnight (right half) at z = 100 m and y = 90 km. Wind fields are represented by arrows (arrows ending with squares are low speed wind). The outline of the island is drawn in thick line; isolines of vertical speeds (cm/s) - in bold line; isolines of temperature (degrees, Centigrade) - in broken line.

As compared to version 2, in the third version the outward wind depends on time; its speed in the range 3 hrs $\leq t \leq$ 15 hrs is given by expression

$$U(t) = [3 + 5 \sin\left(\frac{t - 12}{12}\pi\right)], \quad V(t) = 0 ,$$

while at other moments it is considered constant $\{ U(t) = 3$ m/s, $V(t) = 0\}$. During daytime the local circulation and outward flow are unidirectional over the western part of the island upto an altitude of 1200 m. This results in stronger wind. But over the eastern part the wind gets weaker. Near the eastern shore, a zone of convergence is formed by 16 hrs in which vertical currents and temperature take on extreme values. At night, local circulation is opposite to that in daytime. For this reason, the flow in lower layers, while approaching the island, slows down as if flowing round two sides of the island. Figure A.4 shows results calculated as in figure A.3.

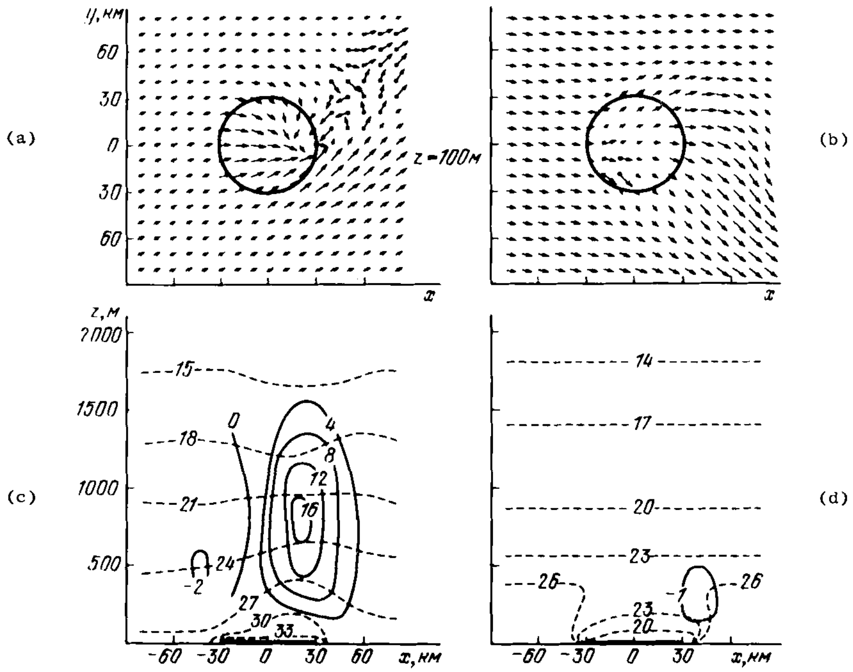


FIGURE A.4

Now let us consider the influence of external wind on diurnal variation of components of heat balance (figure A.2c) and ground temperature (figure A.2d) in the center of the island. In daytime, when wind enhances turbulent mixing, the maximum temperature on the earth's surface is 4°C lower than in the second version. At night, also due to external wind, turbulent flows of heat and moisture do occur but take on small values, but during the whole night they do not change direction, therefore the minimum v_o is 3°C higher than without wind.

The fourth version takes account of the influence of land relief on the development of local circulation. On the island, as compared to the first version, there is an exisymmetric 500 m high mountain whose surface is described by the expression $\delta(r) = (213 + 300 \cos (\pi\ r/40))$ where r is the distance from the center of the island. The time variation process intensity is approximately the same as in the second version, the differences being completely related to the relief. In daytime, circulation intensity hardly varies. Wind speed increases by a mere 1 m/s. Ascending currents, whose range gets narrower with altitude, reach 23 cm/s over the center of the mountain. At night, the mountain influence is much greater. The land breeze is almost twice as strong and at midnight it reaches 4 m/s. The descending currents reach 8 cm/s. Figure A.5 shows the isolines of vertical speeds and temperature at 16 hrs (figure A.5a) and at 0 hrs (figure A.5b) at y = 90 km. Notation is the same as in figure A.3.

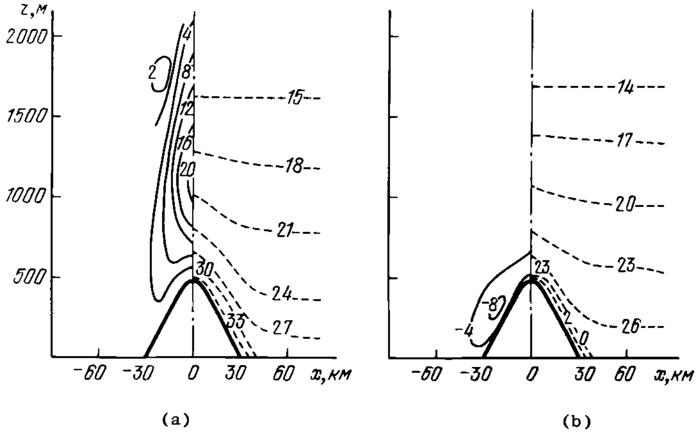


FIGURE A.5

The fifth version refers to the solution of the problem (1.1)-(1.7), (1.14)-(1.18) jointly with the turbulence energy Eqs.(1.36)-(1.38), (1.51)-(1.55). All input parameters are the same as in version 3, only U = -5 m/s, V = 0, V = 0, $\Delta X = \Delta y = 4$ km. Figure A.6a illustrates the isolines of turbulence energy b and vertical turbulence exchange coefficient ν in (x, z) plane at y = 32 km at time, t = 15 hrs. Figure A.6b shows the vertical profiles of the functions b, ν_u and ε at different points for t = 15 hours and figure A.6c for t = 12 hours.

2. Quasihomogeneous ocean layer

World Ocean pollution became an acute problem in the early 1950's due to radioactive fallout from nuclear tests in atmosphere. At present, oil pollution of oceans is increasing and the feasibility of burying decay radioactive products at the ocean bed is being examined. All these factors stimulate the development of mathematical techniques for forecasting impurity propagation into the ocean.

The evolution of conservative impurity concentration field in the Eulerian representation is described by averaged equation of molecular diffusion:

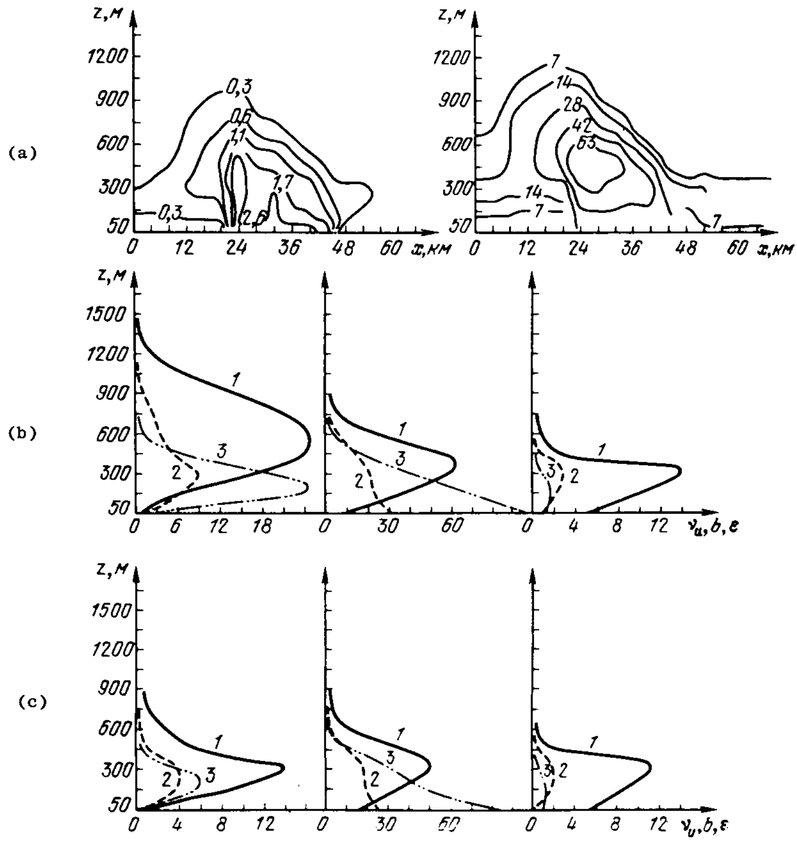


FIGURE A.6

$$\frac{\partial \phi}{\partial t} + u_\alpha \frac{\partial \phi}{\partial x_\alpha} = \mu \Delta \phi - \frac{\partial}{\partial x_\alpha} \overline{u'_\alpha \phi'} + Q\delta(\underline{x} - \underline{x}_o)\delta(t - t_o), \tag{2.1}$$

where ϕ is the impurity concentration, μ is the molecular diffusion coefficient of impurity into the ocean, Q is the power of instantaneous point pollution source.

Impurity turbulent flow vector $u'_\alpha \phi'$ is generally determined by a gradient type (Bussinesq) approximation

$$u'_\alpha \phi' = - k_{\alpha\beta} \frac{\partial \phi}{\partial x_\beta} . \tag{2.2}$$

The turbulent diffusion tensor $k_{\alpha\beta}$ does not depend on passive impurity concentration and is the major characteristic of the turbulent field.

In general, in solving the problem (2.1), (2.2) the velocity field and turbulent diffusion coefficients are assumed to be known. To study the global impurity propagation in the World Ocean, it is necessary to have a large-scale velocity field and tensor field of turbulent diffusion coefficients over the entire ocean. Models of this kind, based on numerical integration of geophysical equations, are being developed both in the USSR and abroad. For the impurity deposited on the ocean surface, of special significance is the forecast of its propagation in the upper boundary layer of the ocean. In this case, stratification being stable or neutral determination of horizontal velocity field and vertical turbulent exchange is considerably simplified. We now take up this problem.

Consider the equations of an *Ekman* oceanic boundary layer with regard to vertical turbulent exchange:

$$\frac{\partial u}{\partial t} - \ell v = \frac{\partial}{\partial z} k \frac{\partial u}{\partial z}, \tag{2.3}$$

$$\frac{\partial v}{\partial t} + \ell u = \frac{\partial}{\partial z} k \frac{\partial v}{\partial z}, \tag{2.4}$$

$$\frac{\partial T}{\partial t} = - \frac{\partial Q}{\partial z}, \tag{2.5}$$

$$\frac{\partial b}{\partial t} = k \left[\left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2 \right] + \frac{\partial}{\partial z} k \frac{\partial b}{\partial z} - \varepsilon - g\alpha\theta, \tag{2.6}$$

$$\frac{\partial \varepsilon}{\partial t} = 1{,}38 \frac{\varepsilon}{b} k \left[\left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2 \right] + \frac{\partial}{\partial z} k \frac{\partial \varepsilon}{\partial z} - 1{,}4 \frac{\varepsilon}{b} \varepsilon - 1{,}4 \frac{\varepsilon}{b} g\alpha\theta, \tag{2.7}$$

$$k = 0{,}08\ b^2/\varepsilon, \tag{2.8}$$

under the boundary and initial conditions

$$z = 0:\ k \frac{\partial u}{\partial z} = -u_*^2,\ k \frac{\partial v}{\partial z} = 0,\ Q = w'T' = Q_o \geqq 0; \tag{2.9}$$

$$k \frac{\partial b}{\partial z} = 0, \quad k \frac{\partial \varepsilon}{\partial z} = 0; \tag{2.10}$$

$$z = H\ (H > h):\quad u = v = 0, \quad b = \varepsilon = 0; \tag{2.11}$$

$$t = 0:\quad u = u^o,\ v = v^o,\ T = T^o,\ b = b^o,\ \varepsilon = \varepsilon^o, \tag{2.12}$$

Here, all quantities in (2.1) are averaged, k is turbulent viscosity coefficient, b is turbulent energy; ε is turbulent dissipation velocity; ℓ is the Coriolis coefficient, g is acceleration due to gravity, h is the depth of the upper quasi-homogeneous layer (UQL) of the ocean, α is thermal expansion coefficient of the medium.

From the viewpoint of numerical solution, problem (2.3)-(2.12) is quite simple. This formulation was used in numerical investigation of storm development. The solution revealed a new phenomenon: storm brings about a local boundary layer at thermal shock. Analysis of numerical solutions demonstrate that analytical solutions of (2.3)-(2.12), which are more illustrative than numerical ones, are extremely important for verification of difference schemes. Let us consider some of them.

Assume that a stationary turbulent surface layer is formed in the ocean under drift motion with a constant coefficient k. The analytical solution of the equation of motion (2.3), (2.4) for a constant coefficient k was first obtained by V.W.Ekman in 1905 ($H \to \infty$):

$$u,\ v = \pm(2k\ell)^{-\frac{1}{2}}\, u_*^2 e^{-\beta z} (\cos \beta z \pm \sin \beta z), \tag{2.13}$$

where $\beta = (\ell/(2k)^{\frac{1}{2}}$. In (2.6)-(2.7) define the function G as a source of turbulence displacement

$$G = k\left[\left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2\right] = \frac{u_*^4}{h}\, e^{-2\beta z}. \tag{2.14}$$

According to dimension theory, the depth of the upper quasihomogeneous layer can be determined as

$$h = \gamma\lambda, \tag{2.15}$$

where $\lambda = u_*/f$ (λ is Ekman scale of length), γ is a function that defines dimensionless parameters in our problem. Equating the depth, at which the turbulence displacement source (2.14) decreases by a factor of e^{π}, i.e.

$$\frac{G_o}{G_h} = e^{\pi}, \quad G_o = k\left[\left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2\right]_{z-0}, \tag{2.16}$$

to the depth of the upper quasihomogeneous layer (2.15), we obtain:

$$k = \frac{2\gamma^2}{\pi^2}\,\frac{u_*^2}{\ell} = \frac{2\gamma^2}{\pi^2}\, u_*\lambda. \tag{2.17}$$

Kinetic energy flow from atmosphere into ocean is

$$-k\frac{\partial}{\partial z}\,\frac{u^2+v^2}{2}\bigg|_{z=0} = u_o u_*^2 = \frac{\pi}{2\gamma}\, u_*^3. \tag{2.18}$$

Assume that the diffusion term $\frac{\partial}{\partial z} k \frac{\partial b}{\partial z}$ in (2.6) is small compared to others. For a known k, the quantities b and ε are readily found in this case from (2.6), (2.8). Equation (2.7) turns to be superfluous:

$$\varepsilon = \frac{\pi^2}{2\gamma^2}\,\frac{u_*^3}{\lambda}\,(e^{-2\beta z} - e^{-\pi}), \quad b = \frac{5}{\sqrt{2}}\, u_*^2(e^{-2\beta z} - e^{-\pi})^{\frac{1}{2}}. \tag{2.19}$$

The dimensionless function γ is found from the condition that there is no turbulence at $z \geqq h$, i.e. $\varepsilon = 0$ at $z = h$:

$$\gamma = (\pi/\sqrt{2})\ e^{-\pi/2}\ \mu^{-\frac{1}{2}}, \tag{2.20}$$

where $\mu = \lambda/L$ is a dimensionless stratification parameter, $L = u_*^3/(g\alpha Q)$ is Monin-Obukhov length scale. Substituting γ from (2.20) into (2.15) we obtain

$$h = \gamma\lambda = \frac{\pi}{\sqrt{2}}\ (e^{\pi}\mu)^{-\frac{1}{2}}\lambda = \frac{\pi}{\sqrt{2}} \sqrt{\frac{\mu}{e^{\pi}}}\ L. \tag{2.21}$$

We can also define h as $h = \gamma L$; in this case $\gamma = \frac{\pi}{\sqrt{2}} \sqrt{\frac{\mu}{e^{\pi}}}$. Both definitions of h are equivalent in case of stable stratification (for $Q > 0$). For neutral stratification ($Q = 0$) there are no parameter μ and scale L, therefore the most general definition of h is (2.15).

Stationary solutions can be used for evaluating nonstationary processes. Relaxation time Δt of dynamic and thermal perturbations in the boundary layer and characteristic time τ in which turbulence adapts to hydrodynamic environment are:

$$\Delta t = \frac{h^2}{k} = \frac{\pi}{4}\left(\frac{2\pi}{\ell}\right), \tag{2.22}$$

$$\tau \sim \frac{b}{\varepsilon} = \frac{5\sqrt{2}\ e^{-\pi}(e^{-2\beta z} - e^{-\pi})^{-\frac{1}{2}}}{\mu\ell}. \tag{2.23}$$

These solutions derived are determined as functions of two dimensionless parameters: μ and z/λ. The analysis is based on the classical Ekman solution of equations of motion, the only difference being that the vertical turbulent exchange coefficient is consistent with the external parameters of the problem. This analysis is valid, provided the surface turbulent layer is thicker than the quasilaminar sublayer:

$$h > 10\ k_o/u_*, \quad \gamma > 10\ k_o\ell/u_*^2 = 10\ k_o/(u_*\lambda),$$

if no account is taken of the wave processes on the ocean surface. Here, coefficient k_o take the minimal value found from the condition $Re_t = k/\nu \geqq 10$, under which turbulence equations (2.6)-(2.8) hold, hence $k_o = 10\nu$. The condition $h > 10\ k_o/u_*$ is chosen by analogy with the laminar sublayer thickness equal to $10\ \nu/u_*$ from Laufer experiment (1951), ν is a kinematic factor of molecular viscosity. On the other hand, for $\gamma > 0.4$ the medium can be considered neutrally stratified and we can take $\gamma = 0.4$. Let us formulate the analysis applicability condition:

$$10^2\ \nu/(u_*\lambda) < \gamma < 0{,}4. \tag{2.24}$$

The qualitative solution is based on the assumption that k is constant. Numerical solutions of (2.3)-(2.12) indicate that k diminishes with depth. Suppose that k is defined by a power function:

$$k = k_1 x^2, \quad x = (1 - z/H). \tag{2.25}$$

In this case, the solutions of (2.3), (2.4) under the boundary conditions (2.9), (2.12) can be written as

$$u, v = \pm \frac{u_*^2 H}{k_1} \frac{x^m}{(m^2+n^2)^{1/2}} [\cos(q - n \ln x), \sin(q - n \ln x)],$$

$$G = \frac{u_*^4}{k_1} x^{2m}, \quad \mathrm{tg}\, q = \frac{n}{m}, \quad m = \frac{1}{2}\left[\left(\frac{a^2+1}{2}\right)^{\frac{1}{2}} - 1\right], \tag{2.26}$$

$$n = \frac{1}{2}\left(\frac{a^2-1}{2}\right)^{\frac{1}{2}}, \quad a^2 = \left(1 + \frac{16H^4 f^2}{k_1^2}\right)^{\frac{1}{2}}.$$

Flow of kinetic energy from atmosphere into the ocean is

$$u_o u_*^2 = \frac{m}{m^2 + n^2} \frac{H}{k_1} u_*^4. \tag{2.27}$$

Define ε, b as

$$\varepsilon = \frac{u_*^4}{k_1} x^{2m} - g\alpha Q, \tag{2.28}$$

$$b = \frac{5}{\sqrt{2}} (u_*^4 x^{2m+2} - k_1 x^2 g\alpha\Theta)^{\frac{1}{2}}. \tag{2.29}$$

To solve the problem, we have to find the depth of the upper quasihomogeneous layer h, k_1 and the depth H. Beside the conditions

$$h = \gamma\lambda, \quad G_o/G_h = e^{\pi}, \quad \varepsilon\Big|_{z=h} = 0 \tag{2.30}$$

we impose the constraint on k at the boundary of turbulence domain:

$$k = k_1 \left(1 - \frac{h}{H}\right)^2 = k_o. \tag{2.31}$$

Solutions of (2.30), (2.31) are

$$k_1 = e^{-\pi} u_* L, \tag{2.32}$$

$$H = \frac{e^{-\pi/2}}{\sqrt{2}} (\lambda L)^{\frac{1}{2}} A(Re_t), \tag{2.33}$$

$$\gamma = \frac{H}{\lambda}\left(1 - \sqrt{\frac{k_o}{k_1}}\right), \tag{2.34}$$

$$h = \left(1 - \sqrt{\frac{k_o}{k_1}}\right) H, \tag{2.35}$$

where

$$Re_t = k_1/k_o = u_* Le^{-\pi}/k_o,$$

$$A(Re_t) = \{[2(1 + 2\pi/\ln Re_t)^2 - 1] - 1\}^{1/4}.$$

The characteristic time of hydrodynamic and turbulent relaxation is of the form

$$\Delta t \sim H^3 / \int_0^H k dz = \frac{3}{4} A^2 (Re_t)/\ell, \tag{2.36}$$

$$\tau \sim b/\varepsilon = (5/\sqrt{2})\, e^{-\pi} x (x^{2m} - e^{-\pi})^{-\frac{1}{2}}/(\mu\ell). \tag{2.37}$$

In addition to (2.24) the condition for applicability of our analysis is $k_1 > K_o$, i.e. $Re_t > 1$; hence, it is natural that $k_1 > \min k$. Moreover, the inequalities $H > 0$, $\nu > 0$, $0 < h < H$, $m > 0$, $n > 0$ always hold.

Substituting (2.32)-(2.35) into (2.26)-(2.29), we obtain the solution which depends on three dimensionless parameters: $z/\sqrt{\lambda}\, L$, Re_t and μ. For $\gamma > 0.4$ the medium is neutrally stratified, $\mu = 0$. Then, k_1, H are given by equations

$$k_1 = k_o(1 - h/H)^{-2}, \quad h = 0{,}4\lambda, \tag{2.38}$$

$$H = (k_1/(4\ell))^{\frac{1}{2}} \{[2(1 + 2/\ln Re_t)^2 - 1]^2 - 1\}^{1/4} \tag{2.39}$$

and the solution depends on two dimensionless parameters:

$$\lambda \Big/ \sqrt{\frac{k_o}{\ell}} = \frac{\lambda}{\lambda_o}, \quad \frac{z}{\lambda_o} \left(\lambda_o = \sqrt{\frac{k_o}{\ell}}\right).$$

Let us analyse solutions of versions A: $k = \text{const}$, and B: $k = k_1 x^2$. For the sake of convenience, write them as version A: $k = e^{-\pi}\mu^{-1}u_*\lambda$;

$$u, v = \pm(e^{\pi}/2)^{\frac{1}{2}} \mu^{\frac{1}{2}} u_* e^{-\beta z}(\cos\beta z - \sin\beta z),$$

$$G = e^{\pi}\mu u^3/(\lambda e^{-2\beta z}), \quad \varepsilon = e^{\pi}\mu u_*^3/[\lambda(e^{-2\beta z} - e^{-\pi})],$$

$$b = (5/\sqrt{2})u_*^2(e^{-2\beta z} - e^{-\pi})^{\frac{1}{2}}, \quad \gamma = \pi/(2e^{\pi}\mu)^{-\frac{1}{2}};$$

version B: $k = e^{-\pi}\mu^{-1} u_*\lambda x^2$;

$$u, v = \pm(e^{\pi}\mu/4)^{\frac{1}{2}} A(m^2 + n^2)^{-\frac{1}{2}} u_* x^m \cdot[\cos(q - n\ln x), \sin(q - n\ln x)],$$

$$G = e^{\pi}\mu u_*^3/(\lambda x^{2m}), \quad \varepsilon = e^{\pi}\mu u^3/[\lambda(x^{2m} - e^{-\pi})],$$

$$b = (5/\sqrt{2})\, u_*^2(x^{2m} - e^{-\pi})^{\frac{1}{2}} x,$$

$$\gamma = A(Re_t)[1 - (Re_t)^{-\frac{1}{2}}]/(2e^{\pi}\mu)^{\frac{1}{2}}.$$

The influence of external parameters in both versions is identical; the difference lies in the presence of an additional parameter Re_t in the second version and in functional dependence on depth: exponential and power ones. As flow Q_o increases (L diminishes, μ, A, m increase) the medium stability grows, hence large scale turbulent fluctuations are suppressed. At the same time, the values of coefficient k and thickness diminish, and turbulence dissipation rate and surface flow velocity increase. Surface turbulence energy does not depend on Q_o. Growth of Q_o leads to the growth of β and m; as a result, the profiles of both solutions become steeper.

Analytical solutions correctly reflect particularities of solution of the system (2.3)-(2.12) derived numerically, and in version B the influence of diffusion coefficient k_o is the same as in numerical solution: the growth of k_o leads to growth of UQL thickness: $dh/dk_o > 0$, $d\gamma/dk_o < 0$, $dH/dk_o > 0$. Figure A.7 illustrates the balance of terms of the energy turbulence equation. Diffusion term becomes significant only in the vicinity of the lower UQL boundary. Analytical solutions provide a similar estimate. For example, in case A the relation

$$\frac{d}{dz} k \frac{db}{dz} / \varepsilon = \left(\frac{25}{2}\right)^{\frac{1}{2}} \left(\frac{\gamma}{\pi}\right)^2 e^{\beta z}$$

is small at z = 0 and increases with depth.

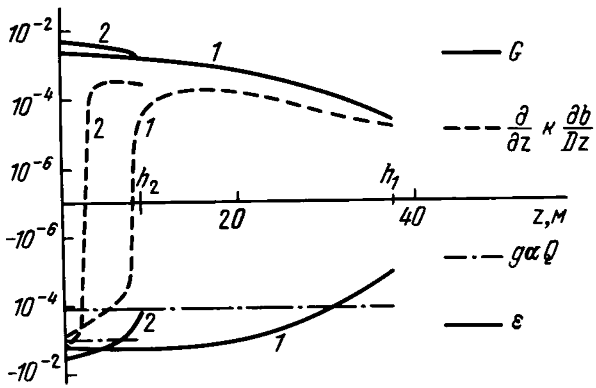


FIGURE A.7

Let us consider nonstationary development of surface turbulent layer. Assume that the solutions are universal functions in nonstationary case, too. Multiplying (2.3), (2.4) by u and ν, respectively, adding them and integrating from 0 to h(t), we obtain

$$\frac{\partial}{\partial t}\int_0^{h(t)} \frac{u^2+v^2}{2}\,dz - \frac{u^2+v^2}{2}\Big|_{z=h}\frac{dh}{dt} = k_o\left[u\frac{\partial u}{\partial z} + v\frac{\partial v}{\partial z}\right]_{z=h} + \tag{2.40}$$

$$+ (ku^2)\big|_{z=0} - \int_0^{h(t)} k\left[\left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2\right]dz.$$

Substituting u, v, k from solution B into (2.40) and integrating, we obtain the forecast equation for UQL depth:

$$\frac{uh}{2k_1^2}\,\frac{1}{R_H^2(m^2+n^2)}\left[Re_t^{-m} - \frac{3R_A}{R_H(2m+1)}\right]\frac{dh}{dt} =$$

$$= \frac{u_*}{k_1}\,\frac{R_A}{R_H}\,\frac{n^2-m^2-m}{(m^2+n^2)(2m+1)} + \frac{2h^2}{k_1^2}\,\frac{R_A}{R_H^3(m^2+n^2)(2m+1)}\,\frac{du_*}{dt} + \tag{2.41}$$

$$+ \frac{u_*h^2}{2}\,\frac{d}{dt}\left[\frac{R_A}{k_1^2R_H^2(m^2+n^2)(2m+1)}\right],$$

$$R_H = 1 - Re_t^{-\frac{1}{2}}, \qquad R_A = 1 - Re_t^{-(2m+1)/2}.$$

In deriving (2.41), H(t) has been eliminated through the use of relation (2.35). The quantities $u_*(t)$, Q(h, t), f, k_o are external parameters in (2.41). The quantity Q(h, t) is found from heat Eq.(2.5).

If Q in (2.5) is defined as $Q = -k_1x^2\partial T/\partial z$ with arbitrary boundary conditions for x = 0: $T = T_o(t)$, $Q = Q_o(t)$, then Q(h, t) is found by integrating (2.5) with respect to h. In this case, we arrive at the assumptions underlying the traditional "integral" models of UQL.

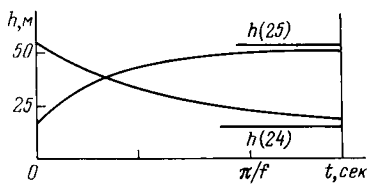


FIGURE A.8

Figure A.8 shows the numerical solutions of (2.41) for the following values of external parameters: $Q = 10^{-4}$ K cm/s, $\ell = 10^{-4}\ s^{-1}$, $k_o = 1$ sq·cm/s:

$$u_* = \begin{cases} 0.5\text{ cm/s}, & t = 0,\\ 1\text{ cm/s}, & t > 0;\end{cases}$$

$$u_* = \begin{cases} 1 \text{ cm/s}, & t = 0, \\ 0.5 \text{ cm/s}, & t > 0. \end{cases}$$

Stationary solutions (2.35) are employed as initial values of h at $t = 0$. Solution of (2.41) as $t \to \infty$ asymptotically approaches the stationary solution (2.35), and in the inertia period $2\pi\ell^{-1}$ the depth h tends to stationary solution.

In concluding the dimensional analysis, let us note that instead of dynamic velocity u_*, as the external parameter, one can also take ε_o, the mean turbulent dissipation rate per mass unit which is the energy flux from atmosphere into the ocean:

$$\varepsilon_o \cong \frac{1}{h} \int_0^H (G - g\alpha Q)\, dz. \qquad (2.42)$$

From ε_o, ℓ, Q one can proceed to the parameters u_*, ℓ, Q by substituting their values obtained from the above solutions into the energy relation (2.42).

In conclusion we may note that this idealization yields analytical solution which clearly demonstrates the effect of external parameters on the development of surface turbulent layer and is consistent with solutions of the system of equations (2.3)-(2.12).

REFERENCES

1) M.E. Berlyand, Modern problems of atmospheric diffusion and atmospheric pollution, Leningrad, Gidrometeoizdat, (1975) (Russian ed.).

2) N.L. Byzova, Impurity diffusion into atmospheric boundary layer, Leningrad, Gidrometeoizdat, (1974) (in Russian).

3) V.S. Vladimirov, Equations of mathematical physics, Moscow, Nauka, (1981) (in Russian).

4) N.L. Karol and G.S. Malakhov, Problems of nuclear meteorology, Moscow, Gosatomizdat, (1962) (in Russian).

5) A.N.Kolmogorov, Equations of turbulent motion of incompressible liquid, Izv. AN SSSR, Fizika, (1942), 6, No.1-2, pp.56-58.

6) K.Ya. Kondratyev, Radiant energy of the Sun, Leningrad, Gidrometeoizdat, (1956) (in Russian).

7) Yu.A. Kuznetsov, On the convergence of splitting method for a system with positively semidefinite matrices, in: Differential and Integral Equations,

Novosibirsk, Computer Center of the Siberian Division of the USSR Academy of Sciences, (1977), pp.112-119 (in Russian).

8) O.A. Ladyzhenskaya, Mathematical problems in the dynamics of incompressible liquid, Moscow, Nauka, (1970) (in Russian).

9) G.I. Marchuk, Methods of nuclear reactor design, Moscow, Atomizdat, (1961) (in Russian).

10) G.I.Marchuk, On certain inverse problems, Doklady AN SSSR, (1964), 156, No.3, pp.503-506.

11) G.I. Marchuk, Eluation for the significance of information from meteorological satellites and formulation of inverse problems, Kosmicheskiye issledovaniya, (1964), 2, No.3, pp.462-477.

12) G.I.Marchuk, On the equations of baroclinic ocean dynamics, Doklady AN SSSR, (1967), 173, No.6.

13) G.I. Marchuk, Numerical methods in weather forecast, Leningrad, Gidrometeoizdat, (1967) (in Russian).

14) G.I. Marchuk, Numerical solution of atmosphere and ocean dynamics problem, Leningrad, Gidrometeoizdat, (1974) (in Russian).

15) G.I. Marchuk, Environment and some optimization problems, Novosibirsk, (1975), Preprint of the Computer Center of Siberian Division of the USSR Academy of Sciences.

16) G.I. Marchuk, Environment and optimization problems of enterprise location, Doklady AN SSSR, (1976), 227, No.5, pp.1056-1059.

17) G.I.Marchuk, Some problems of environmental protection, in: Comprehensive Analysis and its Application, Moscow, Nauka, (1978), pp.375-381 (in Russian).

18) G.I. Marchuk, Methods of computational mathematics, Moscow, Nauka, (1980) (in Russian).

19) G.I. Marchuk, Application of adjoint equations to solution of mathematical physics problems, Uspekhi mekhaniki, (1981), No.1.

20) G.I. Marchuk, V.P. Dymnikov et al., Hydrodynamic model of common circulation of atmosphere and ocean, Information Bull., Novosibirsk, Computer Center of Siberian Division of the USSR Academy of Sciences, (1975).

21) G.I. Marchuk, V.B. Zalesny and V.I. Kuzin, On methods of finite differences and finite elements in problem of global wind circulation of ocean, Izv. AN SSSR, Fizika atmosfery i okeana, (1975), 11, No.12.

22) G.I. Marchuk, V.P. Kochergin, V.I. Klimok and V.A. Sukhorukov, Analytical solutions for the Ekman turbulent layer of the ocean, Doklady AN SSSR, (1979), 247, No.1.

23) G.I. Marchuk, V.P. Kochergin, A.S. Sarkisyan et al., Mathematical models of circulation in the ocean, Novosibirsk, Nauka, (1980) (in Russian).

24) G.I. Marchuk and V.V. Orlov, To theory of conjugate functions, in: Neutron physics, Moscow, Gosatomizdat, (1961), pp.30-45 (in Russian).

25) G.I. Marchuk, V.V. Penenko, A.E. Aloyan and G.L. Lazriyev, Numerical simulation of city microclimate, Meteorologiya i gidrologiya, (1979), No.8, pp.5-15.

26) G.I. Marchuk, Environment and some optimization problems, Lect. Notes Comp. Sci., (1976), 40, No.1, pp.13-30.

27) G.I. Marchuk,V.P. Kochergin, V.I. Klimok and V.A. Sukhorukov, On the dynamics of the ocean surface mixed layer, J. Phys. Oceanogr., (1977), 7, pp.865-875.

28) G.I. Marchuk, V.I. Kuzin and N.N. Obraztsov, Numerical modelling of the distribution sources in a water basin, Novosibirsk, (1979), Academy of Sciences of the USSR, Computing Center, (Preprint).

29) G.I. Marchuk, and V.V. Penenko, Application of optimization methods to the problem of mathematical simulation of atmospheric processes and environment, Proc. of the IFIP, B., (1979), pp.240-252.

30) A.S. Monin and A.M. Obukhov, Basic laws of turbulent mixing in the ground atmospheric layer, Trudy Instituta Geofiziki, the USSR Academy of Sciences, (1954), No.24 (151), pp.163-187.

31) A.S. Monin and A.M. Yaglom. Statistical hydromechanics, Moscow, Nauka, (1965), Vol.1 (in Russian).

32) R.V. Ozmidov, On turbulent exchange in a steadily stratified ocean, Izv. AN SSSR, Fizika atmosfery i okeana, (1965), 1, No.8, pp.853-860.

33) B.L. Rozhdestvensky and N.N. Yanenko, Systems of quasilinear equations and their application to gas dynamics, Moscow, Nauka, (1968) (in Russian).

34) G. Streng and J. Fics, Theory of finite elements method, Moscow, Mir, (1977) (Russian ed.).

35) A.S. Sarkisyan, Numerical analysis and sea current forecast, Leningrad, Gidrometeoizdat, (1977) (in Russian).

36) A.M. Yaglom, On turbulent diffusion in the atmospheric ground layer, Izv. AN SSSR, Fizika atmosfery i okeana, (1972), 9, No.6.

37) R.G. Yanovsky, Environmental protection is a public duty of scientists, in: Methodological Problems of the Modern Science, Moscow, Politizdat, (1979), pp.196-211 (in Russian).

38) V.W. Ekman, On the influence of the earth's rotation on ocean-currents, Arkhiv Mat., Astron och. fizik, (1905), 2, No.11.

This Page Intentionally Left Blank