

## Chapter 2

# A Strategy for Bioremediation of Marine Shorelines by Using Several Nutrient Release Points

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**Abstract** In this chapter, a strategy for the bioremediation of marine shorelines polluted with oil is presented. Several discharge points are chosen in a limited region in order to release a nutrient and reach critical concentration of this substance in the oil-polluted shorelines. The strategy is optimal in the sense that the location of the discharge points and the release rates are planned so as to minimize the amount of the nutrient introduced into the aquatic system. To accomplish this task, a variational problem is solved to find the location of the discharge point in each oil-polluted zone, and to determine a basic (preliminary) shape of its release rate. After that, a quadratic programming problem is solved to specify the strength of these release rates in order to reach the critical concentration in all the polluted zones during the same time interval. An initial-boundary value 3D advection-diffusion problem and its adjoint problems are considered in a limited area to model, estimate and control the dispersion of the nutrient. It is shown that the advection-diffusion problem is well posed, and its solution satisfies the mass balance equation. In each oil-polluted zone, the mean concentration of nutrient is determined by means of an integral formula in which the adjoint model solution serves as the weight function showing the relative contribution of each source. Critical values of these mean concentrations are used as the constraints for the variational problem as well as for the quadratic programming problem. The ability of new method is demonstrated by numerical experiments on the remediation in oil-polluted channel using three control zones.

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## 2.1 Introduction

Crude oil is one of the most important organic pollutants in marine environments. It has been estimated that worldwide approximately  $1.3 \times 10^6$  tons of petroleum impact marine waters and estuaries annually [27]. Massive releases from pipelines, wells and tankers receive the most public attention, but in fact these account for only a relatively small proportion of the total petroleum entering the environment. Almost 50 % comes from natural seeps, and less than 9 % emanates from catastrophic releases. Consumption and urban run-off is responsible for almost 40 % of the input [27]. Independently of the source of pollution, a substantial number of smaller releases of petroleum occur regularly in coastal waters [14], as a result, oil stranded in shorelines has become a common problem which needs attention.

It is well known that oil is comprised of many different toxic compounds which endanger the marine environment involved in a spill, however there are many natural, native microorganisms which are not only capable, but thrive on the decomposition of these toxic compounds. This process of using microorganisms for such cleanup efforts in shorelines is known as bioremediation, and it has proven to be a successful method for the cleanup of marine areas affected by oil spills [7]. There are two different types of bioremediation used for oil spill cleanup: bioaugmentation and biostimulation. Bioaugmentation is the addition of microorganisms capable of degrading the toxic hydrocarbons, in order to achieve a reduction of the pollutants. Biostimulation is the addition of nutrients needed by indigenous hydrocarbon degrading microorganisms in order to achieve maximum degradation of toxic compounds present in the oil. The degradation of hydrocarbons (biodegradation) begins by the conversion of the alkane chain or polycyclic aromatic hydrocarbon (PAH) into alcohol. Oxidation then converts the compound to an aldehyde and then into an acid and eventually into water, carbon dioxide, and biomass. In the case of the PAH, fission occurs which ultimately leads to mineralization [47]. More than 170 genera of microorganisms have been identified in the environment which are able to degrade hydrocarbons, due to such diversity and different conditions at the spill site, hydrocarbons do not all biodegrade at similar rates, and not all hydrocarbons are degradable, but estimates for the biodegradability of different crude oils range from 70 to 97 %. What remain are principally the asphaltenes and resin compounds, which are essentially biologically inert [38].

Although biodegradation is a particularly important mechanism for removing the non-volatile components of oil from the environment, this is a relatively slow natural process and may require months to years for microorganisms to degrade a significant fraction of an oil stranded in shorelines, within the sediments of marine and/or freshwater environments [52]. The simplest way of stimulating biodegradation, and the only one that has achieved experimental verification in the field, is to carefully add nitrogen and phosphorus nutrients. This was first used on a large scale in Alaska, following the 1989 spill from the Exxon Valdez [4, 36, 37]. Two fertilizers were used in the large-scale applications: an oleophilic liquid product designed to adhere to oil, named Inipol EAP22 [19]; and a slow-release granular agricultural product

called Customblen [38]. The bioremediation was very successful, as shown in a joint monitoring program conducted by Exxon, the USEPA and the Alaska Department of Environmental Conservation [36]. Furthermore, this was achieved with no detectable adverse environmental impact [4, 36, 37]. Since then, bioremediation has been used on a limited site as part up of the cleanup of the Sea Empress spill [46], and has been demonstrated on experimental spills in marine or brackish environments on the Delaware Bay [48], a Texas wetland [26], a fine-sand beach in England [45], mangroves in Australia [40], and an Arctic shoreline in Spitsbergen [35].

Due to these successes, it is desirable to include bioremediation in responses to future spills where oil strands on rocky or inaccessible shorelines. In this situation currents can be used to carry the nutrients to the polluted zones instead of release it directly on the site. For such case, an important factor in achieving successful biostimulation, is obtaining an ideal (critical) concentration of nutrients needed for maximum growth of the organisms, and keeping this concentration as long as possible. This can become a difficult task taking into account that appropriate point for releasing the nutrients is unknown, and also because of physical influences, such as differences in densities, wave movements, and tidal influences. Tracer studies are often used to examine how the motion of the water and nutrients are influenced under different situations [2, 3].

In this chapter, a strategy is proposed for the remediation of oil-polluted marine environments which uses the fluid dynamic in a limited water region  $D$  to distribute a nutrient (nitrogen or phosphorus) and stimulate biodegradation in a few oil-polluted zones  $\Omega_i$  of  $D$ ,  $1 \leq i \leq N$ . For example, some recreation or aquaculture areas can be chosen as such zones. By the strategy, the nutrient released at points  $r_1, r_2, \dots, r_N$  of domain  $D$  with discharge rates  $Q_1(t), Q_2(t), \dots, Q_N(t)$  spreads by currents and turbulent diffusion and reaches all the contaminated zones. Moreover, a critical mean concentration of nutrient  $c_i$  (higher than the natural concentration) should be achieved and maintained in each oil-polluted zone  $\Omega_i$  within a certain time to properly stimulate the growth of the oil degrading microorganisms [2]. This time interval is denoted below as  $[T - \tau, T]$ . It should be noted that an adequate set of release rates  $\{Q_i(t)\}_{i=1}^N$  does not always exist, that is at times, this strategy fails. In particular, this can happen when the release points  $\{r_i\}_{i=1}^N$  are improperly chosen with respect to the flow and the location of zones  $\Omega_i$ , or when the time  $T$  is not large enough to let the nutrient to reach all the zones. In order to prevent such situations the problem is solved in two stages. In the first stage, each zone  $\Omega_i$  is considered separately from other and contains just one source. A variational problem is posed and solved in order to find both the optimal location of release point  $r_i$  in the zone and the optimal release rate  $Q_i(t)$  to reach the concentration  $c_i$  in  $\Omega_i$ ,  $1 \leq i \leq N$ . We prove that this problem has unique solution. In the second stage, we consider the process of dispersion of nutrient in all zones together. Due to advection by currents, the nutrient released in one zone can reach other polluted zones. Therefore we need to specify (modulate) the strength of all release rates  $Q_i(t)$  in order to fulfil the critical mean concentrations  $c_i$  in all the polluted zones during the time interval  $[T - \tau, T]$ . To this end, we introduce a positive coefficient  $\gamma_i$  to modulate each release rate

$Q_i(t)$ , such factors are chosen as the solution of a quadratic programming problem. Also, we prove the existence and uniqueness of this optimization problem. Note that a strategy is called optimal if it solves the problem and, at the same time, minimizes the total mass introduced into the aquatic system to mitigate the impact of nutrients on the marine environment and to reduce the remediation cost. Thus, by introducing the least amount of nutrients, the optimal control not only cleans the zones, but also protects the whole ecosystem.

The new strategy considers a few discharge points located so that each oil-polluted zone contains just one discharge point. It generalizes the previous strategy where the only source was used to distribute nutrient in all oil-contaminated areas. Analytical and numerical results for the case of unique source were obtained by considering variational formulations [31], quadratic programming problems [32] and linear programming problems [33].

Taking into account all the above remarks, the variational problem of the optimal two-stage remediation strategy is posed as follows:

$$\text{minimize } m(Q_1, \dots, Q_N) = \frac{1}{2} \sum_{i=1}^N \int_0^T Q_i^2(t) dt \quad (2.1)$$

$$\text{subject to: } c_i - \alpha_i \leq J_i(\phi) = \frac{1}{\tau |\Omega_i|} \int_{T-\tau}^T \int_{\Omega_i} \phi(r, t) dr dt \leq c_i + \beta_i, \quad 1 \leq i \leq N \quad (2.2)$$

$$0 \leq Q_i(t), \quad 0 \leq t \leq T, \quad 1 \leq i \leq N, \quad (2.3)$$

where  $m$  is the functional that represents the total mass of nutrient released into the aquatic system within a time interval  $[0, T]$  and  $\phi = \phi(r, t)$  is the concentration of this substance at point  $r$  in  $D$  at the time  $t > 0$ . Such concentration will be determined with a dispersion model described in Sect. 2.2. Besides, the functional  $J_i(\phi)$  is the mean concentration of nutrient in the  $i$ th zone  $\Omega_i$  within time interval  $[T - \tau, T]$  ( $1 \leq i \leq N$ ). Hereafter, we refer to this functional as the *direct estimation* of nutrient concentration. Without loss of generality, all the zones  $\Omega_i$  considered in this chapter are nonintersecting. The constraints in Eq. (2.2) are imposed to maintain the concentration  $J_i(\phi)$  in a vicinity of the critical concentration  $c_i$  required for optimal biodegradation ( $1 \leq i \leq N$ ). Thus,  $c_i - \alpha_i$  is the minimum concentration of nutrient in the oil-polluted zone  $\Omega_i$  acceptable for efficient stimulation of the biodegradation process, while  $c_i + \beta_i$  is the maximum allowable concentration of nutrient in the oil-polluted zone  $\Omega_i$  established for the protection of aquatic system. Note that the introduction of small positive parameters  $\alpha_i$  and  $\beta_i$  increases the number of feasible solutions of problem (2.1)–(2.3), and therefore this problem is less restrictive than that described by Parra-Guevara and Skiba [29, 31]. Finally, we note that the problem (2.1)–(2.3) can also be used to determine the optimal release parameters in a fairly common case, when the repeated application of nutrients is required

in the oil-contaminated areas due to the slow degradation of the oil in the marine environment. Sufficient conditions for such a methodology are given in Sect. 2.3.

## 2.2 Dispersion Model

The concentration of nutrient  $\phi(r, t)$  in a bounded domain  $D \subset \mathbb{R}^3$  and time interval  $[0, T]$  is estimated by the following dispersion model

$$\frac{\partial \phi}{\partial t} + \mathbf{U} \cdot \nabla \phi - \nabla \cdot \mu \nabla \phi + \sigma \phi + \nabla \cdot \phi_s = \sum_{i=1}^N Q_i(t) \delta(r - r_i) \quad (2.4)$$

$$\phi_s = -v_s \phi \mathbf{k}, \quad \text{in } D \quad (2.5)$$

$$\mu \frac{\partial \phi}{\partial n} = \phi_s \cdot \mathbf{n} - \zeta \phi \mathbf{k} \cdot \mathbf{n} \quad \text{on } S_T \quad (2.6)$$

$$\mu \frac{\partial \phi}{\partial n} = 0 \quad \text{on } S^+ \quad (2.7)$$

$$\mu \frac{\partial \phi}{\partial n} - U_n \phi = 0 \quad \text{on } S^- \quad (2.8)$$

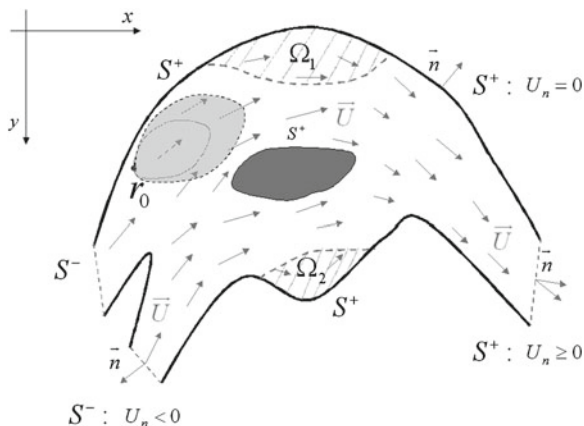
$$\mu \frac{\partial \phi}{\partial n} = 0 \quad \text{on } S_B \quad (2.9)$$

$$\phi(r, 0) = \phi^0(r) \quad \text{in } D \quad (2.10)$$

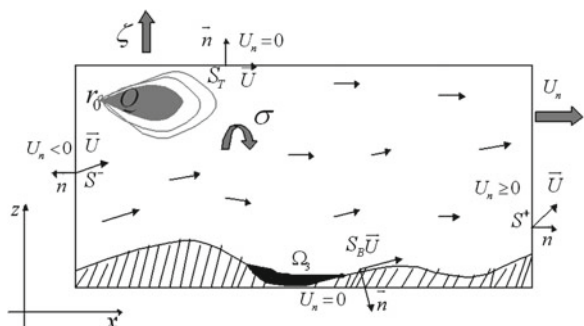
$$\nabla \cdot \mathbf{U} = 0 \quad \text{in } D. \quad (2.11)$$

Here (2.4) is the advection-diffusion equation,  $\mathbf{U}(r, t)$  is the known current velocity that satisfies the incompressibility condition (2.11),  $\mu(r, t)$  is the turbulent diffusion coefficient,  $\sigma(r, t)$  is the chemical transformation coefficient characterizing the decay rate of nutrient in water. Note that the first-order (linear) kinetics  $\sigma \phi$  describing the process of chemical transformation is a reasonable approximation for such nutrients in water as the nitrogen and phosphorus. The term  $\nabla \cdot \phi_s$  in (2.4), describes the change of concentration of nutrient per unit time because of sedimentation with constant velocity  $v_s > 0$ , and  $\delta(r - r_i)$  is the Dirac delta centred at the discharge point  $r_i$ . Equation (2.6) is the boundary condition on the free surface  $S_T$  of domain  $D$ , where  $\zeta(r, t)$  is the coefficient characterizing the process of evaporation of nutrient, and (2.9) represents the boundary condition on the bottom  $S_B$  of domain  $D$ . Equations (2.7) and (2.8) are the corresponding conditions on the lateral boundary of  $D$ , besides,  $S^+$  is the rigid or outflow part of the boundary where  $U_n = \mathbf{U} \cdot \mathbf{n} \geq 0$ , and  $S^-$  is its inflow part where  $U_n < 0$  (Fig. 2.1). Finally, Eq. (2.10) represents the initial distribution of the nutrient at  $t = 0$ . In all equations,  $\mathbf{n}$  is the unit outward normal

**Fig. 2.1** View of domain  $D$  from above



**Fig. 2.2** Cross-sectional area of domain  $D$



vector to the boundary  $\partial D = S_T \cup S^+ \cup S^- \cup S_B$  of domain  $D$ ,  $\partial/\partial n$  is the derivative in the normal direction, and  $\mathbf{k} = (0, 0, 1)^t$  is the unit vector directed upward in the Cartesian coordinate system (Fig. 2.2). We observe that

$$\mathbf{k} \cdot \mathbf{n} = 0 \text{ on } S^+ \cup S^- \text{ and } \mathbf{U} \cdot \mathbf{n} = 0 \text{ on } S_T \cup S_B. \quad (2.12)$$

Also note that the boundary conditions (2.6)–(2.9) are general (i.e., not only for horizontal free and bottom surfaces  $S_T$  and  $S_B$ ), and hence, the dispersion model can take into account free surface wave motion and marine topography.

First of all we show that the solution of dispersion model (2.4)–(2.11) satisfies the mass balance equation. Indeed, integrating Eq. (2.4) over domain  $D$  we get

$$\begin{aligned} \frac{\partial}{\partial t} \int_D \phi \, dr + \int_D \mathbf{U} \cdot \nabla \phi \, dr - \int_D \nabla \cdot \mu \nabla \phi \, dr + \int_D \sigma \phi \, dr + \int_D \nabla \cdot \phi_s \, dr \\ = \sum_{i=1}^N \int_D Q_i(t) \delta(r - r_i) \, dr. \end{aligned}$$

Applying the divergence theorem [18], it is possible to rewrite some integrals as

$$\begin{aligned}\int_D \mathbf{U} \cdot \nabla \phi \, dr &= \int_D \nabla \cdot (\mathbf{U}\phi) \, dr = \int_{\partial D} \mathbf{U} \cdot \mathbf{n} \phi \, dS, \\ \int_D \nabla \cdot \mu \nabla \phi \, dr &= \int_{\partial D} \mu \nabla \phi \cdot \mathbf{n} \, dS = \int_{\partial D} \mu \frac{\partial \phi}{\partial n} \, dS, \\ \int_D \nabla \cdot \phi_s \, dr &= \int_{\partial D} \phi_s \cdot \mathbf{n} \, dS.\end{aligned}$$

Finally, dividing each integral over boundary  $\partial D$  into the four integrals over  $S_T$ ,  $S^+$ ,  $S^-$  and  $S_B$ , and applying Eqs. (2.6)–(2.9) and observation (2.12), we obtain the mass balance equation:

$$\frac{\partial}{\partial t} \int_D \phi \, dr = \sum_{i=1}^N Q_i(t) - \int_D \sigma \phi \, dr - \int_{S^+} U_n \phi \, dS - \int_{S_T} \zeta \phi \mathbf{k} \cdot \mathbf{n} \, dS + \int_{S_B} v_s \phi \mathbf{k} \cdot \mathbf{n} \, dS. \quad (2.13)$$

Since  $\mathbf{k} \cdot \mathbf{n} > 0$  at  $S_T$  and  $\mathbf{k} \cdot \mathbf{n} < 0$  at  $S_B$ , the total mass of the nutrient increases due to the discharge processes ( $Q_i(t) > 0$ ), and decreases because of the chemical transformations ( $\sigma > 0$ ), advective outflow through  $S^+$  ( $U_n > 0$ ), superficial evaporation ( $\zeta > 0$ ) and sedimentation ( $v_s > 0$ ).

We now show that the dispersion problem (2.4)–(2.11) is well posed. Indeed, the model operator is:

$$A\phi = \mathbf{U} \cdot \nabla \phi - \nabla \cdot \mu \nabla \phi + \sigma \phi + \nabla \cdot \phi_s. \quad (2.14)$$

Defining the inner product in  $L_2(D)$  as  $(A\phi, \phi) = \int_D \phi A\phi \, dr$  we obtain the expression

$$(A\phi, \phi) = \int_D \phi \mathbf{U} \cdot \nabla \phi \, dr + \int_D \sigma \phi^2 \, dr - \int_D \phi \nabla \cdot \mu \nabla \phi \, dr + \int_D \phi \nabla \cdot \phi_s \, dr.$$

The divergence theorem allows modifying some integrals in the last equation:

$$\int_D \phi \mathbf{U} \cdot \nabla \phi \, dr = \frac{1}{2} \int_{\partial D} \phi^2 \mathbf{U} \cdot \mathbf{n} \, dS,$$

$$\int_D \phi \nabla \cdot (\mu \nabla \phi) dr = \int_{\partial D} \phi \mu \frac{\partial \phi}{\partial n} dS - \int_D \mu |\nabla \phi|^2 dr,$$

$$\int_D \phi \nabla \cdot \phi_s dr = \frac{1}{2} \int_{\partial D} \phi \phi_s \cdot \mathbf{n} dS.$$

Finally, dividing each integral over  $\partial D$  into the four integrals over  $S_T$ ,  $S^+$ ,  $S^-$  and  $S_B$ , and applying the conditions (2.6)–(2.9) and (2.12), we get

$$\begin{aligned} (A\phi, \phi) &= \int_D \sigma \phi^2 dr + \int_D \mu |\nabla \phi|^2 dr + \int_{S_T} \zeta \phi^2 \mathbf{k} \cdot \mathbf{n} dS \\ &+ \frac{1}{2} \left\{ \int_{S^+} U_n \phi^2 dS - \int_{S^-} U_n \phi^2 dS + \int_{S_T} v_s \phi^2 \mathbf{k} \cdot \mathbf{n} dS - \int_{S_B} v_s \phi^2 \mathbf{k} \cdot \mathbf{n} dS \right\} \end{aligned} \quad (2.15)$$

Since  $U_n < 0$  in  $S^-$ ,  $\mathbf{k} \cdot \mathbf{n} > 0$  at  $S_T$  and  $\mathbf{k} \cdot \mathbf{n} < 0$  at  $S_B$ , Eq.(2.15) can be rewritten as

$$\begin{aligned} (A\phi, \phi) &= \int_D \sigma \phi^2 dr + \int_D \mu |\nabla \phi|^2 dr + \int_{S_T} \zeta \phi^2 \mathbf{k} \cdot \mathbf{n} dS \\ &+ \frac{1}{2} \left\{ \int_{S^+ \cup S^-} |U_n| \phi^2 dS + \int_{S_T \cup S_B} v_s \phi^2 |\mathbf{k} \cdot \mathbf{n}| dS \right\}. \end{aligned}$$

Thus, operator  $A$  is positive semidefinite:  $(A\phi, \phi) \geq 0$ .

Taking the inner product of every term of Eq.(2.4) with  $\phi$  we obtain

$$\left( \frac{\partial \phi}{\partial t}, \phi \right) = (f, \phi) - (A\phi, \phi), \quad f(r, t) = \sum_{i=1}^N Q_i(t) \delta(r - r_i).$$

Using the condition  $(A\phi, \phi) \geq 0$  and the Schwarz inequality [17], the last equation implies the inequality

$$\left( \phi, \frac{\partial \phi}{\partial t} \right) \leq \|\phi\| \|f\|, \quad \|\phi\| = \sqrt{(\phi, \phi)}.$$

Further,

$$\left( \phi, \frac{\partial \phi}{\partial t} \right) = \frac{1}{2} \frac{\partial}{\partial t} \|\phi\|^2 = \|\phi\| \frac{\partial}{\partial t} \|\phi\|$$



and hence,

$$\frac{\partial}{\partial t} \|\phi\| \leq \|f\|.$$

Finally, the integration over time interval  $(0, T)$  leads to

$$\|\phi\| \leq T \max_{0 \leq t \leq T} \|f(r, t)\| + \|\phi^0(r)\|. \quad (2.16)$$

Since the dispersion model (2.4)–(2.11) is linear with respect to  $\phi$ , estimation (2.16) assures that the solution of problem (2.4)–(2.11) is unique and continuously depends on the initial conditions and forcing. Also, using the method described by Skiba and Parra-Guevara [43], it is possible to prove the existence of generalized solution of problem (2.4)–(2.11), that is the model (2.4)–(2.11) is well posed in the sense of Hadamard [13]. Also note that the positive semidefiniteness of operator  $A$  allows us to split the operator  $A$  in coordinate directions, and with the help of numerical schemes by Marchuk [22] and Crank-Nicolson [8] construct unconditionally stable and efficient numerical algorithm of second approximation order in space and time for the solution of problem (2.4)–(2.11) [41].

### 2.3 Adjoint Functions and the Duality Principle

It is rather difficult to analyse and solve the variational problem (2.1)–(2.3) because the constraints in (2.2) are related with the solutions  $Q_i$  of the control problem implicitly through the solution  $\phi$  of the dispersion model (2.4)–(2.11). In order to establish an explicit dependence of the constraints on the control functions  $Q_i$ , we now introduce one more model which is adjoint to the dispersion model (2.4)–(2.11). It means that the operator  $A^*$  is adjoint to the operator  $A$  of the model (2.4)–(2.11) in the sense of the Lagrange identity

$$(A\phi, g) = (\phi, A^*g),$$

where  $(\cdot, \cdot)$  denotes the inner product in the Hilbert space  $L_2(D)$  [22]. Solutions of this adjoint model will be used to establish a duality principle for the mean concentration of the released nutrient in the marine environment. Let us construct the operator  $A^*$ . The inner product  $(A\phi, g)$  is

$$(A\phi, g) = \int_D g\mathbf{U} \cdot \nabla\phi \, dr + \int_D \sigma g\phi \, dr - \int_D g\nabla \cdot \mu\nabla\phi \, dr + \int_D g\nabla \cdot \phi_s \, dr.$$

The integrals in the last expression can be rewritten with the divergence theorem as follows

$$\int_D g\mathbf{U} \cdot \nabla\phi \, dr = \int_{\partial D} g\phi\mathbf{U} \cdot \mathbf{n} \, dS - \int_D \phi\mathbf{U} \cdot \nabla g \, dr,$$

$$\int_D g \nabla \cdot \mu \nabla \phi \, dr = \int_{\partial D} g \mu \frac{\partial \phi}{\partial n} \, dS - \int_{\partial D} \phi \mu \frac{\partial g}{\partial n} \, dS + \int_D \phi \nabla \cdot \mu \nabla g \, dr,$$

$$\int_D g \nabla \cdot \phi_s \, dr = \int_{\partial D} g \phi_s \cdot \mathbf{n} \, dS - \int_D \phi \nabla \cdot \mathbf{g}_s \, dr,$$

where  $\mathbf{g}_s = -v_s g \mathbf{k}$ . Then

$$(A\phi, g) = \int_D \phi (-\mathbf{U} \cdot \nabla g - \nabla \cdot \mu \nabla g + \sigma g - \nabla \cdot \mathbf{g}_s) \, dr$$

$$+ \int_D g \phi \mathbf{U} \cdot \mathbf{n} \, dS + \int_{\partial D} \phi \mu \frac{\partial g}{\partial n} \, dS - \int_{\partial D} g \mu \frac{\partial \phi}{\partial n} \, dS + \int_{\partial D} g \phi_s \cdot \mathbf{n} \, dS.$$

Dividing the integrals over boundary  $\partial D$  into four integrals over  $S_T$ ,  $S^+$ ,  $S^-$  and  $S_B$ , and using conditions (2.6)–(2.9) and (2.12), we obtain that

$$(A\phi, g) = \int_D \phi (-\mathbf{U} \cdot \nabla g - \nabla \cdot \mu \nabla g + \sigma g - \nabla \cdot \mathbf{g}_s) \, dr$$

provided that the function  $g$  satisfies the boundary conditions (2.20)–(2.23) (see below). Thus, the Lagrange identity is fulfilled if

$$A^* g = -\mathbf{U} \cdot \nabla g - \nabla \cdot \mu \nabla g + \sigma g - \nabla \cdot \mathbf{g}_s.$$

On the other hand, multiplying Eq.(2.4) by  $g$  and integrating the result over the space-time domain  $D \times (0, T)$ , we get

$$\int_0^T \int_D g \frac{\partial \phi}{\partial t} \, dr dt + \int_0^T \int_D g A \phi \, dr dt = \int_0^T \int_D g \left\{ \sum_{i=1}^N Q_i(t) \delta(r - r_i) \right\} \, dr dt.$$

Integration by parts of the first integral, together with conditions (2.10) and  $g(r, T) = 0$ , leads to

$$\int_0^T \int_D g \frac{\partial \phi}{\partial t} \, dr dt = - \int_D g(r, 0) \phi^0(r) \, dr - \int_0^T \int_D \phi \frac{\partial g}{\partial t} \, dr dt$$

Applying now Eq. (2.4), the Lagrange identity and the well-known property of the Dirac delta one can obtain

$$\int_0^T \int_D \phi \left\{ -\frac{\partial g}{\partial t} + A^* g \right\} dr dt = \sum_{i=1}^N \int_0^T Q_i(t) g(r_i, t) dt + \int_D g(r, 0) \phi^0(r) dr. \quad (2.17)$$

In order to take advantage of Eq. (2.17), which explicitly relates the discharge rates of nutrient  $Q_i(t)$  with the concentration of nutrient  $\phi(r, t)$  through the adjoint function  $g$ , we consider the following adjoint dispersion model:

$$-\frac{\partial g}{\partial t} - \mathbf{U} \cdot \nabla g - \nabla \cdot \mu \nabla g + \sigma g - \nabla \cdot \mathbf{g}_s = p(r, t), \quad (2.18)$$

$$\mathbf{g}_s = -v_s g \mathbf{k} \text{ in } D, \quad (2.19)$$

$$\mu \frac{\partial g}{\partial n} + \zeta g \mathbf{k} \cdot \mathbf{n} = 0 \text{ on } S_T, \quad (2.20)$$

$$\mu \frac{\partial g}{\partial n} + U_n g = 0 \text{ on } S^+, \quad (2.21)$$

$$\mu \frac{\partial g}{\partial n} = 0 \text{ on } S^-, \quad (2.22)$$

$$\mu \frac{\partial g}{\partial n} = -\mathbf{g}_s \cdot \mathbf{n} \text{ on } S_B, \quad (2.23)$$

$$g(r, T) = 0 \text{ in } D. \quad (2.24)$$

Note that the boundary conditions (2.20)–(2.23) and final condition (2.24) imposed on the solution are those that guarantee the fulfilment of the Lagrange identity. Furthermore, one can see that the first, the second and the fifth terms of Eqs. (2.4) and (2.18) have opposite signs. Thus, the comparison of the equations and boundary conditions of the models (2.4)–(2.12) and (2.18)–(2.24) leads to the important result: if the adjoint model (2.18)–(2.24) is solved backward in time (from  $t = T$  to  $t = 0$ ) then it also has a unique solution, which continuously depends on the forcing  $p(r, t)$ . This result can be immediately shown by the transformation of variable  $t' = T - t$ , cf. [43].

Moreover, the forcing  $p(r, t)$  of Eq. (2.18) can be defined so that the mean concentration of nutrient

$$J_i(\phi) = \frac{1}{\tau |\Omega_i|} \int_{T-\tau}^T \int_{\Omega_i} \phi(r, t) dr dt$$

in an oil-polluted zone  $\Omega_i \subset D$  will be explicitly related with all the discharge rates  $Q_j(t)$ ,  $j = 1, \dots, N$ , and initial concentration of nutrient  $\phi^0(r)$  through the adjoint

solution  $g$ . Indeed, let us take

$$p(r, t) = \begin{cases} \frac{1}{\tau|\Omega_i|}, & r \in \Omega_i \text{ and } t \in (T - \tau, T) \\ 0, & \text{otherwise} \end{cases}$$

where  $|\Omega_i|$  denotes the volume of oil-polluted zone, and  $\tau$  is the time required for the nutrient to reach its critical concentration in the zone. Then the use of this formula in (2.18) leads to

$$J_i(\phi) = \sum_{j=1}^N \int_0^T g_i(r_j, t) Q_j(t) dt + \int_D g_i(r, 0) \phi^0(r) dr, \quad (2.25)$$

also known as the duality principle. Provided that  $\phi^0(r) = 0$  for the first discharge of nutrient, the last formula is reduced to

$$J_i(\phi) = \sum_{j=1}^N \int_0^T g_i(r_j, t) Q_j(t) dt. \quad (2.26)$$

The use of (2.26) in (2.2) for each zone  $\Omega_i$  ( $i = 1, \dots, N$ ), transforms the variational problem (2.1)–(2.3) to a more convenient form for the analysis:

$$\text{minimize } m(Q_1, \dots, Q_N) = \frac{1}{2} \sum_{j=1}^N \int_0^T Q_j^2(t) dt \quad (2.27)$$

$$\text{subject to: } c_i - \alpha_i \leq \sum_{j=1}^N \int_0^T g_i(r_j, t) Q_j(t) dt \leq c_i + \beta_i, \quad 1 \leq i \leq N \quad (2.28)$$

$$0 \leq Q_j(t), \quad 0 \leq t \leq T, \quad 1 \leq j \leq N. \quad (2.29)$$

Note that problem (2.27)–(2.29) uses  $N$  adjoint functions  $g_i(r, t)$ , which, when restricted to the discharge points  $r_j$ ,  $j = 1, \dots, N$ , generate  $N^2$  temporal influence functions  $g_i(r_j, t)$ . Each function  $g_i(r_j, t)$  compresses dynamical information necessary to estimate how a signal emitted at point  $r_j$  impacts the zone  $\Omega_i$ . As a consequence, the duality principle (2.26) quantifies the total effect on zone  $\Omega_i$  due to the signals emitted at points  $r_j$ ,  $j = 1, \dots, N$ .

However, if a repeated discharge of nutrient is needed for degrading oil-residuals, then the nonzero initial concentration of the nutrient must be taken into account (see (2.25)). It should be noted that, due to microbial intake of nutrient in the oil-polluted

zones and the water outflow from region  $D$ , the concentration of nutrient decreases in region  $D$  towards its natural value. Therefore, the following conditions for the mean concentration of nutrient must be fulfilled since the moment  $t_0 > T$ :

$$\frac{1}{|\Omega_i|} \int_{\Omega_i} \phi(r, t) dr < c_i + \beta_i \quad i = 1, \dots, N \quad t \geq t_0 \quad (2.30)$$

The moment  $t_0$  can be determined through monitoring the mean concentration of nutrient in region  $D$  or by using the solution  $\phi$  forecasted by the model (2.4)–(2.11) with the forcing  $Q_j(t)$  equal to zero for  $t > T$  and  $j = 1, \dots, N$ . Once conditions (2.30) are fulfilled, the initial concentration for modelling the next application of nutrient is chosen as

$$\varphi^0(r) = \phi(r, t_0) \quad (2.31)$$

and the next time interval for such modelling is  $[t_0, t_0 + T]$ . Due to the conditions (2.30), the contribution of the new initial condition  $\varphi^0(r)$  to the mean concentrations of nutrient during time interval  $[t_0 + T - \tau, t_0 + T]$  is less than the upper bounds  $c_i + \beta_i$  in  $\Omega_i$ , ( $i = 1, \dots, N$ ). Note that without such conditions the feasibility space for problem (2.1)–(2.3) is empty and there is no solution to the control problem.

Thus, if the conditions (2.30) are fulfilled then one can take  $t_0 = 0$  and consider the problem (2.27)–(2.29) again for modelling the second discharge of nutrient with the following positive parameters:

$$c'_i = c_i - \int_D g_i(r, 0) \varphi^0(r) dr, \quad i = 1, \dots, N. \quad (2.32)$$

Note that the adjoint functions in (2.32) must be calculated in time interval  $[t_0, t_0 + T]$ . Also we assume, without loss of generality, that negative values, if they appear on the left side of the constraints (2.28), are replaced by zero. With these remarks, the variational problem (2.27)–(2.29) represents a general remediation strategy which can be applied repeatedly.

It is important to note that all the adjoint solutions  $g_i(r_j, t)$  which figure in constraints (2.28) are independent of the discharge rates  $Q_j(t)$ . This non-negative solutions are determined by the dynamical processes in region  $D$  and serve in constraints (2.28) as the weight functions characterizing the effect of the discharge of nutrient at a point  $r_j$  on the mean concentration of nutrient in a zone  $\Omega_i$  (see Figs. 2.3, 2.4 and 2.5). In other words, the adjoint solutions are the influence functions (or information functions) in the control theory. That is why the adjoint problem solutions are widely used in the sensitivity study of various models, and in particular, in the atmosphere and ocean model, weather forecast and climate theory [21, 23], data assimilation problems [24], problems of identification of unknown pollution sources, like nuclear accidents [28, 34, 39, 50], simulation of oil pollution [9, 42] and optimal control in pollution problems [1, 15, 16, 20, 22, 30, 33, 49].

## 2.4 Peculiarities of Dual Estimates and Sensitivity Formulas

We now discuss the main features of the dual estimate (2.25), or its simplification (2.26), and show the usefulness of the adjoint estimates in the study of sensitivity of mean concentration  $J_i(\phi)$  to variations in the discharge rates and positions of the sources as well as in the initial distribution  $\phi^0(r)$  of nutrient.

In environmental monitoring, the adjoint estimate (2.25) is a good complement to the direct mean concentration estimate  $J_i(\phi)$ . One can use either direct or adjoint estimates depending on the specific situation. Assume, for example, that the mean concentration  $J_i(\phi)$  of a nutrient is monitored in  $N$  ecologically important zones  $\Omega_i$  of domain  $D$  ( $i = 1, \dots, N$ ). If the number of zones  $N$  is large enough then it is better to solve problem (2.4)–(2.11) and use direct estimate of  $J_i(\phi)$  in each zone. On the other hand, if number  $N$  is rather small then it is more effective and economical to solve adjoint problem (2.18)–(2.24) and use adjoint estimate (2.25). Unlike the direct mean concentration estimate of nutrient, the adjoint estimate (2.25) permits to explicitly evaluate the contribution of each source to value  $J_i(\phi)$ .

In the case of invariable emission rates ( $Q_j(t) = Q_j$ ), evaluation (2.26) becomes even simpler:

$$J_i(\phi) = \sum_{j=1}^N Q_j w_{ij}, \quad (2.33)$$

where

$$w_{ij} = \int_0^T g_i(r_j, t) dt. \quad (2.34)$$

Each weight  $w_{ij}$  depends only on the adjoint solution and characterizes the contribution of the source with emission rate  $Q_j$  to the mean concentration  $J_i(\phi)$  in  $\Omega_i$ .

What is then the basic difference between the direct and adjoint estimates of the mean concentration of nutrient  $J_i(\phi)$ ? The direct estimate, relating to the solution  $\phi(r, t)$  of problem (2.4)–(2.11), is independent of a concrete zone  $\Omega$ , but depends on the discharge rates  $Q_j$  and position  $r_j$  of sources, and also on the initial distribution of nutrient  $\phi^0(r)$  in  $D$ . For this reason such a estimate is preferable if one needs to know the concentration of a substance in many zones of  $D$ , or in each point of  $D \times (0, T)$ . However, in the model sensitivity study, this approach requires much computing time, because the solution  $\phi(r, t)$  of problem (2.4)–(2.11) must be recalculated whenever new values of the parameters  $Q_j$ ,  $r_j$  or  $\phi^0(r)$  are used. Unlike it, the solutions of adjoint problem  $g_i(r_j, t)$  depend on  $\Omega_i$  zone, but are independent of  $Q_j$ ,  $r_j$  or  $\phi^0(r)$ . In the adjoint evaluation (2.25),  $g_i(r_j, t)$  serves as the weight function characterizing the model response to these three parameters. Since the problem is linear, Eq. (2.25) leads to the main sensitivity formula

$$\delta J_i(\phi) = \sum_{j=1}^N \int_0^T g_i(r_j, t) \delta Q_j(t) dt + \int_D g_i(r, 0) \delta \phi^0(r) dr \quad (2.35)$$

that relates a variation  $\delta J_i(\phi)$  in the mean concentration of nutrients in  $\Omega_i$  with variations  $\delta Q_j$  and  $\delta\phi^0$  in the emission rates  $Q_j$  and initial distribution of nutrient  $\phi^0$ . It makes the estimates (2.25) and (2.35) rather efficient and computationally economical, because the solutions  $g_i(r_j, t)$ , once found, can be re-used in these formulas for different values of  $Q_j, r_j$  or  $\phi^0(r)$ .

The effect of changing the position of sources from  $r_j$  to  $r'_j, j = 1, \dots, N$ , is estimated by the formula

$$\delta J_i(\phi) = \sum_{j=1}^N \int_0^T \left\{ g_i(r'_j, t) - g_i(r_j, t) \right\} Q_j(t) dt. \quad (2.36)$$

Finally, we give without proof a general sensitivity formula

$$\begin{aligned} \delta J_i(\phi) = & \sum_{j=1}^N \int_0^T g_i(r_j, t) \delta Q_j(t) dt + \int_D g_i(r, 0) \delta\phi^0(r) dr \\ & - \int_0^T \int_{S_T} g_i(r, t) \phi(r, t) \delta\zeta(r, t) dS dt - \int_0^T \int_D g_i(r, t) B(r, t) dr dt, \end{aligned} \quad (2.37)$$

where

$$B(r, t) = \delta\mathbf{U} \cdot \nabla\phi - \nabla \cdot \delta\mu\nabla\phi + \delta\sigma\phi + \delta v_s \frac{\partial\phi}{\partial z},$$

cf. [43], taking into account arbitrary variations  $\delta Q_j(t)$  and  $\delta\phi^0(r)$ , and small variations  $\delta\mathbf{U}, \delta\sigma, \delta\mu, \delta v_s$  and  $\delta\zeta$  in the domain  $D$ . Unlike the previous formulas, estimate (2.37) is more complicated, because it uses solutions of both problems (2.4)–(2.11) and (2.18)–(2.24) and linearised equations for perturbations.

## 2.5 Main and Adjoint Numerical Schemes of the Dispersion Problem

In this section, balanced and absolutely stable second-order finite difference schemes based on the application of the splitting method by Marchuk [22] and Crank-Nicolson schemes [8] are developed to solve numerically the dispersion model (2.4)–(2.11) and its adjoint formulation (2.18)–(2.24). Since they were described in detail in Skiba [41], we give here only basic results.

Using the continuity Eq.(2.11), the operator  $A$  of Eq.(2.4) can be written as  $A = A_1 + A_2 + A_3$ , where

$$\begin{aligned}
A_1\phi &= \frac{1}{2} \frac{\partial}{\partial x}(u\phi) + \frac{1}{2} u \frac{\partial \phi}{\partial x} - \frac{\partial}{\partial x} \mu \frac{\partial \phi}{\partial x} + \frac{1}{3} \sigma \phi \\
A_2\phi &= \frac{1}{2} \frac{\partial}{\partial y}(v\phi) + \frac{1}{2} v \frac{\partial \phi}{\partial y} - \frac{\partial}{\partial y} \mu \frac{\partial \phi}{\partial y} + \frac{1}{3} \sigma \phi \\
A_3\phi &= \frac{1}{2} \frac{\partial}{\partial z}(\tilde{w}\phi) + \frac{1}{2} \tilde{w} \frac{\partial \phi}{\partial z} - \frac{\partial}{\partial z} \mu \frac{\partial \phi}{\partial z} + \frac{1}{3} \sigma \phi
\end{aligned} \tag{2.38}$$

and  $\tilde{w} = w - v_s$ .

We now show that each one-dimensional split operator  $A_i$  ( $i = 1, 2, 3$ ) is positive semidefinite (or positive definite if  $\sigma > 0$ ), cf. [41]. For simplicity, consider only the case when domain  $D$  is a cube  $[0, X] \times [0, Y] \times [0, Z]$ . Then

$$\int_0^X \phi A_1 \phi dx = \frac{1}{3} \int_0^X \sigma \phi^2 dx + \int_0^X \mu \left( \frac{\partial \phi}{\partial x} \right)^2 dx + \left[ \frac{1}{2} \phi^2 u - \mu \phi \frac{\partial \phi}{\partial x} \right]_0^X.$$

Assume that  $u(0) > 0$  and  $u(X) > 0$ . Then the boundary point  $x = 0$  belongs to  $S^-$ , while point  $x = X$  belongs to  $S^+$ . Applying condition (2.8) at  $x = 0$  and condition (2.7) at  $x = X$ , we get

$$\left[ \frac{1}{2} \phi^2 u - \mu \phi \frac{\partial \phi}{\partial x} \right]_0^X = \frac{1}{2} [\phi^2(X)u(X) + \phi^2(0)u(0)] \geq 0.$$

Since  $\sigma > 0$  and  $\mu > 0$ , we conclude that

$$(A_1\phi, \phi)_{L_2(D)} = \int_0^Z \int_0^Y \int_0^X \phi A_1 \phi dx dy dz \geq 0.$$

In the same way one can show that  $A_2$  and  $A_3$  are also positive semidefinite operators. It should be noted that this proof is also true for any region  $D$  which represents a union of finite number of cubes.

On the other hand, the operator of the adjoint problem (2.18)–(2.24) and (2.11) is the adjoint of  $A$ , and can be written as the sum  $A^* = A_1^* + A_2^* + A_3^*$  where

$$\begin{aligned}
A_1^*g &= -\frac{1}{2} \frac{\partial}{\partial x}(ug) - \frac{1}{2} u \frac{\partial g}{\partial x} - \frac{\partial}{\partial x} \mu \frac{\partial g}{\partial x} + \frac{1}{3} \sigma g \\
A_2^*g &= -\frac{1}{2} \frac{\partial}{\partial y}(vg) - \frac{1}{2} v \frac{\partial g}{\partial y} - \frac{\partial}{\partial y} \mu \frac{\partial g}{\partial y} + \frac{1}{3} \sigma g \\
A_3^*g &= -\frac{1}{2} \frac{\partial}{\partial z}(\tilde{w}g) - \frac{1}{2} \tilde{w} \frac{\partial g}{\partial z} - \frac{\partial}{\partial z} \mu \frac{\partial g}{\partial z} + \frac{1}{3} \sigma g.
\end{aligned} \tag{2.39}$$

Suppose for simplicity that  $\mu = \mu(z)$ , and define the net functions on different grids:



$$\phi_{ijk} = \phi(x_i, y_j, z_k), \quad u_{ijk} = u(x_{i-1/2}, y_j, z_k), \quad v_{ijk} = v(x_i, y_{j-1/2}, z_k)$$

$$w_{ijk} = w(x_i, y_j, z_{k-1/2}), \quad \mu_k = \mu(z_k), \quad v_{ijk} = v(x_i, y_j, z_{k-1/2})$$

The second-order discrete approximation of the operators  $A_i$  and continuity Eq. (2.11) have the following form (invariable indices  $i, j, k$  are omitted)

$$\left(A_1^h \phi\right)_{ijk} = \frac{u_{i+1}\phi_{i+1} - u_i\phi_{i-1}}{2\Delta x} - \frac{\mu_k [\phi_{i+1} - 2\phi_i + \phi_{i-1}]}{(\Delta x)^2} + \frac{\sigma\phi_i}{3} \quad (2.40)$$

$$\left(A_2^h \phi\right)_{ijk} = \frac{v_{j+1}\phi_{j+1} - v_j\phi_{j-1}}{2\Delta y} - \frac{\mu_k [\phi_{j+1} - 2\phi_j + \phi_{j-1}]}{(\Delta y)^2} + \frac{\sigma\phi_j}{3} \quad (2.41)$$

$$\left(A_3^h \phi\right)_{ijk} = \frac{\tilde{w}_{k+1}\phi_{k+1} - \tilde{w}_k\phi_{k-1}}{2\Delta z} - \frac{\mu_{k+1}(\phi_{k+1} - \phi_k) - \mu_k(\phi_k - \phi_{k-1})}{(\Delta z)^2} + \frac{\sigma\phi_k}{3} \quad (2.42)$$

$$\frac{(u_{i+1} - u_i)}{\Delta x} + \frac{(v_{j+1} - v_j)}{\Delta y} + \frac{(w_{k+1} - w_k)}{\Delta z} = 0 \quad (2.43)$$

We immediately obtain the form of adjoint operators  $(A_i^h)^*$  if we substitute  $u, v, \tilde{w}$ , and  $\phi$  in (2.40)–(2.43) by  $-u, -v, -\tilde{w}$ , and  $g$ , respectively. To show how the boundary conditions are discretised, we give only one example (see [41] for more details). Let  $u_{ijk}$  be a positive value of the  $u$ -component of the velocity at the left boundary point  $M = (x_{1/2}, y_j, z_k)$  of the grid domain. Then,  $U_n = -u_{1jk} < 0$ , i.e., the point  $M$  belongs to  $S^-$ , and conditions (2.8) and (2.22) are approximated as

$$\mu_k \frac{(\phi_{0jk} - \phi_{1jk})}{\Delta x} - u_{1jk} \frac{(\phi_{0jk} - \phi_{1jk})}{2} = 0, \quad g_{0jk} = g_{1jk} \quad (2.44)$$

Thus, for any  $i$  ( $i = 1, 2, 3$ ), the discrete operators  $A_i^h$  and  $(A_i^h)^*$  are positive semidefinite, and they are skew-symmetric if  $\mu = \sigma = 0$  and  $S$  is the coast line ( $U_n = 0$  everywhere at  $S$ ).

The problems (2.4)–(2.11) and (2.18)–(2.24) are solved in time with the symmetrized double-cycle componentwise splitting method by Marchuk [23, 41], i.e., within each double time step interval  $(t_n - \Delta t, t_n + \Delta t)$  the main and adjoint numerical schemes have the form

$$\Phi \left[ n - \frac{3-i}{3} \right] - \Phi \left[ n - \frac{4-i}{3} \right] = -\frac{\tau}{2} A_i^h \left( \Phi \left[ n - \frac{3-i}{3} \right] + \Phi \left[ n - \frac{4-i}{3} \right] \right) \quad (i = 1, 2)$$

$$\Phi\left[n + \frac{1}{3}\right] - \Phi\left[n - \frac{1}{3}\right] = -\tau A_3^h \left( \Phi\left[n + \frac{1}{3}\right] + \Phi\left[n - \frac{1}{3}\right] \right) + 2\tau q[n] \quad (2.45)$$

$$\Phi\left[n + \frac{4-i}{3}\right] - \Phi\left[n + \frac{3-i}{3}\right] = -\frac{\tau}{2} A_i^h \left( \Phi\left[n + \frac{4-i}{3}\right] + \Phi\left[n + \frac{3-i}{3}\right] \right) \quad (i = 2, 1)$$

and

$$G\left[n + \frac{3-i}{3}\right] - G\left[n + \frac{4-i}{3}\right] = -\frac{\tau}{2} (A_i^h)^* \left( G\left[n + \frac{3-i}{3}\right] + G\left[n + \frac{4-i}{3}\right] \right) \quad (i = 1, 2)$$

$$G\left[n - \frac{1}{3}\right] - G\left[n + \frac{1}{3}\right] = -\tau (A_3^h)^* \left( G\left[n - \frac{1}{3}\right] + G\left[n + \frac{1}{3}\right] \right) + 2\tau p[n] \quad (2.46)$$

$$G\left[n - \frac{4-i}{3}\right] - G\left[n - \frac{3-i}{3}\right] = -\frac{\tau}{2} (A_i^h)^* \left( G\left[n - \frac{4-i}{3}\right] + G\left[n - \frac{3-i}{3}\right] \right) \quad (i = 2, 1),$$

where  $\Phi$  and  $G$  are the vectors representing the grid values of solutions  $\phi$  and  $g$  at fractional time steps, and  $q$  and  $p$  are the vectors representing the grid values of functions  $Q$  and  $P$  at moment  $t_n$ , respectively [41]. The discretization in time of each one-dimensional split problem is performed with the Crank-Nicolson scheme, and the resulting discrete problem is efficiently solved by the Thomas' factorization method for the tridiagonal matrices [24]. The unconditional stability of the numerical schemes (2.45) and (2.46) directly follows from the inequalities

$$\|\Phi[n+1]\| \leq \|\Phi[n-1]\| + 2\tau \|q[n]\| \quad (2.47)$$

and

$$\|G[n-1]\| \leq \|G[n+1]\| + 2\tau \|p[n]\|, \quad (2.48)$$

where  $\|\cdot\|$  is the Euclidean vector norm [41]. The use of Lagrange identity leads to the equation

$$G^*[n+1]\Phi[n+1] + \tau p^*[n] \left( \Phi\left[n + \frac{1}{3}\right] + \Phi\left[n - \frac{1}{3}\right] \right) = \tau \left( G^*\left[n + \frac{1}{3}\right] - G^*\left[n - \frac{1}{3}\right] \right) q[n] + G^*[n-1]\Phi[n-1] \quad (2.49)$$

in each subinterval  $[t_n - \Delta t, t_n + \Delta t]$ . The sum of such relations over all subintervals in  $[0, T]$  (i.e., over all  $n$ ) and the use of conditions (2.10) and (2.24) leads to a discrete version of adjoint estimate (2.26).

## 2.6 Theoretical Results: Existence, Uniqueness and Formulation of Discharge Parameters

### 2.6.1 First Stage: Discharge Points and Basic Form of Discharge Rates of Nutrient

In order to find the optimal discharge points  $r_i$  in  $D$ , and the basic shape of discharge rates  $Q_i(t)$  at these points, we consider here the variational problem (2.27)–(2.29) for  $N = 1$  and  $\alpha_1 = \beta_1 = 0$ . That is we consider in the first stage of the strategy just a local problem of remediation in which the critical concentration  $c_1$  is reached exactly. Thus, taking into account the corresponding adjoint function  $g_1(r, t)$  for the oil-polluted zone  $\Omega_1$ , the variational problem becomes

$$\text{minimize } m(Q) = \frac{1}{2} \int_0^T Q^2(t) dt \quad (2.50)$$

$$\text{subject to: } \int_0^T g_1(r_1, t) Q(t) dt = c_1 \quad (2.51)$$

$$Q(t) \geq 0, \quad 0 \leq t \leq T \quad (2.52)$$

where, for simplicity, we have omitted the subindex in the release rate, that is  $Q(t) = Q_1(t)$ . At first, the site  $r_1 \in D$  is considered as any point such that

$$P(r_1) = \int_0^T g_1(r_1, t) dt > 0. \quad (2.53)$$

The set of points where condition (2.53) holds is called support of function  $P$  [11]. Note that condition (2.53) is necessary to satisfy constraint (2.51) and that such condition is fulfilled for any point  $r_1$  in the polluted zone  $\Omega_1$ . Moreover, condition (2.53) is also satisfied for points that are outside  $\Omega_1$  but fairly close to this area; such points are adjacent to  $\Omega_1$  and are located on the streamlines coming into the zone. The size of such set of points depends on how large is the parameter  $T$  and the velocity of the flow  $\|\mathbf{U}\|_2$  in a neighbourhood of the zone  $\Omega_1$ .

### 2.6.1.1 Existence and Uniqueness

In this section the existence and uniqueness of solution to variational problem (2.50)–(2.52) is proved. To this end, we remind some properties of the Hilbert space  $H = L_2(0, T)$  together with a strong result of approximation theory (a minimum distance theorem).

**Theorem 2.1** ([5]) *A non-empty closed convex set in a uniformly convex Banach space possesses a unique point closest to a given point.*

**Lemma 2.1** ([5]) *The space  $H = L_2(0, T)$  is a uniformly convex Banach space.*

We point out that the meaning of condition (2.50) is the minimization of the norm (distance) in the space  $H$ . It is for this reason Theorem 2.1 is useful in proving the existence and uniqueness. We now consider the specific set and point in space  $H$  for which Theorem 2.1 is applied.

**Definition 2.1** The feasible space  $F$  for variation problem (2.50)–(2.53) is given as follows

$$F = \left\{ Q \in H; Q(t) \geq 0, 0 \leq t \leq T, \text{ and } \int_0^T Q(t)g_1(r_1, t)dt = c_1 \right\} \quad (2.54)$$

**Lemma 2.2** *The feasible space  $F$  is a non-empty set in space  $H$ .*

*Proof* Because the adjoint solution  $g_1(r_1, t)$  is a non-negative square-integrable function, we have that

$$Q^*(t) = \frac{c_1 g_1(r_1, t)}{\int_0^T g_1^2(r_1, t) dt} \quad (2.55)$$

is a function in  $H$  that fulfils constraints (2.51) and (2.52). Therefore,  $Q^*(t)$  belongs to the feasible space  $F$ . The lemma is proved.

The meaning and usefulness of function  $Q^*(t)$  defined by (2.55) is established in the next section.

**Lemma 2.3** *The feasible space  $F$  is a convex set in  $H$ .*

*Proof* In fact, let  $Q_1, Q_2 \in F$  and  $\lambda \in (0, 1)$ . Then, evidently,  $\lambda Q_1 + (1 - \lambda)Q_2 \geq 0, 0 \leq t \leq T$ . Besides,

$$\int_0^T (\lambda Q_1 + (1 - \lambda)Q_2)g_1(r_1, t) dt = \lambda c_1 + (1 - \lambda)c_1 = c_1$$

and hence,  $F$  is a convex set in  $H$ . The lemma is proved.

**Lemma 2.4** *The feasible space  $F$  is a closed set in  $H$ .*

*Proof* To show this we must prove that  $F = \overline{F}$  [10]. Let  $Q_0$  be an element of  $\overline{F}$ . Then there is a sequence  $\{Q_k\}_{k=1}^{\infty}$  in  $F$  such that

$$\|Q_k - Q_0\| \rightarrow 0 \text{ as } k \rightarrow \infty$$

Assume that  $Q_0(t) < 0$  in some interval  $I \subset (0, T)$  of positive measure  $|I| > 0$ . Then

$$\|Q_k - Q_0\|^2 = \int_0^T (Q_k - Q_0)^2 dt \geq \int_I (Q_k - Q_0)^2 dt \geq \int_I Q_0^2 dt = l > 0$$

The last inequality contradicts the convergence of sequence  $\{Q_k\}_{k=1}^{\infty}$  in  $H$ , and hence,  $Q_0$  is a non-negative function in  $(0, T)$ .

On the other hand, applying the Schwarz inequality we get

$$\begin{aligned} \left| c_1 - \int_0^T Q_0 g_1(r_1, t) dt \right| &= \left| \int_0^T (Q_k - Q_0) g_1(r_1, t) dt \right| \\ &\leq \|Q_k - Q_0\| \|g_1(r_1, t)\| \rightarrow 0 \text{ as } k \rightarrow \infty \end{aligned}$$

and therefore  $\int_0^T Q_0 g_1(r_1, t) dt = c_1$ , that is  $Q_0 \in F$ . The lemma is proved.

Note that the zero function  $q(t) \equiv 0$ ,  $0 \leq t \leq T$ , does not belong to the feasible set  $F$ . Indeed, the constraint (2.51) is not satisfied for such function because  $c_1 > 0$ . This remark allows us to establish the most important result of this section.

**Theorem 2.2** *The variational problem (2.50)–(2.52) has non-trivial unique solution in the space  $H$ .*

*Proof* By Lemma 2.1, the space  $H$  is a uniformly convex Banach space. Besides, by Lemmas 2.1, 2.2 and 2.3, the feasibility space  $F$  is a non-empty closed convex set in  $H$ . Therefore, due to Theorem 2.1, there is a unique function  $Q^* \in F$  that minimizes the distance between the set  $F$  and the point  $q \equiv 0$ . That is according to (2.50), function  $Q^*$  minimizes the objective functional  $m(Q)$ . Finally, we observe that  $Q^* \neq 0$  because  $q \notin F$ , and hence, the unique solution of problem (2.50)–(2.52) is non-trivial. The theorem is proved.

It is shown in the next section that function  $Q^*$ , mentioned in Theorem 2.2, is precisely the function (2.55).

### 2.6.1.2 Optimal Discharge Parameters and the Adjoint Functions

The analytical expression for the optimal discharge rate  $Q^*$ , namely, the solution of variational problem (2.50)–(2.52), can be obtained by means of the method of

Lagrange multipliers [44]. Let

$$L(Q) = \frac{1}{2} \int_0^T Q^2(t) dt - \lambda \left\{ \int_0^T g_1(r_1, t) Q(t) dt - c_1 \right\} \quad (2.56)$$

be the Lagrange functional corresponding to problem (2.50)–(2.52), where  $\lambda$  is the respective Lagrange multiplier. The first variation of  $L$  in the sense of Gateaux [44] is calculated as

$$\delta L(Q; \delta Q) = \frac{\partial}{\partial \varepsilon} L(Q + \varepsilon \delta Q)_{\varepsilon=0} = \int_0^T \{Q(t) - \lambda g_1(r_1, t)\} \delta Q dt \quad (2.57)$$

where  $\delta Q$  is the variation of  $Q$ . A necessary condition for  $Q^*$  to be a minimum is  $\delta L(Q^*; \delta Q) = 0$ , for any  $\delta Q$  [44]. Therefore, from Eq. (2.57) we get

$$Q^*(t) = \lambda g_1(r_1, t), \quad (2.58)$$

where the Lagrange multiplier  $\lambda$  is determined by means of the constraint (2.51) in the way

$$\lambda = \frac{c_1}{\int_0^T g_1^2(r_1, t) dt}. \quad (2.59)$$

The final result is obtained by substituting Eq. (2.59) in (2.58).

Note that, due to Schwarz inequality [17],

$$0 < \int_0^T g_1(r_1, t) dt \leq T^{\frac{1}{2}} \left\{ \int_0^T g_1^2(r_1, t) dt \right\}^{\frac{1}{2}}$$

and therefore  $\int_0^T g_1^2(r_1, t) dt > 0$ , that is function  $Q^*$  is well-defined by the Eqs. (2.58) and (2.59). Besides, since  $g_1(r_1, t) \geq 0$ , we conclude that  $Q^*(t) \geq 0$ ,  $0 \leq t \leq T$ .

We now show that  $Q^*$ , defined by (2.58) and (2.59), also satisfies the sufficient condition to be a minimum. Indeed, let  $Q_0 = Q^* + \delta Q$  be a feasible discharge rate. From constraint (2.51) we have

$$\int_0^T g_1(r_1, t) \delta Q dt = 0, \quad (2.60)$$

where  $\delta Q \neq 0$  is an arbitrary variation of  $Q^*$ . Then,

$$m(Q_0) - m(Q^*) = \int_0^T Q^*(t) \delta Q dt + \frac{1}{2} \int_0^T \delta^2 Q dt. \quad (2.61)$$

Due to Eq. (2.58) and condition (2.60), Eq. (2.61) can be written as

$$m(Q_0) - m(Q^*) = \lambda \int_0^T g_1(r_1, t) \delta Q dt + \frac{1}{2} \int_0^T \delta^2 Q dt = \frac{1}{2} \int_0^T \delta^2 Q dt > 0$$

where  $\lambda$  is given by (2.59). Thus,  $m(Q_0) > m(Q^*)$ , and hence,  $Q^*$  defined by (2.58) and (2.59) is the global minimum of variational problem (2.50)–(2.52). Note that Theorem 2.2 from the previous section ensures the uniqueness of this minimum.

On the other hand, the mass of nutrient introduced into the aquatic system by means of the discharge rate  $Q^*$  is assessed as

$$m(Q^*) = \frac{c_1^2}{2 \int_0^T g_1^2(r_1, t) dt} \quad (2.62)$$

so that, in order to minimize the amount of mass, the integral

$$I(r_1) = \int_0^T g_1^2(r_1, t) dt \quad (2.63)$$

must take its maximum value. Thus, the optimal discharge point  $r_1^*$  is chosen so as to maximize the area under the function  $g_1^2(r_1, t)$ ,  $t \in (0, T)$ . Note that  $I(r_1)$  defined by (2.63) is a continuous non-linear function of three real variables  $r_1 = (x, y, z)$ , which has a global maximum in the closed set  $\overline{\Omega_1}$ . Indeed, according to the definition of the adjoint model forcing  $p(r, t)$ , the greatest values of the adjoint function are always achieved at the points of domain  $\Omega_1$ .

Because all these results can successively be applied to each oil-polluted zone, we conclude that during the first stage of the remediation strategy, the method allows us to determine the discharge points  $r_i^*$ , one in each oil-polluted zone  $\Omega_i$ , as well as to define with Eqs. (2.58) and (2.59) the corresponding basic discharge rates of nutrient:

$$Q_i^*(t) = \lambda_i g_i(r_i^*, t) = \frac{c_i}{\int_0^T g_i^2(r_i^*, t) dt} g_i(r_i^*, t), \quad i = 1, \dots, N. \quad (2.64)$$

Note that all the discharge parameters are calculated by using the adjoint model solutions.

### 2.6.2 Second Stage: Modulation of Basic Discharge Rates

In the second stage of the remediation strategy, we determine positive parameters  $\gamma_1, \gamma_2, \dots, \gamma_N$  such that the new discharge rates of nutrient

$$Q_i(t) = \gamma_i Q_i^*(t), \quad 1 \leq i \leq N \quad (2.65)$$

would satisfy the (global) variational problem (2.27)–(2.29). These parameters modulate the intensity of the basic release rates to fulfil the requirements for the nutrient concentrations in all oil-contaminated zones  $\Omega_i$ . Such correction on the basic discharge rates is needed because the nutrient discharged in one zone could reach the other zones during the time interval  $(0, T)$  due to the processes of advection and diffusion.

Substituting Eq.(2.65) in the variational problem (2.27)–(2.29) we obtain a quadratic programming problem whose solution determines the optimal parameters  $\gamma_i^*$ , and hence, the optimal discharge rates at points  $r_i^*$ ,  $i = 1, \dots, N$ :

$$\text{minimize } m(\gamma_1, \dots, \gamma_N) = \frac{1}{2} \sum_{j=1}^N p_j^2 \gamma_j^2 \quad (2.66)$$

$$\text{subject to: } c_i - \alpha_i \leq \sum_{j=1}^N a_{ij} \gamma_j \leq c_i + \beta_i, \quad i = 1, \dots, N \quad (2.67)$$

$$\gamma_j \geq 0, \quad j = 1, \dots, N \quad (2.68)$$

where  $p_j^2 = \int_0^T [Q_j^*(t)]^2 dt$  and  $a_{ij} = \int_0^T Q_j^*(t) g_i(r_j^*, t) dt$ ,  $i, j = 1, \dots, N$ .

The solution of the quadratic programming problem (2.66)–(2.68) exists because the corresponding feasible space is a compact set in  $\mathbb{R}^N$  and the objective function  $m$  is a continuous function of several real variables [17]. Besides, such a solution is unique because  $m$  is also a strictly convex function and the feasibility space is a convex set in  $\mathbb{R}^N$  [5]. It is assumed here that the feasibility space is a non-empty set due to the introduction of suitable (large enough) parameters  $\alpha_i$  and  $\beta_i$ .

The quadratic programming problem (2.66)–(2.68) can be solved using the *quadprog* routine of MATLAB as soon as the adjoint functions are determined. Regard to this routine, we point out that, when the only constraints of the problem are the upper and lower bounds of variables, i.e., no linear inequalities or equalities are specified, the default *quadprog* algorithm is the large-scale method. Moreover, if the problem has only linear equalities, i.e., no upper and lower bounds or linear inequalities are specified, the default *quadprog* algorithm is also the large-scale method. This method is a subspace trust-region method based on the interior-reflective Newton method described in Coleman and Li [6]. Each iteration involves the approximate solution of a large linear system using the preconditioned conjugate gradient method (PCG). Otherwise, medium-scale optimization is used, and *quadprog* uses an active set method, which is also a projection method, similar to that described in Gill et al. [12]. It finds an initial feasible solution by solving a linear programming problem [25, 51]. Due to the structure of quadratic programming problem (2.66)–(2.68), the second method of *quadprog* routine is applied in the examples.



### 2.7 Numerical Examples of Remediation in a Channel

In order to illustrate the method developed we now consider a two-dimensional example of remediation in a channel of one hundred and twenty metres long  $[0, 120]$  and ten metres wide  $[0, 10]$ . The channel contains three oil-polluted zones  $\Omega_i$  ( $N = 3$ ). The critical nutrient concentrations  $c_i$  ( $\text{grm}^{-3}$ ) in the zones vary from one experiment to another according to Table 2.1. The zones under consideration are:  $\Omega_1 = [20, 30] \times [9, 10]$ ,  $\Omega_2 = [40, 60] \times [9, 10]$  and  $\Omega_3 = [96, 100] \times [0, 2]$ . The parameters of the adjoint model (2.18)–(2.24) have been taken as follows: the velocity vector  $\mathbf{U}$  is directed along the channel and is equal to  $30 \text{ m h}^{-1}$ , the diffusion coefficient  $\mu$  is  $6 \text{ m}^2 \text{ h}^{-1}$ , the coefficient of chemical decay  $\sigma$  is  $1 \text{ h}^{-1}$ , and  $\zeta = v_s = 0$ . The discharge of nutrient is performed from the optimal points during four hours,  $(0, T) \equiv (0, 4)$ , and the mean concentration is controlled within the last one-hour interval  $(3, 4)$ , i.e.,  $\tau = 1 \text{ h}$ .

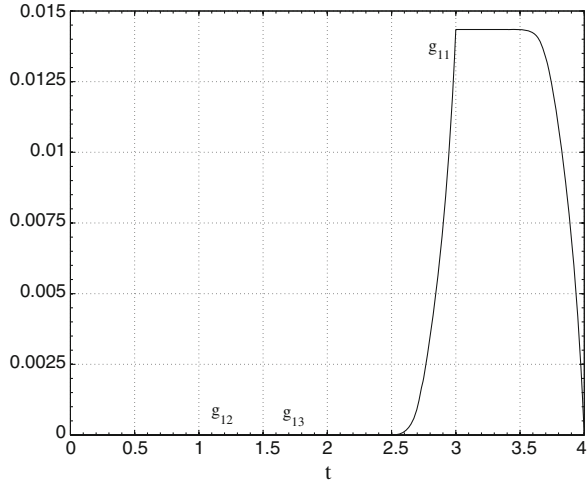
For each oil polluted zone the adjoint model (2.18)–(2.24) was solved by means of the bidimensional version of the splitting-up method (2.45)–(2.46) which is described in Sect. 2.5. The parameters of discretization are the same in all the numerical experiments. The mesh size is the same in both directions, namely,  $\Delta x = \Delta y = 0.4$ , and the corresponding mesh size in the time direction is  $\Delta t = 0.005$ . The function  $I$ , given by Eq. (2.63), was built for each polluted zone through the respective adjoint solution. In each case, by the maximization of function  $I$  we determined the following optimal discharge points:  $r_1^* = (20.2, 9.8)$ ,  $r_2^* = (40.2, 9.8)$  and  $r_3^* = (96.2, 0.2)$ . For this grid (as well as for finer grids) we obtained that the optimal discharge site tends to be the point at the left-superior corner of the zones  $\Omega_1$  and  $\Omega_2$ , and the left-inferior corner of zone  $\Omega_3$ , as it must be in order to have the maximum impact of nutrient in each polluted zone.

The adjoint solutions  $g_{ij} = g_i(r_j^*, t)$ , for the  $i$ th polluted zone and the  $j$ th optimal discharge point, are plotted in Figs. 2.3, 2.4 and 2.5. According to Eq. (2.64), the basic discharge rate for each polluted zone  $\Omega_i$  is a multiple of the adjoint function  $g_{ii} = g_i(r_i^*, t)$ . From the shape of these functions, given in Figs. 2.3, 2.4 and 2.5, one concludes that the basic discharge rates are equal to zero in the time interval  $[0, 2.25]$ . According to Eq. (2.25), this means that a basic discharge rate influences the nutrient concentration of a polluted zone only if the adjoint function of the zone is non-zero in the time interval  $[2.25, 4.0]$ . Figure 2.3 shows that  $g_{12}$  and  $g_{13}$  do not satisfy this condition, and therefore the discharge of nutrients at points  $r_2^*$  and  $r_3^*$  has no influence on its concentration in zone  $\Omega_1$ , as it was to be expected due to the flow direction and the location of zones in the channel.

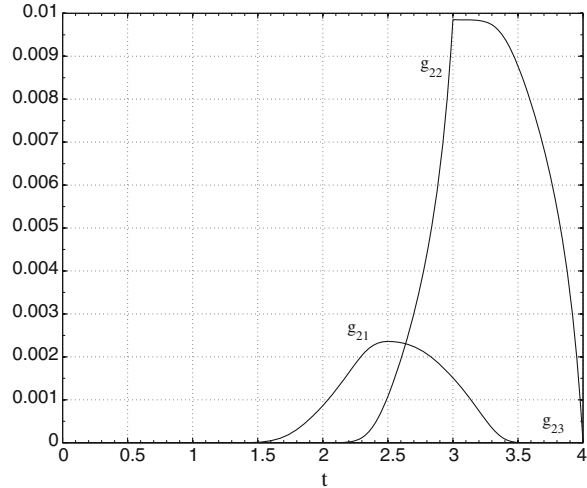
**Table 2.1** Concentrations  $c_i$  ( $\text{grm}^{-3}$ ) in the three polluted zones

Concentration \ Experiment	1	2	3	4	5
$c_1$	0.8	1.0	0.5	1.2	0.6
$c_2$	0.8	0.8	1.0	0.5	1.2
$c_3$	0.8	0.5	1.5	1.2	0.6

**Fig. 2.3** Adjoint functions  $g_{ij} = g_i(r_j^*, t)$  corresponding to zone  $\Omega_1$  ( $i = 1$ ) when they are restricted to the optimal discharge points  $r_j^*$  ( $j = 1, 2, 3$ )



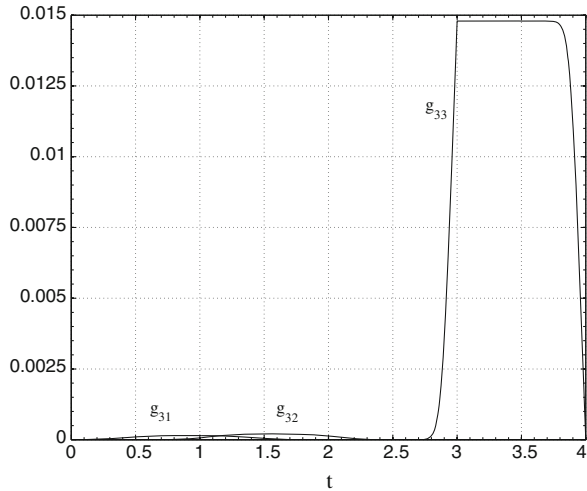
**Fig. 2.4** Adjoint functions  $g_{ij} = g_i(r_j^*, t)$  corresponding to zone  $\Omega_2$  ( $i = 2$ ) when they are restricted to the optimal discharge points  $r_j^*$  ( $j = 1, 2, 3$ )



A similar result follows from Fig. 2.5, since the adjoint functions  $g_{31}$  and  $g_{32}$  are almost zero in the time interval  $[2.25, 4.0]$ , and therefore the discharge of nutrients at points  $r_1^*$  and  $r_2^*$  practically has no influence on its concentration in zone  $\Omega_3$ . However, it follows from Fig. 2.4 that function  $g_{21}$  is positive in the time interval  $[2.25, 4.0]$ , and hence, the discharge of nutrient at point  $r_1^*$  influences its concentration in zone  $\Omega_2$ , as it was expected. Finally, the temporal behaviour of adjoint function  $g_{23}$  allows us to conclude that the discharge at point  $r_3^*$  does not affect the concentration of nutrient in  $\Omega_2$ .

Thus, the polluted zones are not independent with respect to the dispersion process, since the release of nutrient in a particular zone can affect the concentration in

**Fig. 2.5** Adjoint functions  $g_{ij} = g_i(r_j^*, t)$  corresponding to zone  $\Omega_3$  ( $i = 3$ ) when they are restricted to the optimal discharge points  $r_j^*$  ( $j = 1, 2, 3$ )



**Table 2.2** Modulation parameters  $\gamma_i^*$  for the basic discharge rates

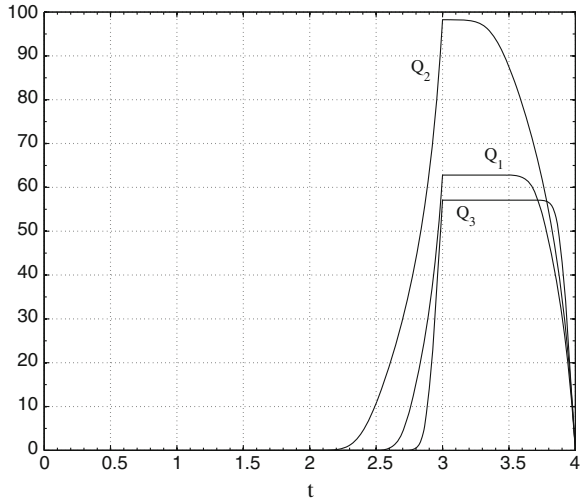
Parameter\Experiment	1	2	3	4	5
$\gamma_1^*$	1.0000	1.0000	1.0000	1.0000	1.0000
$\gamma_2^*$	0.9579	0.9473	0.9789	0.8989	0.9789
$\gamma_3^*$	1.0000	1.0000	1.0000	1.0000	1.0000

other zones. If it is the case, the application of second stage of the remediation strategy is necessary to correct the intensity of the basic discharge rates. To this end, the quadratic programming problem (2.66)–(2.68) was solved by using the adjoint functions  $g_{ij} = g_i(r_j^*, t)$ , the critical concentrations  $c_i$  given in Table 2.1 and the corresponding basic discharge rates. Table 2.2 summarizes the optimal modulation parameters  $\gamma_i^*$  obtained for each experiment.

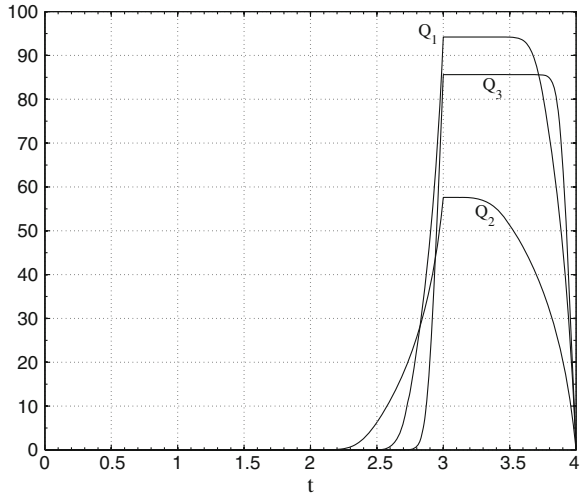
For all the experiments, the slack variables of the quadratic programming problem (2.66)–(2.68) are taken equal to zero:  $\alpha_i = \beta_i = 0$  ( $i = 1, 2$  and 3), hence, each critical concentration  $c_i$  is reached in the respective oil polluted zone exactly. Table 2.2 shows that the only discharge rate which must be corrected is that located in zone  $\Omega_2$  ( $\gamma_2^* < 1$  in the five experiments). This is a consequence of the impact that the discharge of nutrient at point  $r_1^*$  has on the zone  $\Omega_2$ . The optimal discharge rates for experiments 1 and 4 are shown in Figs. 2.6 and 2.7, respectively. As compared with Fig. 2.6, the intensity of functions  $Q_1$  and  $Q_3$  in Fig. 2.7 has increased. This is the result of the raise in the critical concentrations from 0.8 to 1.2 (see Table 2.1. At the same time, the decrease in the intensity of function  $Q_2$  in Fig. 2.7 compared to Fig. 2.6 is explained by the drop in the critical concentration of nutrient from 0.8 to 0.5 and also by the correction of  $Q_2$  through the parameter  $\gamma_2^*$  (see Table 2.2).

It should be noted that in all the experiments, the slack variables are not necessary because the feasible space of problem (2.66)–(2.68) is nonempty when  $\alpha_i = \beta_i = 0$

**Fig. 2.6** Optimal discharge rates  $Q_i(t) = \gamma_i^* Q_i^*(t)$ ,  $i = 1, 2$  and  $3$ , for Experiment 1

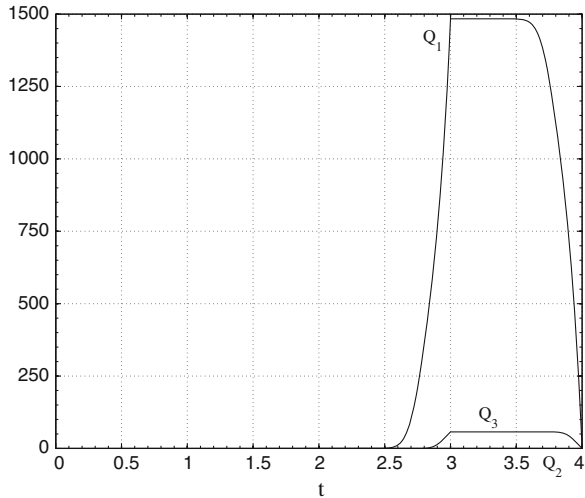


**Fig. 2.7** Optimal discharge rates  $Q_i(t) = \gamma_i^* Q_i^*(t)$ ,  $i = 1, 2$  and  $3$ , for Experiment 4



( $i = 1, 2$  and  $3$ ), and therefore the existence of the optimal solution is assured. However, such variables are required for the general formulation of the strategy. For example, when the critical concentrations for the three polluted zones are  $c_1 = 19.0$ ,  $c_2 = 0.8$  and  $c_3 = 0.8$  then the feasible space of problem (2.66)–(2.68) is empty. Indeed, in this case, the basic discharge rate at point  $r_1^*$  is so intensive that the concentration of nutrient in the zone  $\Omega_2$  cannot be maintained as low as 0.8. On the other side, if nonzero slack variables are introduced as  $\alpha_1 = \beta_1 = 0.1$  and  $\alpha_i = \beta_i = 0$  ( $i = 2, 3$ ), then the feasible space of problem (2.66)–(2.68) is nonempty and we have the optimal solution:  $\gamma_1^* = 0.9947$ ,  $\gamma_2^* = 0.0048$  and  $\gamma_3^* = 1.0000$ . Figure 2.8 shows the optimal discharge rates obtained for the three polluted zones.

**Fig. 2.8** Optimal discharge rates  $Q_i(t) = \gamma_i^* Q_i^*(t)$ ,  $i = 1, 2$  and  $3$ , for the critical concentrations  $c_1 = 19.0$ ,  $c_2 = 0.8$  and  $c_3 = 0.8$ , and slack variables  $\alpha_1 = \beta_1 = 0.1$  and  $\alpha_i = \beta_i = 0$  ( $i = 2, 3$ )



Note that  $Q_2$  is practically zero, and hence, the discharge rate  $Q_1$  is responsible for the concentration reached in zone  $\Omega_2$ .

## 2.8 Conclusions

The main objectives of the mathematical modelling in the environment protection are the identification of emission rates of sources and their positions, the prediction of concentrations of different substances (pollutants, cleaners, nutrients, etc.), the development of the methods which help to prevent dangerous pollution levels (control of emissions) and the search of new strategies for the remediation of polluted zones. In this chapter, we have presented a method for the cleanup of the oil-polluted marine environment through bioremediation. It is assumed that oil is stranded in some zones at the shoreline and the goal is to release a nutrient into aquatic system in order to increase the amount of indigenous microorganisms which degrade the pollutants in such zones. Thus, the specific objective is to determine the appropriate parameters of releasing the nutrient, namely, the discharge sites and the discharge rates, in order to reach critical (necessary) concentrations of the nutrient in the polluted zones. All the unknown parameters are chosen for minimizing the total mass of the released nutrient, with the aim to minimize the impact on the environment and the cost of remediation.

To this end, the problem is solved in two stages. In the first stage, each zone  $\Omega_i$  is considered separately from other and contains just one source. In order to reach the critical concentration  $c_i$  in each polluted zone  $\Omega_i$  ( $1 \leq i \leq N$ ), a variational problem is posed and solved with the aim to find both the optimal location of release point  $r_i$

in the zone and the optimal release rate  $Q_i(t)$ , also named as basic or preliminary discharge rate. We prove that this problem has unique solution.

In the second stage, we consider the process of dispersion of nutrient in all zones together. Due to advection by currents, the nutrient released in one zone can reach other polluted zones. Therefore we must specify (modulate) the strength of all release rates  $Q_i(t)$  in order to fulfil the critical mean concentrations  $c_i$  in all the polluted zones during the time interval  $[T - \tau, T]$ . To this end, we introduce positive coefficients  $\gamma_i$  to replace all release rates  $Q_i(t)$  by  $\gamma_i Q_i(t)$ . These coefficients are chosen as the solution of a quadratic programming problem where the objective function for minimizing is the mass of nutrient introduced by the new discharge rates  $\gamma_i Q_i(t)$ . Also, we prove the existence and uniqueness of this optimization problem.

Both stages of this remediation strategy use the adjoint solutions to assess the mean concentration of nutrient in the oil-polluted zones. Such approach is quite useful. Indeed, in the first stage, the optimal release point for a specific oil-polluted zone is found by maximizing a continuous non-linear function of three real variables. The function is built with the adjoint problem solution corresponding to the selected zone. In addition, the respective basic discharge rate is determined as a multiple of the adjoint solution which is evaluated at the optimal discharge point. Of course, the basic discharge rate also depends on the critical concentration for the respective oil-polluted zone. And in the second stage, the adjoint solutions, evaluated at the optimal discharge points, are also used to pose the constraints for the quadratic programming problem.

Thus, this new remediation method is strongly based on the adjoint estimates. Nevertheless, it also uses the direct concentration estimates of nutrient in the polluted zones when various discharges of the nutrient are needed. Therefore, the two equivalent (direct and adjoint) estimates complement each other well in the assessment of nutrients and control of pollutants. The direct estimates, utilizing the solution of the advection-diffusion problem, enable making the comprehensive analysis of ecological situation in the whole area. On the other hand, the adjoint estimates use solutions of the adjoint problems and explicitly depend on the positions of sources, their discharge rates, and also on the initial distribution of nutrient in the region. Besides, the solutions of adjoint problem serve as influence (weight) functions, which show the impact of the location of discharge source and its intensity on the concentration of nutrient in each oil-polluted zone. Therefore, the adjoint estimates are effective and economical in the sensitivity study of the concentrations of nutrient to variations in the model parameters.

Owing to special boundary conditions, both the main and adjoint problems are well-posed according to Hadamard, that is the solution of each problem exists, is unique and stable to initial perturbations. These conditions are reduced to the well-known and natural boundary conditions in the non-diffusion limit (pure advection problem) and also in the case of a closed sea basin (when the boundary is the coast line).

Finite difference schemes for the solution of the main and adjoint transport problems are also given. The schemes are balanced, unconditionally stable, of second-order approximation, and are based on using the splitting method and Crank-Nicolson

scheme. In the absence of dissipation and sources, each scheme has two conservation laws. All one-dimensional discrete equations obtained at every fractional step of the splitting algorithm are efficiently solved by the Thomas factorization method for tridiagonal matrices.

Finally, we point out that the adjoint technique described in this chapter can also be used for the solution of such problems as the control of industrial emissions, the detection of the enterprises which violate the emission rates prescribed by a control, and the estimation of the intensity of a pollution source in the case when its position is known. For example, the last cases include a nuclear (or chemical) plant accident or nuclear bomb explosion (testing, terrorist attacks, and others). In all these situations, the source position is known or can easily be located (from a satellite or other monitoring equipment), and then our method gives a lower bound of the source intensity, which can be useful in the assessment of the scale of accident.

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