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Numerical Methods for Parameter Estimation
and Optimal Control of the Red River Network

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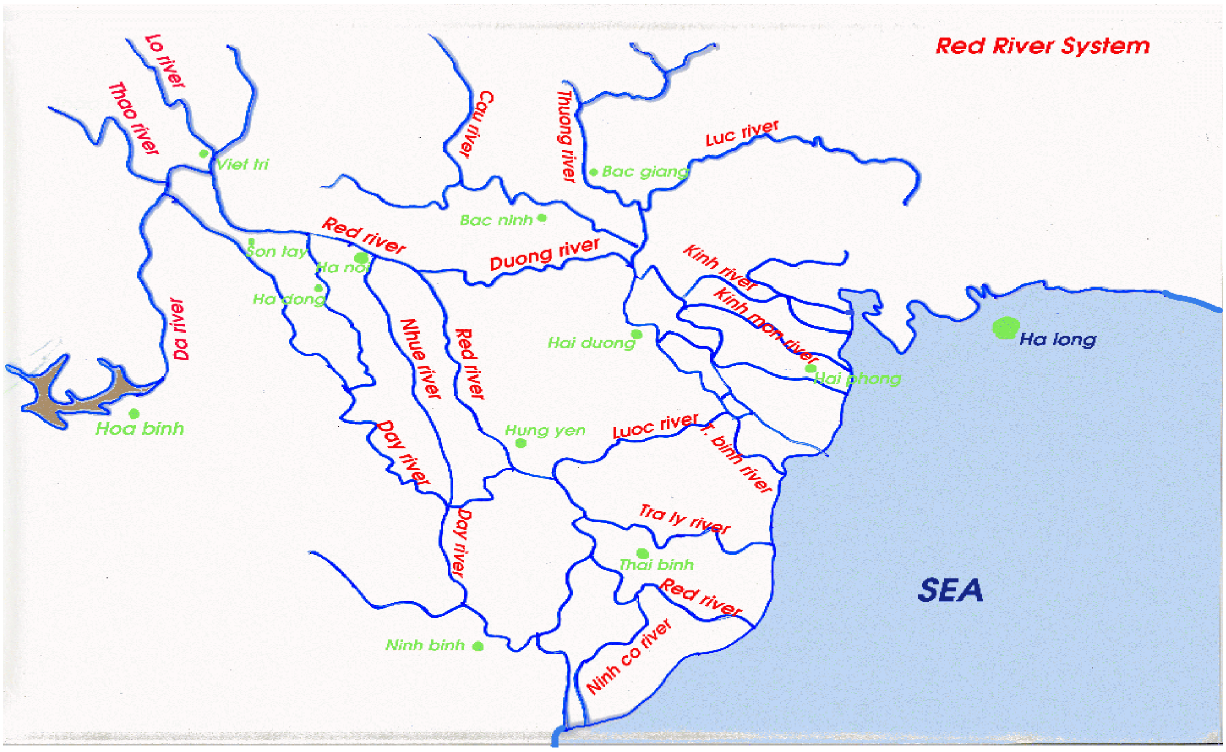

Abstract

In this thesis efficient numerical methods for the simulation, the parameter estimation, and the optimal control of the Red River system are presented.

The model of the Red River system is based on the Saint-Venant equation system, which consists of two nonlinear first-order hyperbolic Partial Differential Equations (PDE) in space and in time. In general a system of equations of this type can not be solved analytically. Therefore I choose a numerical approach, namely the Method Of Lines (MOL) combined with the Backward Differentiation Formulae (BDF) method implemented in the solver DAESOL, which is developed at IWR (University of Heidelberg), for the solution of the Saint-Venant equation for the simulation of the Red River system.

In a river, there are geometrical and hydraulic parameters, e.g. friction coefficients, river bed slope, etc., which are very expensive or – even worse – impossible to measure. The Red River system is a large system, therefore the number of the unknown parameters is also large, thus manual parameter estimation, as often done by hydrologists, does not work effectively. To overcome this problem and to come up with accurate parameter values, we estimate these parameters by solving a corresponding least-squares problem. This high dimensional nonlinear constrained optimization problem is solved by applying a special reduced Gauss-Newton method implemented in the software packages for parameter estimation PARFIT and FIXFIT. Based on the code FIXFIT we have developed a numerical tool for solution of simulation and parameter estimation problems for river flows that are modeled by hyperbolic PDE.

Using the validated model, we formulate an optimal control problem for preventing floods in the Red River lowland. This problem is solved by the direct multiple shooting method within the software package MUSCOD-II. We propose an online optimization approach with a *nonlinear model predictive control* (NMPC) technique to reduce the maximum flood level at Ha Noi by controlling the water discharge at the output of the reservoir Hoa Binh. The potential of our approach is demonstrated in real-life test cases corresponding to the flood season in the year 2000.

Kurzfassung

In dieser Arbeit werden effiziente numerische Methoden für die Simulation, für Aufgaben der Parameterschätzung sowie für Optimal-Steuerungsprobleme beim Rote-Fluss-System im Norden Vietnams vorgestellt.

Das Modell des Rote-Fluss-Systems beruht auf der Saint-Venant-Gleichung, einer instationären räumlich eindimensionalen nichtlinearen hyperbolischen partiellen Differentialgleichung (PDE) erster Ordnung, die aus zwei Komponenten besteht. Da ein Differentialgleichungssystem dieses Typs nicht analytisch gelöst werden kann, wählen wir einen numerischen Ansatz. Mit der Linienmethode (MOL) wird die PDE in eine hochdimensionale gewöhnliche Differentialgleichung überführt und mit "Backward-Differentiation-Formulae" (BDF) in Zeitrichtung diskretisiert. Für die in dieser Arbeit durchgeführten Simulationen der Saint-Venant-Gleichung des Rote-Fluss-Systems wird der am IWR der Universität Heidelberg entwickelte BDF-Löser mit variabler Schrittweite und Ordnung (DAESOL) verwendet.

In ein Modell für einen Fluss gehen geometrische und hydraulische Parameter ein, z.B. Reibungskoeffizienten oder Gefällwerte des Flussbettes, die in der Praxis oft nur sehr aufwändig oder überhaupt nicht durch Messungen direkt ermittelt werden können. Da das Rote-Fluss-System sehr ausgedehnt ist, treten eine hohe Anzahl unbekannter Parameter auf. Eine "händische" Schätzung dieser Parameter, wie sie vielfach von Hydrologen durchgeführt wird, erwies sich als ineffektiv. Um diese Schwierigkeit zu überwinden und zu genauen Parameterwerten zu kommen, bestimmen wir die Parameter durch Lösung eines geeigneten Least-Squares-Problems, wobei als Messdaten Pegelstände verwendet werden. Die numerische Lösung dieses hochdimensionalen beschränkten Optimierungsproblems wird durch Anwendung einer speziellen reduzierten Gauß-Newton-Methode, die in den Softwarepaketen PARFIT und FIXFIT implementiert ist, vorgenommen. Auf der Grundlage des Codes FIXFIT haben wir ein Werkzeug zur Simulation und Parameterschätzung von Fluss-Modellen entwickelt, die in Form von hyperbolischen PDE vorliegen.

Unter Verwendung des validierten Modells formulieren wir ein Optimal-Steuerungsproblem mit dem Ziel der Vermeidung von Überflutungen im Tiefland des Rote-Fluss-Systems. Dieses Problem wird mit einer direkten Mehrzielmethode, wie sie im Softwarepaket MUSCOD-II realisiert ist, gelöst. Darüber hinaus schlagen wir eine Regelungsstrategie im Rahmen des "Nonlinear Model Predictive Control" (NMPC) vor. Hierbei wird Echtzeit-Optimierung eingesetzt, um die Wasserzufuhr beim Reservoir Hoa Binh unter wechselnden sonstigen Bedingung online so zu bestimmen, dass der maximale Pegelstand bei Hanoi so niedrig wie möglich gehalten wird. Das Potenzial unseres Ansatzes wird anhand von

Testfällen, die der Situation während der Hochwasserphase im Jahre 2000 entsprechen, nachgewiesen.

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Contents

List of Selected Symbols

	Lowercase Latin Characters	
b	river width	[m]
c	wave speed	[ms^{-1}]
g	gravity acceleration	[ms^{-2}]
h	water deepth	[m]
q	lateral in flow	[$\mathrm{m}^2\mathrm{s}^{-1}$]
y	water level	[m]
t	time varialbes	[s]
u	control function	
v	velocity component	[ms^{-1}]
x	space varialbe	[m]
	Uppercase Latin Characters	
A	cross-sectional area	[m^2]
B	river width	[m]
D	hydraulic diameter	[m]
F	force	[N]
F_g	gravity force	[N]
F_f	friction force	[N]
F_p	pressure	[N]
P	hydraulic perimeter, parameter	
R	hydraulic radius	[m]
S_0	river bed slope	
S_{0x}	component of the river bed slope in x axis	
S_{0y}	component of the river bed slope in y axis	
S_f	river bed friction	
S_{fx}	component of the river bed friction in x axis	
S_{fy}	component of the river bed friction in y axis	
Q	water discharge	[$\mathrm{m}^3\mathrm{s}^{-1}$]
Q^{in}	input water discharge	[$\mathrm{m}^3\mathrm{s}^{-1}$]
Q^{out}	output water discharge	[$\mathrm{m}^3\mathrm{s}^{-1}$]
U	flow velocity vector	[$\mathrm{m}^3\mathrm{s}^{-1}$]
V	water volume	[m^3]
W_p	wetted perimeter	[m]

Lowercase Greek Characters

ρ	density	[kg m^{-3}]
ξ	water elevation	[m]

Chapter 1

Introduction

Every year the Red River system collects 115–117 billion m^3 water from a drainage-basin of about 169 000 km^2, among them 86 660 km^2 (51%) in Vietnam. This water amount is an essential factor for the life of 17 million people in the lowland of the Red River system, both in the positive and the negative sense. It provides resources for living and production. For instance, the hydroelectric power plant Hoa Binh (on this river system) delivers about 40% of the electric energy of Vietnam. But the Red river from time to time also causes strong floods which kill people and damage many valuable things. In consequence of natural disasters in the Red River lowland, for example in 1996 [48], 312 persons died and 610 persons were injured, 36700 dwelling-houses and 15190 classrooms were damaged, and 383000 ha of area under cultivation were destroyed. Such disasters impend every year, and people living there are often in danger. So the control of the Red River system is a very important problem for Vietnam.

One possibility for preventing floods is the strengthening of the dike system. But to do it for nearly 3000 km dike, which were built since 866 to date and reaches now the height of 14,5–15,0 m in Ha Noi, this is unfortunately too expensive, especially for such a week economy like Vietnam's. Therefore, the control of this river system by means of hydroelectric reservoirs is a more practical solution. There are two most important reservoirs in northern Vietnam. With a volume of $2,94 \times 10^9\,m^3$ and a drainage-basin of $4,3\,\%$ of the entire area of the Red River until Son Tay, the smaller reservoir Thac Ba plays only a reserve role in flood prevention. The main duty is taken by Vietnam's largest reservoir Hoa Binh, whose volume is $9,45 \times 10^9\,m^3$. But both reservoirs are far away to be enough to prevent floods in the Red River whose discharge may be $37\,800\,m^3/s$ as in August 1971, when the water level in Ha Noi reached the record level of 14,6 m. It remains a very hard question for the Vietnamese government, for all responsible institutions and experts, how to control these reservoirs to minimize flood in the Red River lowland.

There are many difficulties in answering the above mentioned question. They can be listed as follows,

- geographical, meteorological and hydrological data are lacking and inaccurate, both for the past and for the present time,
- there are no suitable methods or software for operative forecast of floods,
- knowledge of the dependencies of the flood in lowland on the working regimes of the reservoirs is lacking.

The main goal of this thesis is to contribute to the solution of the above listed problems with the ultimate goal to find a method for optimal control of the reservoirs. Here, we focus on the control of the reservoir Hoa Binh. Our work can be formally broken down into the following parts:

- formulating the model of the Red River system.
- using numerical methods to simulate the Red River system,
- estimating unknown parameters of the Red River system by means of optimization and
- finding an optimal control for the reservoir Hoa Binh to minimize flood in the lowland. The criterion for minimizing flood in the Red River lowland is minimizing the water level in Ha Noi.

The research approach of this thesis is interdisciplinary and motivated by the applicational aspect.

The mathematical model of the river flows is based on the Saint-Venant equation system. This is a system of two hyperbolic Partial Differential Equations (PDE), which can be solved by numerical methods, e.g. finite element methods, finite volume methods, or finite difference methods. To treat the instationary case, we use finite difference for the spatial discretization. The resulting large-scale time dependent Ordinary Differential Equation (ODE) system connected by algebraic constraints, is treated by the BDF method implemented in the solver DAESOL which was developed by Prof. Bock, Dr. Schlöder and their team at the Interdisciplinary Center for Scientific Computing (IWR). There exist already software and methods for modelling river flows, e.g. the comercial software MIKE developed by "DHI Water and Environment", WENDY and RIBASIM developed at Delft Hydraulics, Holland, *etc.* which are based on fixed stepsize methods in time. In contrast to those software and methods, in this thesis a stepsize control strategy is applied in order to improve the computing time and stability of the numerical methods.

One noticeable problem arising in the modelling procedure of the Red River system is caused by the fact that there are geometrical and hydraulic variables which can not be measured, e.g. the friction coefficients, river bed slope, *etc.* In previous work these variables are determined manually based on the experiences of hydrologists. However, the number of these variables is very big due to the spatial discretization of the Saint-Venant equations (up to some thousands) and, even worse, they are strongly correlated with each other, therefore the manual estimations for the unknown variables of the river flows are not sufficiently effective. In order to avoid this problem and to come up with a good model for the Red River system, in this thesis, the variables which can not be measured, are treated as unknown parameters and their values are estimated by means of optimization. Here, the values of water levels at the gauging stations, which was measured in the past, are used. To the best of the author's knowlegde this is the first time that optimization based parameter estimation is carried out for a river system. To realize this idea, we formulate an optimization problem fitting the model response to the measurement data. This is a least squares problem constrained by a large scale ODEs. For the solution of this problem, the Generalized Gauss-Newton method developed and implemented in the codes PARFIT by Bock (1981 [10], 1983 [11], 1987 [12]), and Bock et al. (2001 [13]), and the Reduced Gauss-Newton method which was developed and implemented in the code FIXFIT by Schlöder (1987 [54]) and Dieses (2001 [27]) are used as a framework. Based on the code FIXFIT we have developed a tool for solution of simulation and parameter estimation for river flows (see Thai et al. [14]). This software can be applied for solution of simulation and parameter estimation problems which are constrained by hyperbolic and parabolic PDEs.

The values of unknown parameters of the Red River system are estimated and their statistical reliability is assessed, i.e., in terms of the variance-covariance matrix or confidence intervals. A validation and a verification for the estimated parameters is made. This shows that the model response is fitted well to the measurement data.

In order to find an optimal control for the reservoir Hoa Binh to minimize the water level in Ha Noi, an optimization problem is formulated. This problem is solved by MUSCOD-II, a powerful software package for simulation and optimization, which has been developed in the research group of Professor Bock. This software is based on the boundary value problem (BVP) approach, that is simulation and optimization are done at the same time, and it has been applied very successfully to many application problems. MUSCOD-II solves the optimal control problem with a reduced SQP-method (see Bock et al. [15] and Leineweber [42]) based on the direct multiple shooting discretization. As results, we recommend new strategies for optimal control of the reservoir Hoa Binh in order to minimize the water level in Ha Noi.

This thesis is organized in 7 chapters:

In Chapter 2 the Saint-Venant equation system is chosen for modelling the Red River system. A derivation of this equation system is recalled to explain all dependencies between the variables in the equation system.

Chapter 3 describes mathematical methods for the solution of the Saint-Venant equation. We first show how the original model equations are discretized in space to obtain a large system of ODEs connected by algebraic constraints, and then how the BDF method which is implemented in the solver DAESOL is applied to obtain the solution of the model equations. The stability, convergence, and accuracy of the numerical method applied to our problem are discussed.

Chapter 4 is dedicated to the presentation an efficient numerical method for solution of the parameter estimation problem. The parameter estimation problem for the Red River system is a least-squares problems constrained by the Saint-Venant equation, i.e. by the PDEs. In this chapter a discussion about numerical methods for solution of this optimization problem is made, and based on that the Reduced Gauss-Newton method developed and implemented in the code FIXFIT is chosen for the framework of parameter estimation in this thesis.

Chapter 5 presents numerical results of parameter estimation and simulation of the Saint-Venant equations for the Red River system. In the first part of this chapter the introduction to the Red River system is made. In the second part we present the values of the estimated parameters with their confidence intervals. A validation and a verification of the estimated parameters is made, and these show good coincidence between the model response and the measurement data. In the third part of the chapter, numerical results for simulation of the Saint-Venant equations are presented for the estimated parameters. These show the values of the state variables, i.e. water discharge and water level at every river cross-sectional node depending on the time.

The mathematical model of the Red River system can then be used for optimal control problems: in Chapter 6 the optimization problem is formulated in order to find an optimal control of the reservoir Hoa Binh to minimize the maximal water level in Ha Noi. For the solution of this problem the software package for optimization MUSCOD-II is applied.

Finally, in Chapter 7 we summarize the results and give an outlook to further research directions.

Chapter 2

Dynamical Modelling of a River System

This chapter contains an introduction to the mathematical modelling of river flows. The first section gives an outline of existing models for open channel flows. In the second section, the hydraulic model is considered in more detail. The parameterization of hydraulic functions for the Red River system is shown in the third section. Based on this description, we can neglect weakly influential terms in the mathematical physics equations for the Red River system. This leads to the specific case of Saint-Venant equation, which is significantly simplified. The aim of this chapter is to choose a suitable model for the considered Red River system.

2.1 Model Classification for River Flows and a Suitable Model of the Red River System

The main task of modelling of river flows is to determine the nonlinear dynamic relationship between hydraulic quantities, i.e., water discharge (or water velocity), water level (or cross-sectional area) and the time. This has called attention from many experts over the past hundreds of years. Mathematical models of a hydraulic system are ranging from very simply computable models to complex computer-based, physically-based models. They can be classified into the following types [48], [68]:

- Metric Models
- Conceptual Models
- Hydraulic Models

Metric Models, e.g. black-box models, time-series models, are based on observational data and seek to characterize flow response largely on the basis of these data, using some form of statistical estimation or optimization (see [68],[51], [37], and [65]). These models ignore physical laws, and are usually simple as no deeper knowledge of the studied processes is needed and no expensive morphometric and physical measurements are required. Usually, metric models are lumped, i.e. they do not attemp in any way to represent the processes occuring within the river channel, not even in a simplified manner.

Conceptual (see [48], [68]) models are partly physically based. In a conceptual type model the internal descriptions of various subprocesses are modelled attemping to represent, in a simplified way, the known physical process.

Hydraulic Models represent processes in a mathematical-physics form, based on physical laws (see [4, 59]) and are solved in an approximated manner via finite difference or finite element methods.

In the present project a hydraulic type model is chosen for the modelling of processes in the Red River system because of a number of reasons. Hydraulic models allow to describe completely and exactly the processes in the Red River system. By a hydraulic model, we can easily express all dependencies between hydraulic variables, e.g. the water level, the water discharge *etc.*, the knowledge of which is very important for the control of the Red River flows. One more reason to use a hydraulic model to modelling the Red River system is that it does not require availability of detailed hydraulic data in the past time, which are not available in Vietnam.

The main problem of a hydraulic type model is the inability of measuring some hydraulic quantities, e.g. river bed friction, river bed slope, etc. To avoid that and to come up with accurate values of these hydraulic quantities, we treat these unmeasurable quantities as unknown parameters and estimate them from measurements by means of optimization. We will discuss this in detail in Chapter 4.

2.2 Hydraulic Models for River Flows

In nature, water flow in the river is unstationary, i.e. it varies in time and space, and has a free surface. The basic flow equations mathematically describing unsteady river flow are the continuity equation, derived from the principle of conservation of mass, and the momentum equation from Newton's second law, the principle of conservation of momentum. J.-C. Barre de Saint-Venant [22] derived those equations more than a century ago, long before the techniques to solve them became available. These are called the Saint-Venant equation system. However, the first version of the Saint-Venant equation is not complete: the forces upon the investigated system are not described, some important quantities are missing, e.g. the lateral in (out) water discharge.

To continue Saint-Venant's work, in the last decades many scientists have recalled and completed the derivation of the Saint-Venant equation using new performances in mathematics. Different ways of generating this equation system can be found in books of hydrology or physics like Maniak [45], Chow *et al.* [17], Somojlovich [57], or Stoker [62]. It is not our intention to give a complete overview of all these methods. In this section, using material from the above literature, we outline the establishment of the Saint-Venant equation. The main goal here is to explain the dependencies of all hydraulic variables.

2.2.1 Assumptions for the Derivation of the Saint-Venant Equation for River Flows

The commonly used model for river flows is the one-dimensional Saint-Venant equation. In deriving it the following assumptions are made:

- Flow in the channels can well be approximated by a flow with uniform velocity over each cross-section,
- The channel is straight enough so that its course can be considered as a straight line,
- the pressure in the water obeys hydrostatic pressure law,
- the slope of the river bed is small,
- the effects of friction and turbulence can be modelled by a friction slope S_f.

2.2.2 Derivation of the Saint-Venant Equation

Consider a control volume between two cross sections x and $x + dx$ and between two level ξ and $\xi + d\xi$ as shown in Figure 2.1.

2.2.2.1 Continuity Equation

Let x $[m]$, t $[s]$ be the space and the time variables: $t \geq 0$, $x_0 \leq x \leq x_1$, $A(x, h(x,t))$ $[m^2]$ be the cross-section area, dA be the normal area vector, dV be the elemental volume, and U be the velocity vector with $|U| = u[ms^{-1}]$, and its direction is the direction of the flow. Then the continuity equation for this control volume can be written as follows

$$\frac{d}{dt}\iiint\limits_{c.v.} \rho dV + \iint\limits_{c.s.} \rho U \cdot dA = 0, \tag{2.1}$$

Where:

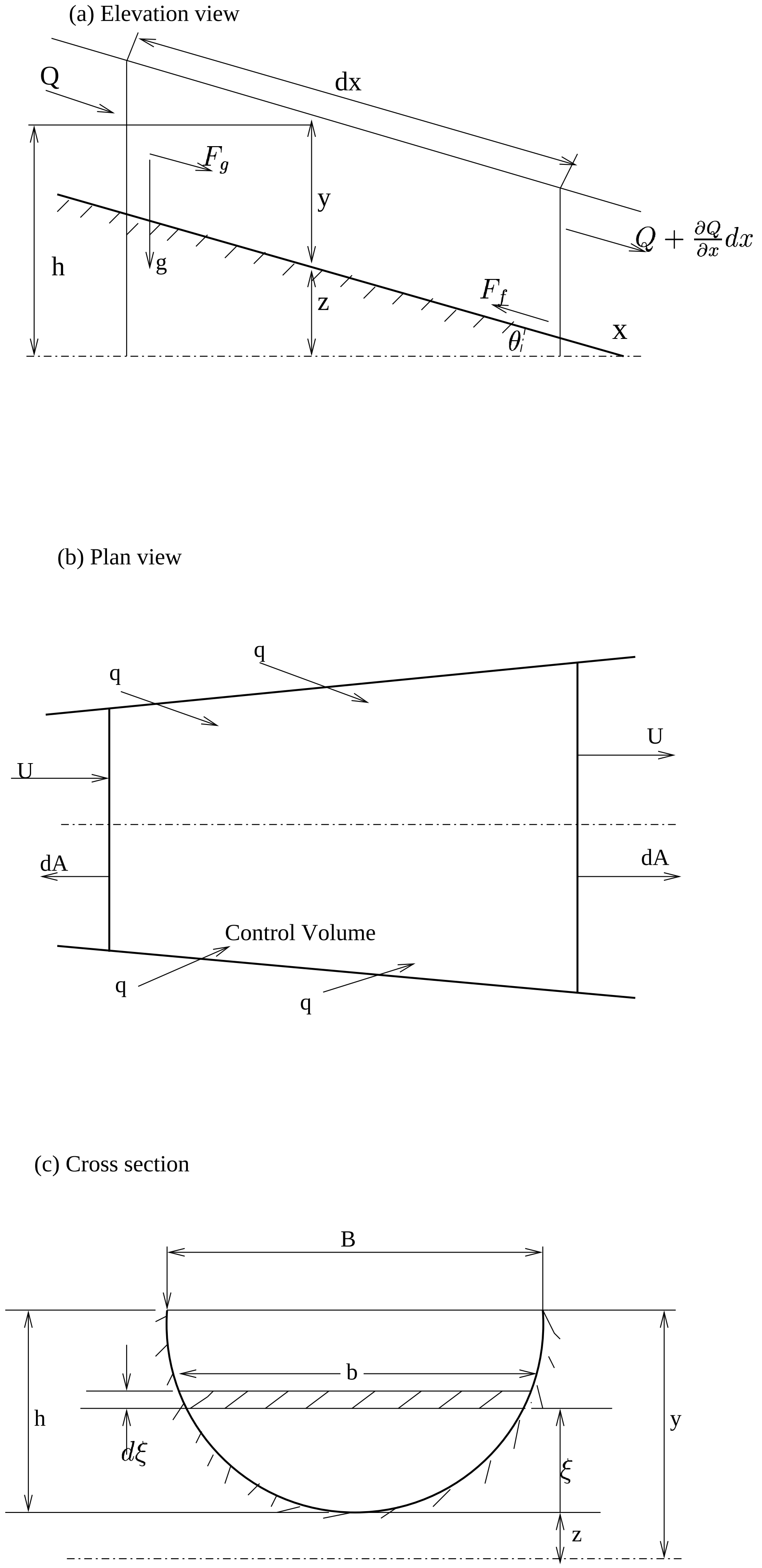

Figure 2.1: An elemental control volume for derivation of Saint-Venant Equations

- $\iiint_{c.v.}$ and $\iint_{c.s.}$ indicate the integration over the control volume and the integration over its surface, respectively.
- $U \cdot dA$ is the vector dot product of the vector U and the normal area vector dA, which is defined as

$$U \cdot dA = |U| \cos(\widehat{U, dA})|dA|$$

- ρ is the water density.

The first member of (2.1) is the rate of change of mass stored within the control volume. If $A(x, h(x,t))$ is the average cross-sectional area and dx is the length of the elemental control volume, then

$$\frac{d}{dt} \iiint_{c.v.} \rho dV = \frac{\partial(\rho A(x, h(x,t))dx)}{\partial t} \tag{2.2}$$

Here the partial derivative is used because the control volume is defined to be fixed in size (though the water level may vary within it)

The second member of (2.1) is total outflow of mass from the control volume. This can be computed as follows

$$\iint_{c.s.} \rho U \cdot dA = \iint_{inlet} \rho U \cdot dA + \iint_{outlet} \rho U \cdot dA \tag{2.3}$$

If we call $Q(x,t) = uA$ [m^3s^{-1}] the flow discharge, $q(x,t)$ [m^2s^{-1}] the lateral in- or outflow per unit length and assume that the density is constant, then

$$\iint_{inlet} \rho U \cdot dA = -\rho(Q(x,t) + qdx) \tag{2.4}$$

and

$$\iint_{outlet} \rho U \cdot dA = \rho(Q(x,t) + \frac{\partial Q(x,t)}{\partial x} dx) \tag{2.5}$$

Substituting Eqs (2.2)-(2.4) into (2.1) and simplifying by dividing by ρdx, we obtain

$$\frac{\partial Q(x,t)}{\partial x} + \frac{\partial A(x,h(x,t))}{\partial t} - q = 0 \tag{2.6}$$

Equation (2.6) is the continuity equation for a river flow.

2.2.2.2 Momentum Equation

Newton's second law for the considered control volume:

$$\rho\frac{d}{dt}(A(x,h(x,t))udx) = \sum F \tag{2.7}$$

where F are the forces acting on the control volume .

Using the Reynold's transport theorem (see [17, 1])

$$\rho\frac{d}{dt}(A(x,h(x,t))u\Delta x) = \frac{d}{dt}\iiint\limits_{cv} u\rho dV + \iint\limits_{c.s.} u\rho U \cdot dA$$

we can rewrite (2.7) as follows

$$\frac{d}{dt}\iiint\limits_{cv} u\rho dV + \iint\limits_{c.s.} u\rho U \cdot dA = \sum F \tag{2.8}$$

There are five forces acting on the considered volume:

$$\sum F = F_g + F_f + F_e + F_w + F_p \tag{2.9}$$

where F_g is the gravity force due to the weight of the water in the control volume, F_f is the friction force along the bottom and sides of the control volume, F_e is the contraction/expansion force produced by abrupt changes in the channel cross section, F_w is the wind shear force on the water surface, and the F_p is the unbalanced pressure force. In our modelling, we will neglect F_e and F_w. Each of the remaining three forces is evaluated in the following paragraphs.

Gravity

The weight of our considered volume is $\rho qA(x,h(x,t))dx$. Here g is the gravity acceleration. In Fig. 2.1 we can see that F_g is given by

$$F_g = \rho gA(x,h(x,t))dx sin\theta \tag{2.10}$$

We assume that θ is very small. Hence the bed slope $S_0 = tan\theta \approx sin\theta$. Substituting this to (2.10) gives

$$F_g = \rho g A(x, h(x,t)) S_0 dx \tag{2.11}$$

Friction

The friction force can be evaluated by the empirical formula

$$F_f = -\frac{C_n \rho g A(x, h(x,t)) u|u| dx}{R^{\frac{4}{3}}} \tag{2.12}$$

where C_n is the Manning Coefficient and R is the hydraulic radius.

Pressure

There two components of the pressure force:

- Pressure over the vertical surface F_{pv}, which is computed by

$$F_{pv} = -\frac{\partial}{\partial x}\left\{\int_0^{h(x,t)} \rho g(h(x,t) - \xi) b(x,\xi) d\xi\right\} dx \tag{2.13}$$

- Pressure over the part of slice in contact with the banks of the river F_{ph}, which is computed by

$$F_{ph} = \left\{\int_0^{h(x,t)} \rho g(h(x,t) - \xi) b_x(x,\xi) d\xi\right\} dx \tag{2.14}$$

Let us now consider equation (2.13). Using the Leibniz integral rule, we can rewrite the right hand side of this equation as follows

$$\begin{aligned}
&-\frac{\partial}{\partial x}\left\{\int_0^{h(x,t)} \rho g(h(x,t) - \xi) b(x,\xi) d\xi\right\} dx \\
&= -\left\{\int_0^{h(x,t)} \frac{\partial}{\partial x}\left(\rho g(h(x,t) - \xi) b(x,\xi)\right) d\xi\right\} dx \\
&\quad - \left\{\left(\rho g \underbrace{(h(x,t) - h(x,t)}_{=0} b(x, h(x,t)) \frac{\partial h(x,t)}{\partial x}\right)\right\} dx \\
&\quad + \left\{\left(\rho g(h(x,t) - 0) b(x,0) \underbrace{\frac{\partial 0}{\partial x}}_{=0}\right)\right\} dx \\
&= -\left\{\int_0^{h(x,t)} \frac{\partial}{\partial x}\left(\rho g(h(x,t) - \xi) b(x,\xi)\right) d\xi\right\} dx
\end{aligned}$$

Hence, we can compute F_p as follows

$$\begin{aligned}
F_p &= F_{pv} + F_{ph} \\
F_p &= -\left\{\int_0^{h(x,t)} \frac{\partial}{\partial x}\left(\rho g(h(x,t)-\xi)b(x,\xi)\right)d\xi\right\}dx \\
&\quad + \left\{\int_0^{h(x,t)} \rho g(h(x,t)-\xi)b_x(x,\xi)d\xi\right\}dx \\
&= -\int_0^{h(x,t)} \rho g h_x(x,t)b(x,\xi)d\xi dx
\end{aligned}$$

Note that $h_x(x,t)$ is independent of ξ and the cross section area is computed by $A(x,h(x,t)) = \int_0^{h(x,t)} b(x,\xi)d\xi$. We can rewrite this equation as follows

$$\begin{aligned}
F_p &= -\int_0^{h(x,t)} \rho g h_x(x,t)b(x,\xi)d\xi dx \\
&= -\rho g h_x(x,t)\int_0^{h(x,t)} b(x,\xi)d\xi dx = -\rho g A(x,h(x,t))h_x(x,t)dx. \qquad (2.15)
\end{aligned}$$

Now let us consider the left hand side (LHS) of (2.8). The first member of the LHS is computed by

$$\frac{d}{dt}\iiint_{cv} u\rho dV = \rho dx \frac{\partial}{\partial t}\left(Q(x,t)\right) \qquad (2.16)$$

The second member of the LHS can be computed as follows:

$$\begin{aligned}
\iint_{c.s.} u\rho u.dA &= \iint_{inlet} u\rho u.dA + \iint_{outlet} u\rho u.dA \\
&= -\rho u(Q(x,t)+qdx) + \left(\rho u Q(x,t) + \frac{\partial}{\partial x}(\rho u Q(x,t))dx\right) \\
&= -\rho q u dx + \frac{\partial}{\partial x}(\rho u Q(x,t))dx \qquad (2.17)
\end{aligned}$$

Now substituting equations (2.11), (2.12), (2.15), (2.16), and (2.17) into (2.8) and simplifying gives

$$\frac{\partial Q(x,t)}{\partial t} + \frac{\partial}{\partial x}\left(\frac{Q(x,t)^2}{A(x,h(x,t))}\right) = -A(x,h(x,t))gh_x(x,t) + A(x,h(x,t))g(S_0 - S_f) + qu, \tag{2.18}$$

where $S_f = \frac{F_f}{\rho g A(x,h(x,t))} = \frac{C_n u|u|}{R^{\frac{4}{3}}}$ is called friction slope.

The two differential equations (2.6) and (2.18) are the basic equations for the modelling of river flows, and called the Saint-Venant equations.

2.2.3 Alternative Formulations

There are other ways of representing the Saint-Venant equations which are expressed in terms of different pairs of the state variables:

2.2.3.1 Using $Q(x,t)$ and $h(x,t)$

Equations (2.6) and (2.18) can be rewritten in term of $Q(x,t)$ and $h(x,t)$ as follows:

$$\begin{cases} \dfrac{\partial h(x,t)}{\partial t} = -\dfrac{Q_x(x,t)}{A_h(x,h(x,t)} + \dfrac{q}{A_h(x,h(x,t))} \\ \dfrac{\partial Q(x,t)}{\partial t} = -\dfrac{\partial}{\partial x}\left(\dfrac{Q(x,t)^2}{A(x,h(x,t))}\right) - A(x,h(x,t))gh_x(x,t) \\ \qquad + A(x,h(x,t))g(S_0 - S_f) + qu. \end{cases}$$

2.2.3.2 Using $Q(x,t)$ and $y(x,t)$

In the current time, by applying new technologies, at any gauging station we can measure the absolute water level $y(x,t)$, i.e. the water level with respect to the null level. In Figure 2.1 the relation between $h(x,t)$ and $y(x,t)$ is shown:

$$y(x,t) = h(x,t) + z(x) \tag{2.19}$$

Here, $z(x)$ is the bed height. By definition we have

$$z_x(x) = -S_0(x), \qquad \text{where } S_0 \text{ is the bed slope.} \tag{2.20}$$

Differentiating (2.19) and substituting into (2.20) we get

$$y_x(x,t) = h_x(x,t) - S_0(x) \tag{2.21}$$

By using (2.19), (2.20) and (2.21) we can represent the cross-sectional area and its partial derivatives as follows

$$\begin{aligned} A(x,h(x,t)) &= A(x,y(x,t)-z(x)) =: \tilde{A}(x,y(x,t)), \\ \tilde{A}_t(x,y(x,t)) &= \tilde{A}_y(x,y(x,t))y_t(x,t) \qquad (2.22) \\ &= A_h(x,h(x,t))h_t(x,t) \qquad (2.23) \end{aligned}$$

Substituting (2.19), (2.20), (2.21), and (2.23) into (2.6) and (2.18), we obtain the system

$$\begin{cases} y_t(x,t) = -\dfrac{Q_x(x,t)}{\tilde{A}_y(x,y(x,t))} + \dfrac{q}{\tilde{A}_y(x,y(x,t))} \\ Q_t(x,t) = -2\dfrac{Q(x,t)}{\tilde{A}(x,y(x,t))}Q_x(x,t) \\ \qquad + \left(\dfrac{Q(x,t)}{\tilde{A}(x,y(x,t))}\right)^2 \tilde{A}_x(x,y(x,t)) \\ \qquad -g\tilde{A}(x,y(x,t))(y_x(x,t)+S_f)+qu \end{cases} \tag{2.24}$$

The equation system (2.24) is the Saint-Venant equation expressed in term of $Q(x,t)$ and $y(x,t)$ and has the following advantages

- An unique coordinate system for the whole system. Because the null level is unique for the Red River system.
- S_0 is eliminated from the equation system. That reduces the number of unknown parameters.

By doing an analogous transfer, we can rewrite the Saint-Venant equation in term of $u(x,t)$ and $h(x,t)$ or $u(x,t)$ and $y(x,t)$ as follows

2.2.3.3 Using $u(x,t)$ and $h(x,t)$

The flow velocity $u(x,t)$ is computed by

$$\begin{aligned} u(x,t) &= \frac{Q(x,t)}{A(x,h(x,t))} \\ &= \frac{Q(x,t)}{\tilde{A}(x,y(x,t))} \end{aligned}$$

Then, the Saint-Venant equation can be rewritten in the following form

$$\begin{cases} h_t(x,t) &= -\dfrac{A(x,h(x,t))}{B(x,h(x,t))}u_x(x,t) - \dfrac{u(x,t)A_x(x,h(x,t))}{B(x,h(x,t))} + \dfrac{q}{B(x,h(x,t))} \\ u_t(x,t) &= -u(x,t)u_x(x,t) - gh_x(x,t) - g(S_f - S_0) + \dfrac{qu(x,t)}{A(x,h(x,t))} \end{cases} \tag{2.25}$$

Here, $B(x,h(x,t))$ denotes the width of the river at the location x and corresponding to the water depth $h(x,t)$.

2.2.3.4 Using $u(x,t)$ and $y(x,t)$

$$\begin{cases} y_t(x,t) &= -\dfrac{\tilde{A}(x,y(x,t))}{\tilde{B}(x,y(x,t))}u_x(x,t) - \dfrac{u(x,t)\tilde{A}_x(x,h(x,t))}{\tilde{B}(x,y(x,t))} + \dfrac{q}{\tilde{B}(x,h(x,t))} \\ u_t(x,t) &= -u(x,t)u_x(x,t) - gy_x(x,t) - gS_f + \dfrac{qu(x,t)}{\tilde{A}(x,y(x,t))} \end{cases}$$

Here, $\tilde{B}(x,h(x,t))$ denotes the width of the river at the location x and corresponding to the water level $y(x,t)$.

2.3 Parameterization for Hydraulic Functions of Saint-Venant Equation

In order to describe our system completely, in this section we will discuss how to parameterize the following hydraulic functions, which occur in the Saint-Venant equation:

- Lateral water flow q
- Cross-sectional area $\tilde{A}(x,y(x,t))$
- Friction slope S_f

2.3.1 Lateral Water Flow

Lateral water inflow to a river channel includes following components:

- Rainfall q_r (positive),
- Underground water source $q_{\rm uw}$ (negative),
- Water used for farm products $q_{\rm farm}$ (negative),
- Water used for living $q_{\rm live}$(negative),
- Evaporating water $q_{\rm evap}$(negative).

The two last components are very small compared to the first three components. Hence, we investigate only the first three components.

Rainfall

The investigation of the water balance in Vietnam [34] shows that the mean of the rainfall in the Red River lowland is about 1.50 m per year, or 4.76×10^{-8} [m/s]. For the Red River system, the width of the river varies from 2.00×10^2 to 2.00×10^3 [m]. Correlatively, the discharge of rainfall per unit of length q_r varies from 9.52×10^{-6} to 9.52×10^{-5} [m^3/s]

Underground Water Sourses

The total resource of underground water for the Red River system is 0.27×10^2 [m^3/s]. If the total length of Red River is 5.50×10^5 [m], then per unit of length, the value of underground water is 4.91×10^{-5} [m^3/s]

Water used for farm products

The total of water required for farm products is 10^{10} [m^3] per year (see [34]), or 3.17×10^2 $[m^3/s]$. If the total length of Red River is 5.50×10^5 [m], then, the value of the the water used for farm per unit of length is $q_{farm} = 5.76 \times 10^{-4}$ [m^3/s].

Summarzing the above investigation, we get Table 2.1 for the water balance

Water resource	Notation	$Value$ [m^3/s]
Underground water	$q_{\rm uw}$	4.91×10^{-5}
Water used for farm	$q_{\rm farm}$	5.76×10^{-4}
Rainfall	q_r	$9.52 \times 10^{-6} \div 9.52 \times 10^{-5}$
Total lateral water	q	$\simeq 6.00 \times 10^{-4}$
Water discharge in Ha Noi	Q	$3.00 \times 10^3 \div 9.00 \times 10^3$

Table 2.1: Evaluation of Water Resource

In this table, we can see that $q \ll Q$, and consequently the lateral water q can be neglected.

2.3.2 Cross-Sectional Area

Cross-sectional area is a function of x and y

$A = \tilde{A}(x, y)$

If at every location x, we define the river width $b(x, y)$ as a function of the water level y and the location x, then the cross-sectional area can be computed as follows

$$\tilde{A}(x, y) = \int_{y_0(x)}^{y} b(x, y)dy \tag{2.26}$$

where $y_0(x)$ is the river bed level at the location x, i.e. the level, in which $b(x, y_0) = 0$.

Wetted perimeter is the length of the cross section along which there is friction between the fluid and the boundary. It is denoted by W_p and computed as follows

$$W_p(x, y) = \int_{y_0(x)}^{y} \sqrt{1 + b_y(x, y)^2} dy \tag{2.27}$$

In Equation (2.12) the **hydraulic radius** R appears. It is defined as

$$R(x, y) = \frac{\tilde{A}(x, y)}{W_p(x, y)} \tag{2.28}$$

In practice, at some location x, the relation between the river width and the water level is given in the table form

Water level y	y_1	y_2	$\ldots$	y_n
River width $b(x, y)$	b_1	b_2	$\ldots$	b_n

Table 2.2: Definition of Cross section

In Table (2.2), n is the number of measured points in the y direction.

Then, as an approximation of the solution of equations (2.26) and (2.27) we compute $\tilde{A}(x, y)$ and $W_p(x, y)$ at arbitrary $y = y_i$, for $i = 1, 2, .., n$

$$\tilde{A}(x, y_i) = \sum_{j=1}^{i-1} b_j (y_{j+1} - y_j) \tag{2.29}$$

$$W_p(x, y_i) = \sum_{j=1}^{i-1} \sqrt{(b_{j+1} - b_j)^2 + (y_{j+1} - y_i)^2} \tag{2.30}$$

2.3.3 Friction Slope

By rewriting the Manning equation and replacing $u = \frac{Q}{A}$, we get

$$S_f = -\frac{C_n Q|Q|}{A^2 R^{\frac{4}{3}}} \tag{2.31}$$

The hydraulic radius can be easily computed by the equation (2.28). The only unknown function is the Manning coefficient C_n. That is an unmeasurable quantity, and our task now is to estimate it.

The investigation of the U.S. Army Corps of Engineers for the Mississippi River [67] shows that the Manning coefficient C_n depends on the water discharge and this relation is also a function of the time. This is illustrated in the Figure 2.2.

Based on the results of this investigation, we assume that C_n is a function of the discharge Q. We propose that C_n for the river channel i_{chan}, at the cross-sectional area i_{cross} is defined by a polynomial as follows

$$C_n(x_{i_{\text{chan}}}^{i_{\text{cross}}}, Q(x_{i_{\text{chan}}}^{i_{\text{cross}}}, t)) = \sum_{i=0}^{n_p(i_{\text{chan}})} p(i_{\text{chan}}, i) \left(\frac{Q_{\max}(i_{\text{chan}})}{Q(x_{i_{\text{chan}}}^{i_{\text{cross}}}, t)} \right)^i, \tag{2.32}$$

where: $x_{i_{\text{chan}}}^{i_{\text{cross}}}$ is the location at the cross-sectional area i_{cross} of the channel i_{chan}; $Q(x_{i_{\text{chan}}}^{i_{\text{cross}}}, t)$ and $Q_{max}(i_{\text{chan}})$ are the water discharge in the location $x_{i_{\text{chan}}}^{i_{\text{cross}}}$ at the time t and the maximal value of the water discharge for the channel i_{chan}; $p(i_{\text{chan}}, i)$, $i = 0, 1, \ldots, n_p(i_{\text{chan}})$ is the parameter number i of the channel i_{chan}, with $n_p(i_{\text{chan}})$ is number of the all parameters of channel i_{chan}.

There are two problems we have to solve

- Determine the number of all the parameters $n_p(i_{\text{chan}}) + 1$
- Determine the values of all parameters $p(i_{\text{chan}}, i)$

The second problem is solved by means of optimization, minimizing the difference between the value of the water level measured at some gauging stations and the value of the water level at the same gauging stations, but computed from the simulation of the Red River system. We will discuss it in more detail in the next section.

For the first problem, we assume that the second problem is solved, i.e. we can determine the values of all parameters if we know $n_p(i_{\text{chan}})$. Then $n_p(i_{\text{chan}})$ can be determined by using the F-test for linear hypotheses testing (see [5], [55]). The main idea of this is to answer to the question: for a given number i, are the $i+1$ parameters significantly better than i parameter?

The main steps for taking the decision are:

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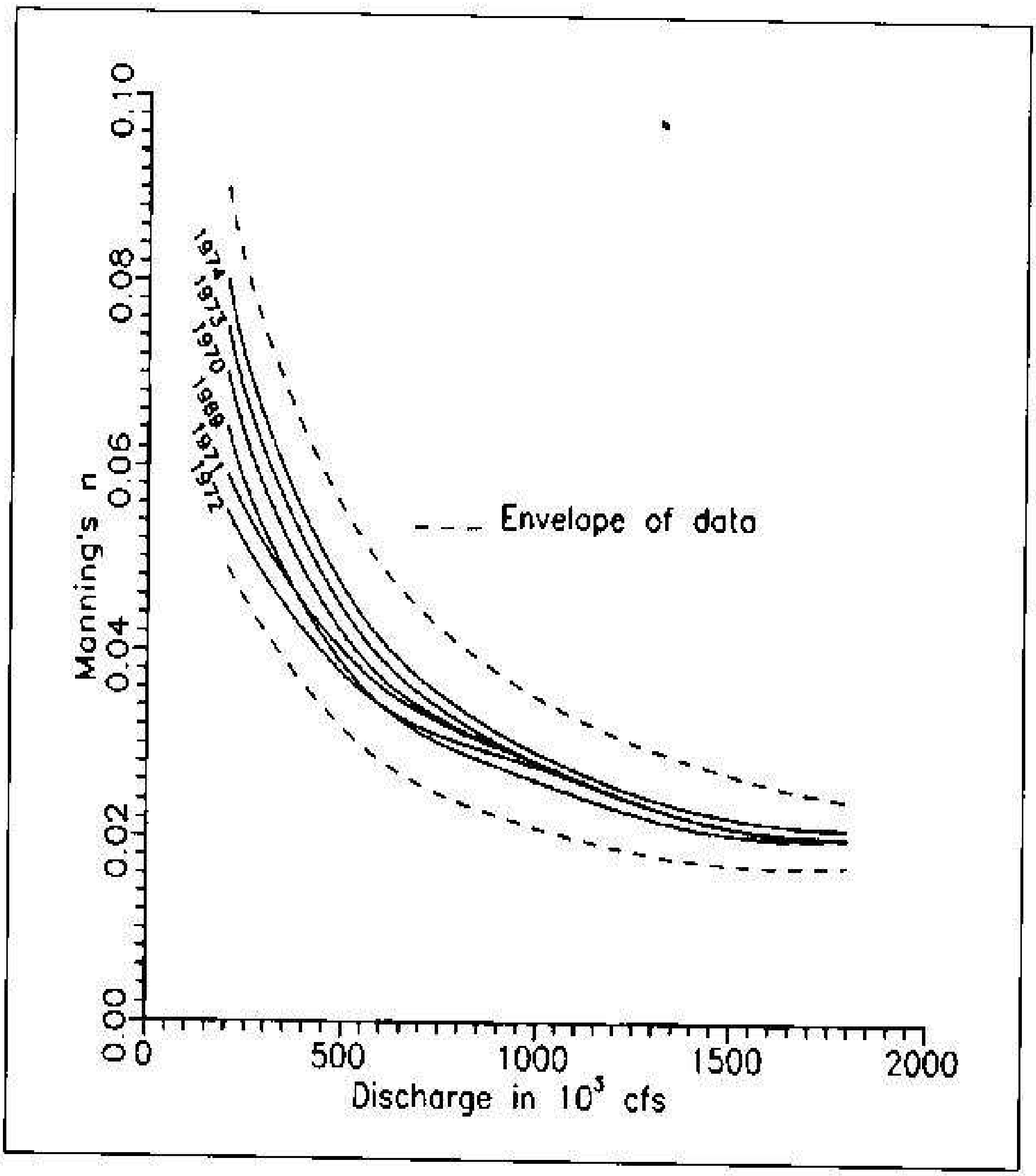


Figure D-14. Variation of Manning's *n* with discharge for the Mississippi River at Arkansas City (Source: St. Louis District, U.S. Army Corps of Engineers)

Figure 2.2: Variation of Manning's C_n (Source: St. Louis District, U.S. Army Corps of Engineers [67])

- **Step 1:** starting from $i = 1$, i.e. there is only one parameter.
- **Step 2:** Determining parameter p_i for $n_p = i$ and the corresponding residual S_i.
- **Step 3:** Determining parameter p_{i+1} for $n_p = i + 1$ and the corresponding residual S_{i+1}.
- **Step 4:** Computing the test function

$$F_{test} = \frac{S_i - S_{i+1}}{S_{i+1}} \frac{n_m - n_p}{n_p},$$

  where n_m, n_p are the number of measurements and number of parameters, respectively.

  - **If** $F_{test} \geq F_{n_p, n_m - n_p}$ then p_{i+1} is significantly better than p_i. We set $i = i + 1$ and go to step 2,
  - **Else** the suitable parameter number $n_p = i$. Stop.

Here, $F_{n_p, n_m - n_p}$ denotes the quantile of the Fisher distribution on the some probability confidence level, say 0.95, with the degrees of freedom n_p and $n_m - n_p$ (see e.g. [47]).

2.3.4 The River Network Models

2.3.4.1 Internal Boundary Condition

It is important to have a good model for the junction of two channels in order to connect several single channels to a river network. In Figure 2.3, the basic notations of two joint river channels are shown: the channels 1 and 2 join to channel 3 at the location $\bar{x}$. x_1, x_2, x_3 are respectively the locations of the beginning points of the channels 1 and 2, and the last point of the channel 3.

The precise hydraulic description of the flow at channel junctions is rather complicated and difficult because of the hight degree of flow mixing, separation, turbulence, and energy loss. We assume that the energy losses are neglected, and the junction is point-type. Then the conditions for the water flow at the joint point are:

$$Q_3(\overline{x}, t) = Q_1(\overline{x}, t) + Q_2(\overline{x}, t) \quad (2.33)$$

$$h_1(\overline{x}, t) = h_3(\overline{x}, t) \quad (2.34)$$

$$h_2(\overline{x}, t) = h_3(\overline{x}, t) \quad (2.35)$$

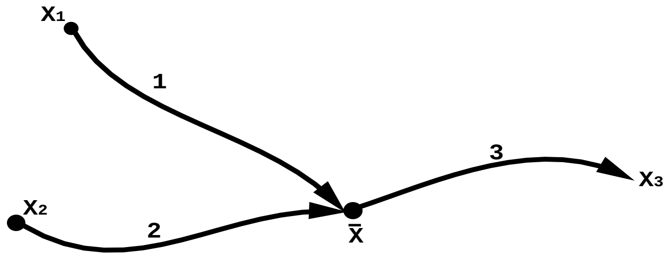


Figure 2.3: Junction of two river channels

The flow directions shown in Figure 2.3 play only a formal role. In the case that the flow in any channel has a converted direction, the equation (2.33)-(2.35) are also valid with the change that the sign of the discharge of this channel is converted in the equation (2.33).

2.3.4.2 Boundary Condition

Figure 2.4 illustrates a scheme of the Red River system. As it will be menioned later in Chapter 3 for an unique solution of the simulation of the Red River system, the following boundary conditions should be given:

- Upper boundary conditions, i.e. a state variables at the input nodes of the system, namely Hoa Binh, Phu Tho, and Vu Quang. In our study of the Red River system the water discharge at these three input nodes are given as functions in time $Q(x^{\text{upper}}, t)$, where x^{upper} is the location of the upper boundaries.
- Lower boundary conditions, i.e. a state variables at the output nodes of the system, namely Thuong Cat, Trieu Duong, Nam Dinh, Phu Le, Ba Lat, and Dinh Cu. In our study the water level at these listed output nodes of the Red River system are given as functions in time $y(x^{\text{lower}}, t)$, where x^{lower} is the location of the lower boundary nodes.

Let z denote

- the state variables, which are given in the left hand site of Equations (2.33)-(2.35) as the internal boundary conditions,
- and the variables $Q(x^{\text{upper}}, t)$, and $y(x^{\text{lower}}, t)$, which are given as the boundary conditions of the Red River system.

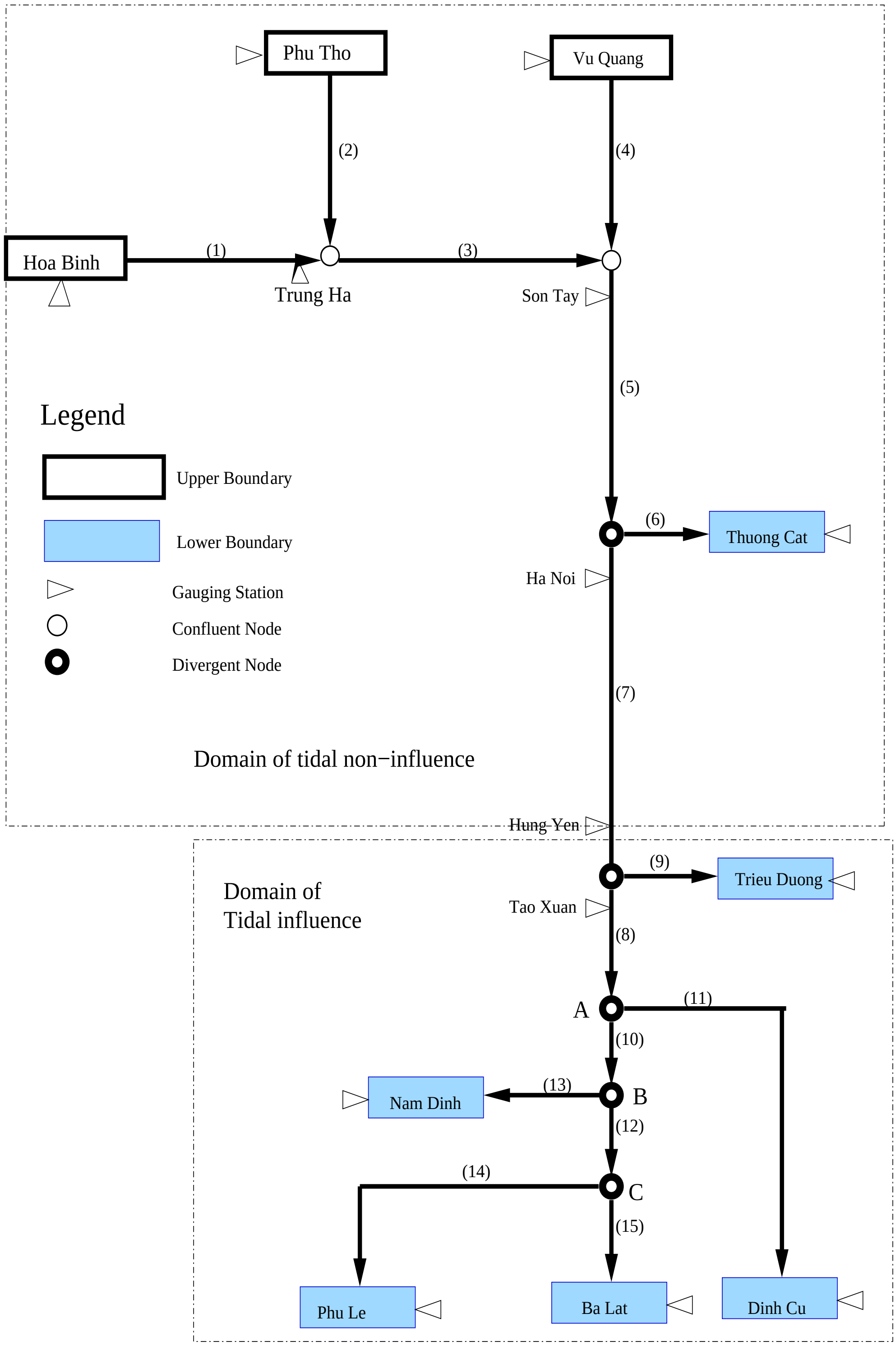


Figure 2.4: The Red River Network

Then, we can summary all internal boundary conditions and all boundary conditions in the following general form:

$$z = \phi(t, w; p). \tag{2.36}$$

Here:

- $z \in I\!R^{n_z}$, with $n_z = 2 \cdot n_{\text{chan}}$, where n_{chan} is the number of all channels of the Red River system,
- t is the time variable: $t \in I := [t_0, t_{end}]$ and x is the space variable $x \in X := [x_0, x_{end}]$,
- $w(t, x, w, z; p)$ is the state variable, i.e. water discharge Q or water level y at the point x. And z is the state variable which is given as boundary condition or determined by equations (2.33)-(2.35): $z \in I\!R^{n_z}$, with n_{chan} is the number of the channel members and $n_z = 2 \times n_{chan}$ is the number of boundary conditions including internal boundary conditions,
- p is the parameter: $p \in I\!R^{n_p}$, with n_p the number of parameters,
- $\phi(t, w; p)$ is the vector of the right hand side of the equation for boundary condition for channel members: $\phi : I \times I\!R^{n_w} \times I\!R^{n_p} \to I\!R^{n_z}$.

For the ease of presentation, later in this thesis we call (2.36) the boundary conditions of the Red River system.

2.3.4.3 The Model for a River Connected Network

The Saint-Venant equation for all channel members in the river network coupled with the boundary conditions and the internal boundary condition determined by the equation (2.36) and initial conditions establishes the model of the river network. It can be written in the following general form:

Saint-Venant equation

$$\dot{w}(x, t, w, w_x, z; p) = f(t, x, w, w_x, z; p), \tag{2.37}$$

Boundary conditions

$$z = \phi(t, w; p),$$

Initial Conditions

$$w(t_0, x) = w_0(x),$$

where:

- t is the time variable: $t \in I := [t_0, t_{end}]$ and x is the space variable $x \in X := [x_0, x_{end}]$,
- $w(t, x, w, z; p)$ is the state variable, i.e. water discharge Q or water level y at the point x. And z is the state variable which is given as boundary condition or determined by equations (2.33)-(2.35): $z \in I\!R^{n_z}$, with n_{chan} is the number of the channel members and $n_z = 2 \cdot n_{chan}$ is the number of boundary conditions including internal boundary conditions,
- p is the parameter: $p \in I\!R^{n_p}$, with n_p the number of parameters,
- $f(t, x, w, w_x, z; p)$ is the vector of the right hand side of the Saint-Venant equation for channel members: $f : I \times X \times I\!R^{n_w} \times I\!R^{n_z} \times I\!R^{n_p} \rightarrow I\!R^{n_w}$
- $\phi(t, w; p)$ is the vector of the right hand side of the equation for boundary condition for channel members: $\phi : I \times I\!R^{n_w} \times I\!R^{n_p} \rightarrow I\!R^{n_w}$,
- w_0 is the initial condition: $w_0 : X \rightarrow I\!R^{n_w}$.

Chapter 3

Numerical Methods for Simulation of the Saint-Venant Equation

In the last chapter the mathematical equations model for the river flows are described. Now it is shown how these can be solved.

As it has been mentioned in the last section, the Saint-Venant equation for river flows is a pair of two first-order nonhomogeneous hyperbolic partial differential equation. In Section 3.1 the introduction the equation of this type is given. The focus of this section is existence and uniqueness of solutions of the considered initial-boundary value problems.

It is well-known that a hyperbolic partial differential equation cannot be solved analytically except by making some very strict assumptions which are unrealistic for most situations. Therefore a numerical approach has to be used. In the next sections, the numerical methods for simulation of the Saint-Venant equation for river flows are outlined. In Section 3.2 it is shown how to discretize the Saint-Venant equation in space. That leads our PDE system into a large stiff system of semi-implicit ordinary differential equations. For the solution of this system, we use the solver DAESOL which has been developed in the research group of Bock and Schlöder by Bauer [6, 8]. This is a stable and efficient integrator. The theoretical basis of the solver DAESOL is given in Section 3.3.

Due to the problem that the number of characters is limited, in this chapter some letters, e.g. y, z, u, and w are used as the notation of mathematical variables or functions and not related with the physical variables which have the same notations in the model equations.

3.1 Introduction to Hyperbolic PDE

The investigation of general hyperbolic PDE has been described in many textbooks of mathematics like Tveito [66], Morton [46], or textbooks of computer science and scientific computing like Ames [2], or university lectures scripts like Sleigh *et al.* [56]. In this section, using the material from the above listed literature the author will make clear some important properties of hyperbolic PDE, which are useful for the numerical solution of the Saint-Venant equation - a specific case of a hyperbolic PDE.

3.1.1 The Characteristics of the Saint-Venant Equation

The general form of a linear first-order hyperbolic partial differential equation is

$$\begin{aligned} w_t + a(x,t)w_x &= f(x,t) \\ w(x,0) &= w_0(x) \end{aligned} \tag{3.1}$$

with state variable $w \in I\!R$, spatial variable $x \in I\!R$, time variable $t \in I\!R$, $t \geq 0$. a, f, and w_0 are given smooth functions.

For simplicity we assume that w is scalar. However the results of the following discussion is also valid for the case, when the state variable w is a vector.

Definition 3.1.1 *Any solution of*

$$\begin{aligned} \frac{dx}{dt} &= a(x(t),t) \\ x(0) &= x_0 \end{aligned} \tag{3.2}$$

is called the characteristic of hyperbolic PDE (3.1)

Remark 3.1.2 *By choosing different values of x_0, we have a family of characteristics of (3.2).*

In Figure 3.1 an example for the family of characteristic curves is illustrated. Along a characteristic curve the solution $w(x,t)$ satisfies

$$\begin{aligned} \frac{dw}{dt} &= \frac{\partial w}{\partial t} + \frac{\partial w}{\partial x}\frac{dx}{dt} \\ &= \frac{\partial w}{\partial t} + a(x(t),t)\frac{\partial w}{\partial x} \\ &= f(x,t) \end{aligned} \tag{3.3}$$

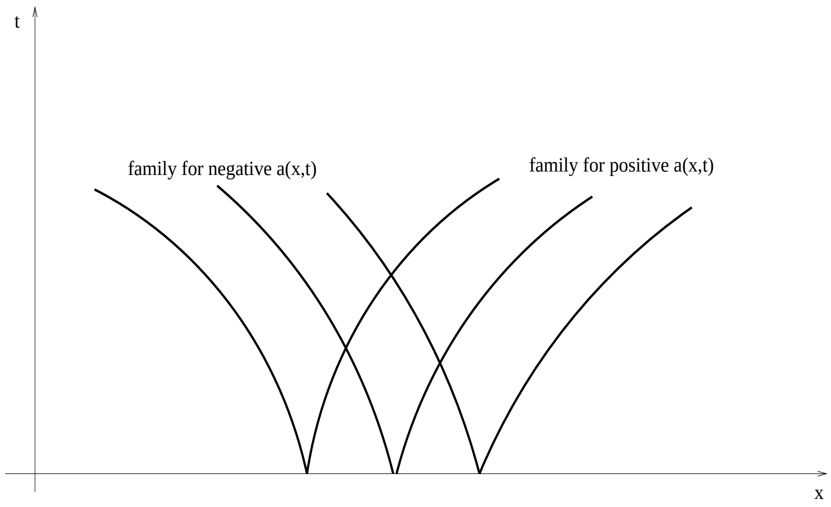


Figure 3.1: A family of characteristics of a hyperbolic PDE

The same principles can be applied to the case

$$\begin{aligned} w_t + a(w)w_x &= f(x,t) \\ w(x,0) &= w_0(x) \end{aligned} \tag{3.4}$$

where if $\dfrac{dx}{dt} = a(w)$ then

$$\begin{aligned} \frac{dw}{dt} &= \frac{\partial w}{\partial t} + \frac{\partial w}{\partial x}\frac{dx}{dt} \\ &= \frac{\partial w}{\partial t} + a(w)\frac{\partial w}{\partial x} \\ &= f(x,t) \end{aligned} \tag{3.5}$$

Now let us define the characteristics for the Saint-Venant equation. Firstly, we have to arrange our equation system in the form of (3.4). For simplicity, we consider a simplest river channel which has rectangular cross section area A of constant river width b and constant bed slope S_0. The result of this consideration is valid for rivers in general, i.e. with a cross section area of any form, where the river width and the bed slope are functions of water depth and space, respectively.

If we define the wave speed $c(x,t)$ by

$$c = \sqrt{gh},$$

then

$$h = \frac{c^2}{g},$$

and consequently, we have

$$dh = \frac{2c}{g} dc.$$

Now by replacing all the terms involving h of equation system (2.25), and replacing $A = b.h$, as it has been assumed above, we get

Continuity equation

$$\begin{aligned} & b\frac{\partial h}{\partial t} + bu\frac{\partial h}{\partial x} + bh\frac{\partial u}{\partial x} &= 0 \\ \Longleftrightarrow \quad & \frac{2c}{g}b\frac{\partial c}{\partial t} + \frac{2c}{g}bu\frac{\partial c}{\partial x} + b\frac{c^2}{g}\frac{\partial u}{\partial x} &= 0 \\ \Longleftrightarrow \quad & 2\frac{\partial c}{\partial t} + 2u\frac{\partial c}{\partial x} + c\frac{\partial u}{\partial x} &= 0 \end{aligned}$$

The last equation uses c and u as state variables.

Momentum equation

Analogously, for the momentum equation, we get

$$\frac{\partial u}{\partial t} + 2c\frac{\partial c}{\partial x} + u\frac{\partial u}{\partial x} = g(S_0 - S_f) \tag{3.6}$$

Adding and subtracting (3.6) and (3.6) give

$$\begin{aligned} \frac{\partial u}{\partial t} + (u+c)\frac{\partial u}{\partial x} + 2\frac{\partial c}{\partial t} + 2(u+c)\frac{\partial c}{\partial x} &= g(S_0 - S_f) \\ \frac{\partial u}{\partial t} + (u-c)\frac{\partial u}{\partial x} - 2\frac{\partial c}{\partial t} - 2(u-c)\frac{\partial c}{\partial x} &= g(S_0 - S_f) \end{aligned}$$

These equations can be rearranged as

$$\frac{\partial(u+2c)}{\partial t} + (u+c)\frac{\partial(u+2c)}{\partial x} = g(S_0 - S_f) \tag{3.7}$$

$$\frac{\partial(u-2c)}{\partial t} + (u-c)\frac{\partial(u-2c)}{\partial x} = g(S_0 - S_f) \tag{3.8}$$

The equation system (3.7) and (3.8) is the Saint-Venant equation written in the general form of (3.1), where

$$w = \begin{pmatrix} u + 2c \\ u - 2c \end{pmatrix} \qquad a = \begin{pmatrix} u + c \\ u - c \end{pmatrix} \qquad f = g \begin{pmatrix} S_0 - S_f \\ S_0 - S_f \end{pmatrix}$$

By definition (3.2) the equations of the two characteristics C_1 and C_2 of the Saint-Venant equation are

$$\begin{aligned} C_1 : \quad & \frac{dx}{dt} = u + c \\ C_2 : \quad & \frac{dx}{dt} = u - c \end{aligned} \tag{3.9}$$

using equation (3.3) we have the relationship between u and c along the curve C_1

$$\frac{d(u + 2c)}{dt} = g(S_0 - S_f) \tag{3.10}$$

and along the curve C_2

$$\frac{d(u - 2c)}{dt} = g(S_0 - S_f) \tag{3.11}$$

Definition 3.1.3 *Flows can be classified as follows*

- *If the flow velocity is greater than the wave speed: $u > c$, then the flow is called supercritical*
- *If the flow velocity is equal to the wave speed: $u = c$, then the flow is called critical*
- *If the flow velocity is lower than the wave velocity: $u < c$, then the flow is called subcritical*

3.1.1.1 The Domain of Dependence and the Zone of Influence

For any river flow, the velocity is always less than the wave velocity, i.e. $|u| < c$. Consequently, from now and through this thesis we consider only subcritical flows.

As it is shown in Figure 3.3, the state variables at the point P are determined by the equations of two characteristics C_1 and C_2, which are crossed at P. Only the domain, bounded within two characteristics can influence the conditions at P. Any disturbance

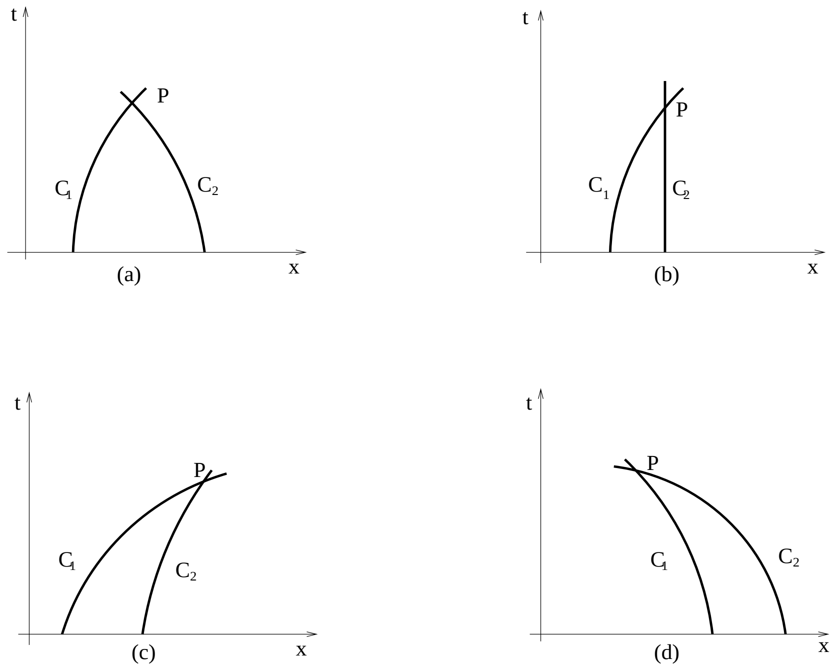


Figure 3.2: Characteristics and flow classification: (a) subcritical flow; (b) critical flow; (c) supercritical flow in a positive direction; (d) supercritical flow in a negative direction

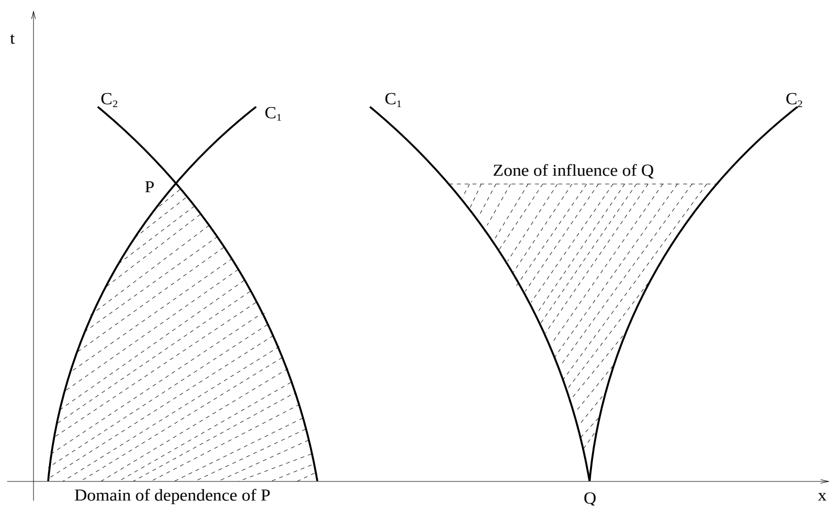


Figure 3.3: Domain of dependence and zone of influence

outside of this domain will not influence the flow at P. This domain is called domain of dependence of P.

Conversly, any disturbance occuring at some point Q, as shown in Figure 3.3 can be propagated in both upstream and downstream by the curves C_1 and C_2. This means that the conditions at Q can influence only the zone that is bounded within the two curves C_1 and C_2. This zone is called zone of influence of Q.

Knowledge of the characteristics and of the domain of dependence and influence is important in the study of the influence of initial and boundary conditions to uniqueness of the solution of the system.

3.1.2 Existence and Uniqueness of the Solution for the Saint-Venant Equation

If we denote $w_1 = u + 2c$, $w_2 = u - 2c$, $a_1 = u + c$, $a_2 = u - c$, $e = g(S_0 - S_f)$, then the Saint-Venant can be rewritten as follows

$$\begin{cases} \dfrac{\partial w_1}{\partial t} + a_1 \dfrac{\partial w_1}{\partial x} & = & e \\ \dfrac{\partial w_2}{\partial t} + a_2 \dfrac{\partial w_2}{\partial x} & = & e \end{cases} \tag{3.12}$$

Boundary conditions and internal boundary conditions: let w_z be the state variables, which are given as the boundary conditions and the internal boundary conditions as mentioned in Section 2.3, then Equation 2.36 of the boundary conditions and the internal boundary conditions can be rewritten in the following form

$$w_z = \tilde{\phi}(t, w_1, w_2; p).$$

Initial Conditions

$$w_1(t_0, x) = w_1^0(x), \qquad w_2(t_0, x) = w_2^0(x).$$

This is a system of two simultaneous first-order hyperbolic partial differential equations. Let us now specify which initial and boundary conditions determine unique solutions for this equation system. The following theorems are taken from Ames [2]. Their proofs and additional information can be found in Bernstein [9], Garabedian [32], and Courant and Hilbert [20].

Theorem 3.1.4 *[2] Let us suppose that continuously differentiable values of w_1 and w_2 are specified on the noncharacteristic curve CD of Fig. 3.4 (a), and assume that CD to be continuously differentiable. A solution to Eqns (3.12), assuming these prescribed*

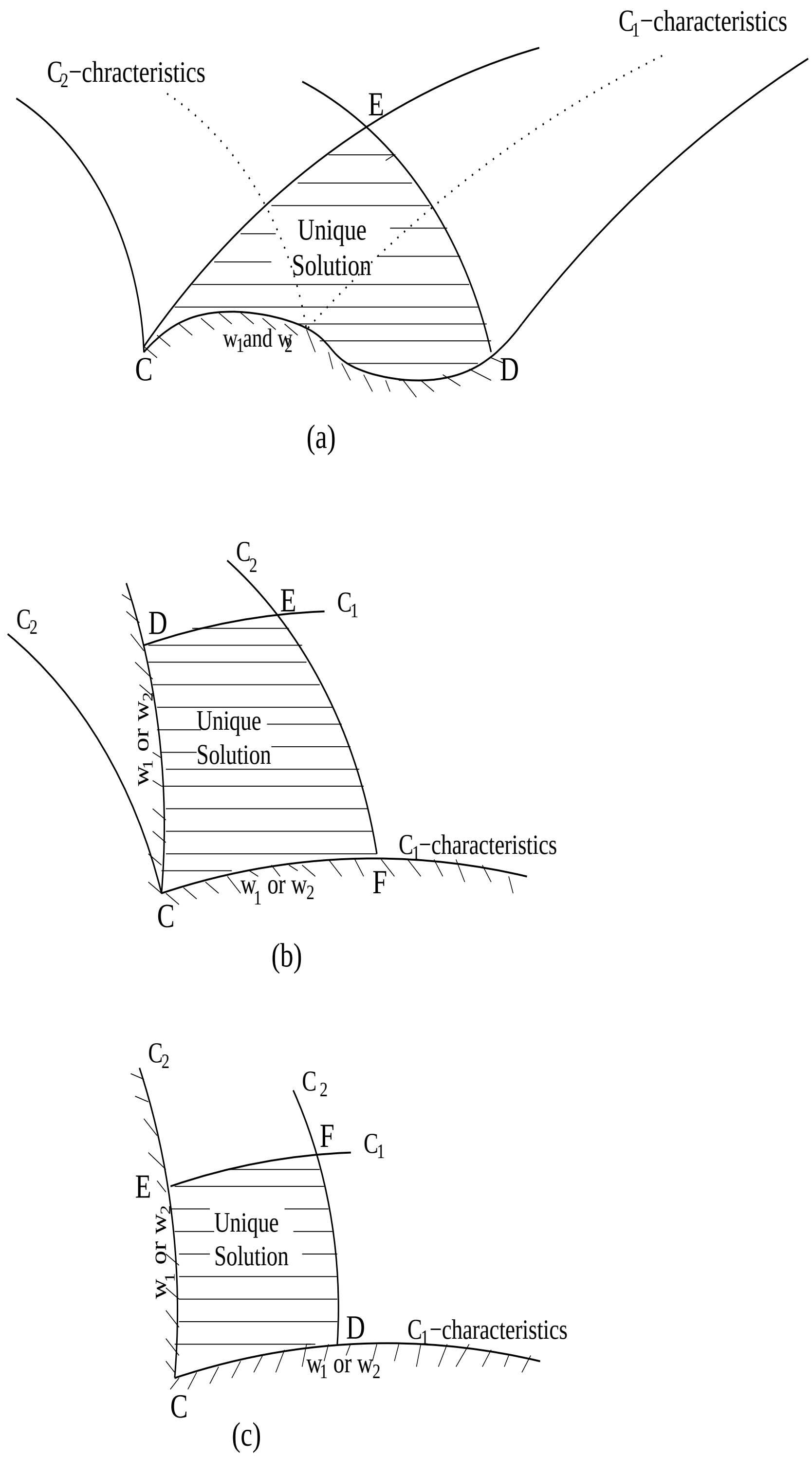


Figure 3.4: Uniqueness domains for hyperbolic systems [2]

values, is uniquely determined in the region CDE bounded by the initial curve CD, the C_1 characteristics CE, and the C_2 characteristics DE. The direction of propagation is assumed to be upward, but if it were reversed there would be a corresponding "triangle" of uniqueness below CD.

Theorem 3.1.5 *[2] Let us suppose that CD is a noncharacteristic curve that is continuously differentiable. An unique solution is determined in the region $CDEF$ of Fig. 3.4 (b), where DE and EF are characteristics, provided that w_1 and w_2 are known at C and continuously differentiable values of w_1 or w_2 are given along each of segments CD and CF. The values at C must be compatible with the characteristics. An unique solution can sometimes be assured even when a discontinuity appears at C.*

Theorem 3.1.6 *[2] In the case sketched in Fig. 3.4 (c), with CD and CE characteristics, an unique solution is determined in the region $CDFE$, where EF and FD are characteristics, when w_1 and w_2 are known at C and continuously differentiable values of w_1 or w_2 are given along CD and CE. The values at C must be compatible with the characteristics.*

From these theorems the extent to which initial and boundary conditions determine the unique solution of the Saint-Venant equation can be deduced. That is stated in the following corollary.

Corollary 3.1.7 *Suppose that*

- *at the initial moment of time, the values of both state variables of (3.12) are given,*
- *on the left boundary, the values of both state variables of (3.12) for the considered time interval are given,*
- *in the right boundary, the values of both state variables of (3.12) for the considered time interval are given,*

Then the solution to the Saint-Venant equation (3.12) is unique.

Remark 3.1.8 *The results of the corollary (3.1.7) can be applied for the Saint-Venant equations expressed in terms of different pairs of state variables, i.e. (w_1, w_2), or (u, h), or (u, y), or (Q, h), or (Q, y), or (Q, A), because the relationship between those pairs of variables are unique.*

3.1.3 An Introduction to Numerical Methods for Solving the Saint-Venant Equation

Let us now to discuss numerical methods to solve the Saint-Venant equation for the Red river system, which is described in Chapter 2. We recall Equation (2.37) with the correrre-sponding initial and boundary conditions, which is written in the general form as follows,

Saint-Venant equation

$$\dot{w}(x,t,w,w_x,z;p) = f(t,x,w,w_x,z;p)$$

Boundary conditions

$$z = \phi(t,w;p),$$

Initial Conditions

$$w(t_0,x) = w_0(x),$$

where:

- t is the time variable: $t \in I := [t_0, t_{end}]$ and x is the space variable $x \in X := [x_0, x_{end}]$,
- $w(t,x,w,z;p)$ is the state variable, i.e. water discharge Q or water level y at the point x. And z is the state variable which is given as boundary condition or determined by equations (2.33)-(2.35): $z \in \mathbb{R}^{n_z}$, with n_{chan} is the number of the channel members and $n_z = 2 \cdot n_{chan}$ is the number of boundary conditions including internal boundary conditions,
- p is the parameter: $p \in \mathbb{R}^{n_p}$, with n_p the number of parameters,
- $f(t,x,w,w_x,z;p)$ is the vector of the right hand side of the Saint-Venant equation for channel members: $f : I \times X \times \mathbb{R}^{n_w} \times \mathbb{R}^{n_z} \times \mathbb{R}^{n_p} \to \mathbb{R}^{n_w}$
- $\phi(t,w;p)$ is the vector of the right hand side of the equation for boundary condition for channel members: $\phi : I \times \mathbb{R}^{n_w} \times \mathbb{R}^{n_p} \to \mathbb{R}^{n_w}$,
- w_0 is the initial condition: $w_0 : X \to \mathbb{R}^{n_w}$.

The idea of numerical methods is that to transform this continuous problem into a discrete form in space. This results in a system of algebraic equations, which can be solved by numerical methods, e.g. Newton-like methods. The solution to the newly obtained system of algebraic equations is an approximation to the solution of the original continuous problem. There are four fundamental concepts in the context of discretization methods: accuracy, consistency, stability and convergence. The following discussion about those four concepts is based on the material from [2], [3], [21], [46] and [60].

3.1.3.1 Accuracy

There are two quantities for the measure of how well the numerical solution represents the exact solution of the problem:

- Truncation (or local) error which shows how well the difference equations match the differential equations
- Global error which reflects the overall error between the numerical solution and the exact solution.

It is impossible to find the global error, because the exact solution is unknown.

An expression of the truncation error of a numerical method can be obtained by substituting the known exact solution of the problem into the discretization, leaving a remainder which is then a measure of the error. Or, alternatively, the exact solution of the discretized problem could be substituted into the differential equation and the obtained remainder is the expression of the truncation error. In our case, the exact solution the Saint-Venant equation of the Red river system is not available, therefore the second way of obtaining an expression of the truncation error for a numerical method is preferable.

For the equation (3.1), the truncation error τ is a function of the time step Δt and the space step Δx: $\tau = \tau(\Delta t, \Delta x)$. If $\tau = O(\Delta t^p, \Delta x^q)$, then the method is said to be *pth* order in time and *qth* order in space.

3.1.3.2 Consistency

A method is said to be consistent if the truncation error decreases as the step size is reduced. This is satisfied when $p, q \geq 1$.

3.1.3.3 Stability

A numerical method is said to be stable if any error in the numerical solution, which is obtained by this method, will remain bounded. For a hyperbolic PDE as the criterion for the stability of a numerical method we can use the restrictions on the size of the grid, i.e. Δx and Δt at the location x and at the time t, which is introduced by Courant, Friedrichs and Lewy (1928). This is called the CFL condition and stated for Equation (3.4) at an arbitrary location x and arbitrary time t as follows [46]

$$|a|\Delta t \leq \Delta x, \tag{3.13}$$

where $a = a(w(x,t))$ is the coefficient of Equation (3.4), which is determined at the location x and at the time t.

Physically, the condition (3.13) means that the set of the points used for the computation enclose the domain of dependence as shown in Figure 3.5 (a). In this figure, PQ is the characteristic of the considered equation.

Figure 3.5 (b) illustrates the situation in which the CFL condition is violated. Either of the characteristics PQ or PR lies outside of the computing triangle. As we have mentioned in the last section, the values of the state variables at Q and R must alter the solution of the differential equation at P by the relationship along the characteristic curves. The numerical solution at P however, remains unaltered, since the numerical data of the set of points used for calculation are unchanged. The error in the solution therefore is not bounded or we can say by other words, the numerical scheme is not stable.

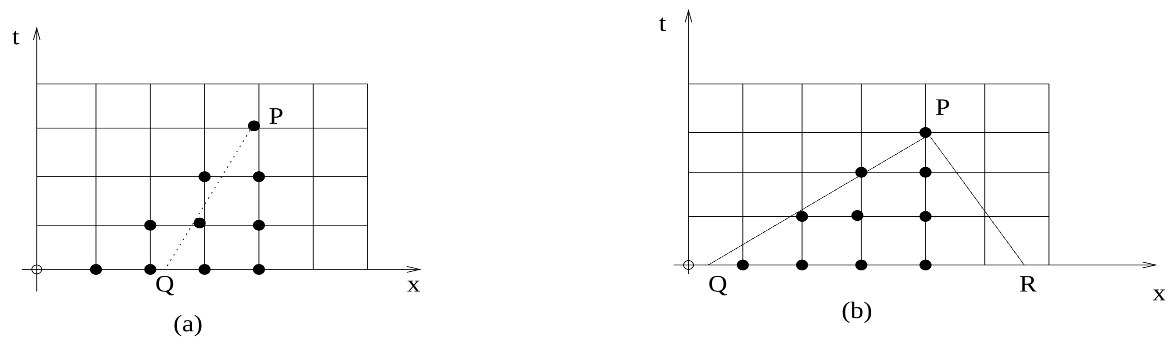


Figure 3.5: CFL Condition (a) and the violation (b) [46]

3.1.3.4 Convergence

The method is said to be convergent, if the numerical solution tends to the exact solution as the grid size is reduced to zero.

A detailed study of the stability and the convergence of the particular numerical method which is used for simulation of the Saint-Venant equation is given in Section 3.3.

3.1.4 Classification of Numerical Methods and the Available Software for Simulation of River Flows

3.1.4.1 Numerical Methods

There are many techniques available to transform a continuous problem into a discrete system. These techniques can be used either for a spatial discretization or for a time discretization. The three most popular methods for general fluid flow problems are,

- Finite Difference Methods (FDM) (see e.g. Lions *et al.* [19]), in which the derivative terms in the model equations are approximated by algebraic relations of the values at particular points or nodes. These techniques are simple to implement, but require a high degree of regularity within the mesh and so this limits their application to complex problems, i.e. problems of high dimensions or complex boundary.
- Finite Element Methods (FEM) (see e.g. Johnson [35]), the basis of which is to divide the computing domain into elements such as triangles or quadrilaterals and to place within each element nodes, where the numerical solution is determined. The solution at any position is then represented by a series expansion of the nodal values within the local vicinity of this position. The nodal distributions are multiplied by basis functions and the particular way in which the basis functions are defined determines the choice of variant of FEM.
- Finite Volume Methods (FVM) (see e.g. Leveque [44]) which are based on forming a discretization from an integral form of the model equations, and entails subdividing the domain into a number of finite volumes. Within each volume, the conservation within each cell is achieved.

The methods of the two last categories are usually used for simulation of complex systems, i.e. systems of high dimension. They require complete geometrical information of the system and their computational cost is high. This disadvantage limits their applicability for large scale problems.

For open channel flows, the one dimensional models are applied due to the fact that water in channels is flowing mainly in the direction along the river channel. Hence, for simulation of river flows, the finite difference method is used.

3.1.4.2 Available Software for Simulation of the Red River

Let us now make a review of the available software packages for simulation of river systems in Vietnam. The material for the following analysis is taken from [4], [63], and [64].

The commonly used software packages for simulation of river flows in open channels in Vietnam are:

1. Software based on conceptual models: HMC, developed by the Russian National Centre for Meteorology; SSARR (Stream Synthesis And Reservoir Regulation), developed by Rockwood, US Army (1957);
2. Software based on hydraulic models: VRSAP (Vietnam River System And Plains), developed by Prof. Nguyen Nhu Khue (1978); WENDY and RIBASIM developed at Delft Hydraulics, Holland; MITSIM, developed at the Massachusetts Institute of Technology (1977-1978); MIKE, developed at DHI Water and Environment, Denmark.

3.1.4.3 An efficient Numerical Approach for Simulation of the Red river

As mentioned above, through out this thesis we will consider only hydraulic models, i.e. of the software of the second group. These software packages are based upon finite difference methods and have been applied for simulation of some parts or of the whole river system. Practical application shows that they have the following advantages:

- They are already available!
- They produce acceptable results for simulation of river systems,
- They have user friendly interfaces (e.g. MIKE).

Besides these advantages, there are many disadvantages:

- Some of them are old, e.g. SSARR, VRSAP, MITSIM. Therefore they have problems in providing the amount of needed memory for large problems,
- Most of the newly developed software packages, e.g. MIKE, are commercial, therefore licences are required. Moreover, it is difficult to modify or integrate commercial software with others, e.g. with software for optimization, because normally source codes of commercial software are not released.
- They are based upon numerical methods which use a fixed stepsize technique. That means during the computation the space and the time steps are fixed. They are chosen before computing process and restricted by the CFL stability condition (3.13). Therefore the time step can not be chosen large and consequently, the computation cost is high.

- They do not allow to identify unknown parameters of the system from the measured data, which was collected in the past, by means of parameter estimation. That is very uncomfortable because the quality of simulation results strongly depends on the values of some unknown parameters of the system which vary in time, e.g. the friction coefficient of river channels.

In order to avoid the above listed limitations of the software, already available for simulation of river flows, we come up with an efficient software for simulation which satisfies the following conditions:

- produces good results for simulation of river flows,
- runs fast,
- is easy to use,
- can be easily integrated with other software packages, e.g. for parameter estimation or optimization,
- Estimates unknown parameters for the system by means of optimization, minimizing the difference between the the measured values of the state variable and the values of this state variable, which are computed from a model of the system, at some given gauging stations.

We introduce an efficient numerical approach for solving the Saint-Venant equation with step control techniques. The main points are:

- Using the Method of Lines (MOL) to transform the Saint-Venant equation into a large system of differential algebraic equations (DAE). This point is described in detail in Section 3.2
- Using a multistep method, namely the BDF method, to lead the DAE system which is established in the last step into the nonlinear algebraic system. The mathematical background of this point is discussed in Section 3.3
- Using a Newton-like method to solve the algebraic system which has to be solved within each step of the BDF method.

We integrate this simulation technique with powerful software packages for parameter estimation PARFIT (Bock[11, 12]) and FIXFIT (Schlöder [54]) as well as for optimization, MUSCOD (Bock and Plitt [15]). This yields an efficient tool for simulation, parameter estimation and optimal control of river flows.

3.2 Spatial Discretization

Recall the model equation for a river network (2.37). For simplicity we drop p from the equations. This gives:

Saint-Venant equation

$$\dot{w} = f(t, x, w, w_x, z), \tag{3.14}$$

Boundary conditions

$$z = \phi(t, w), \tag{3.15}$$

Initial Conditions

$$w(t_0, x) = w_0(x), \tag{3.16}$$

where:

- t is the time variable: $t \in I := [t_0, t_{end}]$ and x is the space variable $x \in X := [x_0, x_{end}]$,
- $w(t, x, w, z)$ is the state variable, i.e. water discharge Q or water level y at the point x and z is the state variable which is given as boundary condition or determined by equations (2.33)-(2.35): if n_{chan} is the number of the channel members of the Red River system, then $z \in \mathbb{R}^{n_z}$, where $n_z = 2 \times n_{\text{chan}}$ is the number of boundary conditions including internal boundary conditions,
- $f(t, x, w, w_x, z)$ is the vector of the right hand side of the Saint-Venant equation for channel members: since the Saint-Venant equation system of a single river channel consists of two equations, then the number of all equations of the Saint-Venant equation system for the Red River system, which consists of n_{chan} channels is $n_w = 2 \times n_{\text{chan}}$, and $f : I \times X \times \mathbb{R}^{n_w} \times \mathbb{R}^{n_w} \times \mathbb{R}^{n_z} \to \mathbb{R}^{n_w}$,
- $\phi(t, w)$ is the vector of the right hand side of the equation for boundary condition for channel members: $\phi : I \times \mathbb{R}^{n_w} \to \mathbb{R}^{n_z}$,
- w_0 is the initial condition: $w_0 : X \to \mathbb{R}^{n_w}$.

Substituting (3.15) into 3.14 yields an ODE in w:

Saint-Venant equation

$$\dot{w} = f(t, x, w, w_x, \phi(t, w)), \tag{3.17}$$

with the initial condition 3.16.

In this section we outline the method of lines (MOL) to discretize the model equations in space. This leads the Saint-Venant system into a large system of ODEs.

3.2.1 Method of Lines

Discretize the space interval into N subintervals:

$$x_0 < x_1 < ... < x_{N-1} < x_N = x_{end},$$

then the step size Δx is determined by

$$\Delta x = \frac{x_N - x_0}{N}$$

The main idea of the MOL is to approximate the differentials by differences in the solution at discretized points. There are many ways to approximate the first derivative of w w.r.t. x, and the three most popular difference formula are:

- Forward difference

$$(w_x)_i = \frac{w_{i+1} - w_i}{\Delta x} + O(\Delta x) \tag{3.18}$$

- Central difference

$$(w_x)_i = \frac{w_{i+1} - w_{i-1}}{2\Delta x} + O(\Delta x^2) \tag{3.19}$$

- Backward difference

$$(w_x)_i = \frac{w_i - w_{i-1}}{\Delta x} + O(\Delta x) \tag{3.20}$$

In practical applications many other difference formula can be derived for different problems being modelled. We will discuss the choise of a suitable difference formula for the spatial discretization of the Saint-Venant equation for the Red River system in the next paragraph.

Substituting the approximations of w_x into (3.14) gives an ODE-system of dimension $n_y = 2 \times N$. Let the values of w at the discretization points be denoted by w_i, $i = 1, 2, ..., N$. Define a function of dimension n_y

$$y = (w_1, w_2, ..., w_N).$$

The Saint-Venant is now transformed into the following ODE system

$$\dot{y} = \bar{f}(t, y), \tag{3.21}$$

with the initial conditions

$$y(t_0) = y_0.$$

This system of ODEs can be solved by linear multistep methods which are introduced in Section 3.3.

3.2.1.1 Practical Realization

As it is shown in Equations (3.18)-(3.20) the three-point forward difference formula and the three-point backward difference formulas are first-order of accuracy, and the three-point central formula is a second order of accuracy. In practice, based on the physical properties of the investigated system, i.e. the type of the model equation systems, and the possible requirement of an increase in the order of accuracy we can derive different differentiation formulas using more points in the approximation formulas, e.g., five points instead of three. For hyperbolic PDE, there are different routines that can be used for approximation of first derivatives w.r.t the spatial variable x, e.g. the routine DSS002 of order two based on a central difference scheme of two points, or the routine DSS004 of order four based on a central difference scheme of four points, or the routine DSS020 considering the flow direction. The investigation made by Schiesser [52, 53] shows that the use of higher order schemes, e.g. DSS004, DSS020 have the effect to reduce the numerical oscillation, which appears when the boundary condition changes in jumps. For our considered system, water discharge and water level in a river can not jump. Hence, there is no big difference when using different scheme for spatial discretization. In Figures 3.6 and 3.7 the numerical results of the water level along a river channel, say channel 1, at 7h00, July 27, 2000, and of the water level at a arbitrary spatial node, say at the location $x = 24000$ m in the distance from Hoa Binh in the time period from 1h00, July 15, 2000 to 13h00, July 27, 2000, discretized by different schemes, e.g. DSS002, DSS004, and DSS020 are shown.

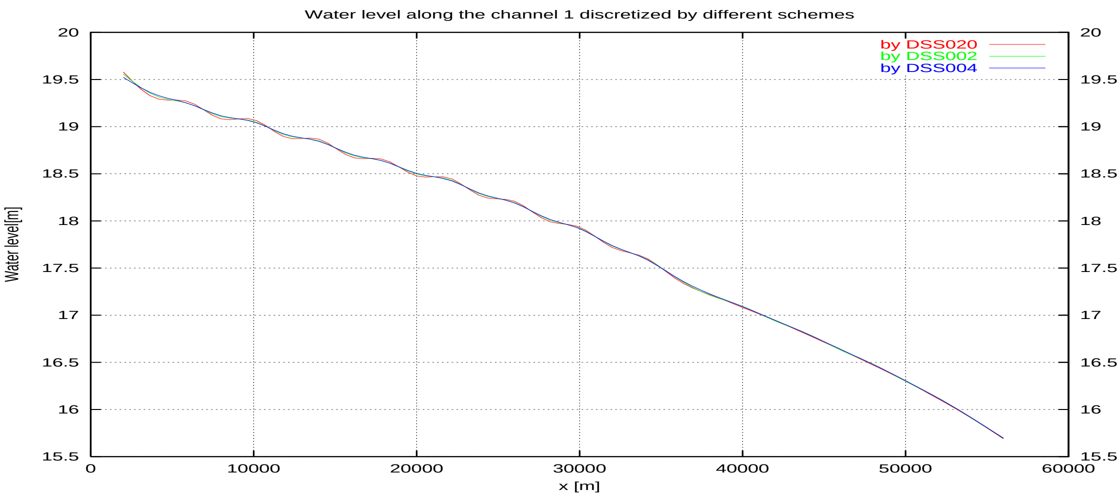


Figure 3.6: Water level along Channel 1 discretized by different schemes

It is observed that the differences between the values of the water level discretized by schemes DSS002, DSS004, and DSS020 are under 2×10^{-3} m, i.e. efficiently small. Consequently, any from these three schemes is acceptable. For the purpose of reducing the cost of computation, the routine DSS002 is applied in our approach.

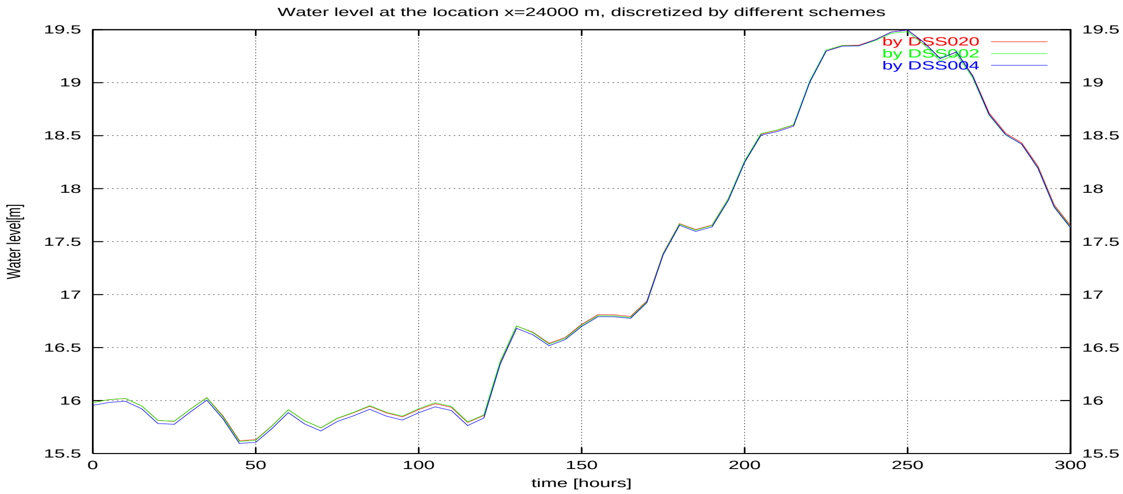


Figure 3.7: Water level at location $x = 24000$ m, discretized by different schemes

3.3 Time Discretization

In this section we give an outline of the theory of multistep methods for the ODE system (3.21)-(3.22), in particular of the BDF method which is implemented in the solver DAESOL in our research group *"Simulation and Optimization"* at the Interdisciplinary Center for Scientific computing (IWR), Heidelberg. The material for the following discussion can be found in [3, 6, 8].

3.3.1 Linear Multistep Method

The aim of a multistep method is to find the solution $y \in C^1([t_0, t_{end}], I\!R^n)$ of the initial value problem

$$\dot{y} = f(t, y), \qquad y(t_0) = y_0 \tag{3.22}$$

We first discretize the interval of integration by a mesh

$$\Delta = \{t_0 < t_1 < ... < t_{N-1} < t_N\}$$

and let $h_i = t_i - t_{i-1}$ be the ith step size. Then we construct appoximations

$$y_\Delta : \Delta \to I\!R^n : t_i \to y_\Delta(t_i)$$

where $y_i := y_\Delta(t_i)$ is an approximation of $y(t_i)$ for $i = 0, ..., N$.

Assume that we have equidistant discretization, i.e. $h_i = h$ for $i = 0, ..., N$.

3.3.1.1 Definition of the Multistep Method

The main idea of multistep methods is to use information from previous integration step to construct high-order approximations of the solution at the computed node. The general form of a $k-$step linear multistep method for an equidistant discretization problem is given by [3, 60]

$$\sum_{j=0}^{k} \alpha_j \, y_{n-j} = h \sum_{j=0}^{k} \beta_j \, f_{n-j}. \tag{3.23}$$

where α_j, β_j are the method's coefficients. Let us assume that $\alpha_0 \neq 0$, and $|\alpha_k| + |\beta_k| \neq 0$. By scaling, we can set $\alpha_0 = 1$. If $|\beta_0| = 0$, then the linear multistep method is explicit, otherwise implicit.

Alternatively, with the purpose to discuss stability the linear multistep method can be expressed in terms of the characteristic polynomials

$$\rho(\xi) := \sum_{j=0}^{k} \alpha_j \, \xi^j, \tag{3.24}$$

$$\sigma(\xi) := \sum_{j=0}^{k} \beta_j \, \xi^j. \tag{3.25}$$

In the following discussion we will look in more detail at the properties of the linear multistep method (3.23) with respect to Consistency, Stability and Convergence.

3.3.1.2 Consistency

Define the linear operator $L(t, y, h)$ by

$$L(t, y, h) := \sum_{j=0}^{k} [\alpha_j y(t - jh) - h\beta_j \dot{y}(t - jh)],$$

where $y(t) \in C^\infty([t_0, t_{end}], I\!R^n)$. By definition the truncation error of the linear multistep (3.23), τ_n can be written as

$$\tau_n = h^{-1} L(t, y, h),$$

where $y(t)$ is the exact solution of (3.22).

Definition 3.3.1 *The linear multistep method (3.23) is said to be consistent of the order p if*

$$L(t, y, h) = O(h^{p+1})$$

for all t and h, such that $[t, t + kh] \in [t_0, t_{end}]$

A linear multistep method is consistent if it has order $p \geq 1$. The necessary and the sufficient conditions for the consistency of the multistep method (3.23) are stated in the following theorem, the proof of which can be found in [3]

Theorem 3.3.2 *A linear multistep method (3.23) is consistent iff*

$$\sum_{j=0}^{k} \alpha_j = 0, \qquad \sum_{j=0}^{k} j\alpha_j + \sum_{j=0}^{k} \beta_j = 0$$

A multistep method expressed in terms of the characteristic polynomials (3.24) and (3.25) is consistent iff $\rho(1) = 0$, $\dot{\rho}(1) = \sigma(1)$

3.3.1.3 Stability

The multistep method is essentially a difference equation which approximates the differential equation. In general, we can rewrite the equation (3.23) as follows

$$\sum_{j=0}^{k} \alpha_j y_{n-j} = q_n, \qquad n = k, k+1, ... \tag{3.26}$$

The homogeneous difference equation of (3.26) is defined as

$$\sum_{j=0}^{k} \alpha_j y_{n-j} = 0, \qquad n = k, k+1, ... \tag{3.27}$$

Definition 3.3.3 *The multistep (3.23) is said to be stable if its homogeneous difference equation (3.27) is stable*

Stability is defined as below:

Theorem 3.3.4 *Define the equation*

$$\phi(\xi) = \sum_{j=0}^{k} \alpha_j \xi^{k-j} = 0. \tag{3.28}$$

The difference equation (3.26) is stable if all k roots ξ_i of $\phi(\xi)$ satisfy $|\xi_i| \leq 1$, for $i = 1, 2, ..., k$, and $|\xi_i| = 1$, then ξ_i is a simple root.

3.3.1.4 Convergence

Before discussing the convergence of the multistep method, first let us take a look at the stability of the method in the limit $h \to 0$, i.e. 0-stability.

Definition 3.3.5 *Given a mesh*

$$\Delta = \{t_0 < t_1 < ... < t_{N-1} < t_N\},$$

and let $h_i = t_i - t_{i-1}$ be the ith step size. Then the function y_h defined as

$$y_h : \Delta \to \mathbb{R}^n : t_i \to y_h(t_i)$$

is called a mesh function.

Definition 3.3.6 *The linear method (3.23) is said to have* 0*-stability if there are positive constants h_0 and K such that for any mesh functions x_h and z_h with $h \leq h_0$,*

$$|x_l - z_l| \leq K \left\{ \sum_{i=0}^{k-1} |x_i - z_i| + \max_{k \leq n \leq N} \left| h^{-1} \sum_{j=0}^{k} \alpha_j (x_{n-j} - z_{n-j}) \right.\right.$$
$$\left.\left. - \sum_{j=0}^{k} (\beta_j f(t_{n-j}, x_{n-j}) - f(t_{n-j}, z_{n-j})) \right| \right\}, \qquad 1 \leq l \leq N$$

If we plug in y_n instead of x_n and $y(t_n)$ instead of z_n into the stability condition of the definition (3.3.6), then we obtain that if the k initial values are accurate to order p and the method has order p, then the global error is $O(h^p)$.

Definition 3.3.7 *The multistep method (3.23) is said to be convergent if*

$$\lim_{h \to 0} y_n = y(t_n), \qquad n = 1, 2, ..., N$$

Theorem 3.3.8 *The linear multistep method is* 0*-stable iff all roots ξ_i of the characteristic polynomials $\rho(\xi)$ satisfy*

$$|\xi_i| \leq 1,$$

and if $|\xi_i| = 1$, then ξ_i is a simple root, $1 \leq i \leq k$.

If the root condition is satisfied, the method is accurate to order p, and the initial values are accurate to order p, then the method is convergent to order p

3.3.1.5 Absolute and Relative Stability

Applying the linear multistep method (3.23) to the test problem $\dot{y} = \lambda y$ gives

$$\sum_{j=0}^{k} \alpha_j \, y_{n-j} = h\lambda \sum_{j=0}^{k} \beta_j \, y_{n-j}.$$

If we let $y_n = \xi^n$ then ξ must satisfy

$$\sum_{j=0}^{k} \alpha_j \, \xi^{k-j} = h\lambda \sum_{j=0}^{k} \beta_j \, \xi^{k-j}. \tag{3.29}$$

or if it is in terms of characteristic polynomials, then

$$\rho(\xi) = h\lambda\sigma(\xi) \tag{3.30}$$

Definition 3.3.9 *The linear multistep method is said to be absolutely stable if the value* $|y_n|$ *does not grow with* n*. This is equivalent to the condition that all roots of (3.29) satisfy* $|\xi| \leq 1$.

The region, where $z = h\lambda$ satisfy the condition (3.29) or (3.30) is called a the region of absolute stability. The boundary of this region for the linear multistep method (3.23) can be found by plotting

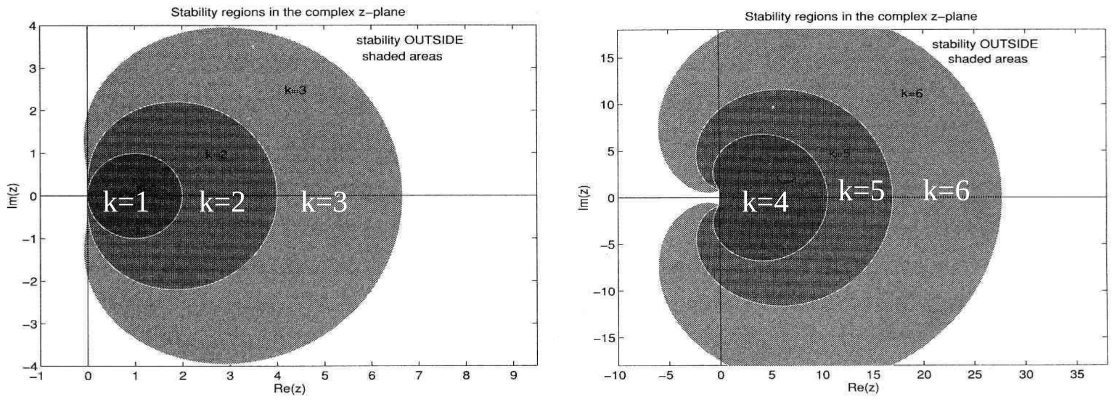
$$z = \frac{\rho(e^{i\theta})}{\sigma(e^{i\theta})}$$

Definition 3.3.10 *The linear multistep (3.23) is called A-stable if its region of absolute stability contains the left half-plane* $hRe(\lambda) < 0$.

Theorem 3.3.11 *An explicit linear multistep method cannot be A-stable.*

Theorem 3.3.12 *The order of an A-stable linear multistep method cannot exceed* 2.

The region of absolute stability for the BDF method introduced in the next section is illustrated in Figure 3.8. It shows that the region where the condition for absolute stability is violated increases with the number of steps k. The methods become unstable for $k > 6$.



(a) BDF $k = 1, 2, 3$ (b) BDF $k = 4, 5, 6$

Figure 3.8: *BDF* absolute stability regions. The stability regions are outside the shaded area for each method [3].

3.3.2 Practical Implementation of the BDF-method

3.3.2.1 The BDF method

BDF-methods (**B**ackward **D**ifferentiation **F**ormulae) are multistep-methods, based on polynomial interpolation of the last, already computed values.

An interpolation polynomial can be defined from the already computed values of the last $k+1$ values y_n, y_{n-1}, ...,y_{n-k} at the next value y_{n+1} by

$$P(t; y_{n+1}, y_n, ..., y_{n-k}) = \sum_{i=n-k}^{n+1} L_i(t) \cdot y_i \tag{3.31}$$

and in consequence,

$$\dot{P}(t; y_{n+1}, y_n, ..., y_{n-k}) = \sum_{i=n-k}^{n+1} \dot{L}_i(t) \cdot y_i, \tag{3.32}$$

where L_i is a Lagrange Basis polynomial:

$$L_i(t) = \prod_{\substack{j=n-k \\ j \neq i}}^{n+1} \frac{t - t_j}{t_i - t_j}, \quad i = n-k, \ldots, n+1.$$

$\dot{P}(t_{n+1}; y_{n+1}, y_n, ..., y_{n-k})$ is an approximation of $\dot{y}(t_{n+1})$:

$$\dot{y}(t_{n+1}) \approx \dot{p}(t_{n+1}; y_{n+1}, y_n, \ldots, y_{n-k}) =: \frac{1}{h} \left(\alpha_0 \cdot y_{n+1} + \sum_{i=1}^{k+1} \alpha_i \cdot y_{n+1-i} \right) \tag{3.33}$$

The coefficients of the linear multistep method are determined from (3.31) and (3.32):

$$\alpha_i = h \cdot \dot{L}_{n+1-i}(t_{n+1}), \quad i = 0, \ldots, k+1.$$

For simplicity, let us abbreviate

$$\beta := \sum_{i=1}^{k+1} \alpha_i \cdot y_{n+1-i}.$$

Then, equation (3.33) becomes

$$\dot{y}(t_{n+1}) \approx \dot{P}(t_{n+1}; y_{n+1}, y_n, \ldots, y_{n-k}) =: \frac{1}{h}\left(\alpha_0 \cdot y_{n+1} + \beta\right) \tag{3.34}$$

3.3.2.2 Practical Implementation of the BDF-method in the solver DAESOL

The code DAESOL was implemented especially for the solution of initial value problems for DAEs of index 1 of the following type

$$\begin{aligned} A(t,y,z,p)\,\dot{y} &= f(t,y,z,p) \\ 0 &= g(t,y,z,p), \\ & y(t_0) = y_0,\ z(t_0) = z_0, \end{aligned}$$

where:

- t is the time variable: $t \in [t_0, t_l]$,
- $y \in I\!R^d$, and $z \in I\!R^{m-d}$ denoting the state variables,
- $p \in I\!R^{n_p}$ the parameters,
- $A : I\!R \times I\!R^m \times I\!R^{n_p} \to I\!R^{(d,d)}$, $f : I\!R \times I\!R^m \times I\!R^{n_p} \to I\!R^d$ and $g : I\!R \times I\!R^m \times I\!R^{n_p} \to I\!R^{m-d}$ being functions with $m \geq d > 0, n_p \geq 0$.

We assume that the following conditions are satisfied:

- The functions A, f and g have to be differentiable efficiently often respect to the time t, and for sensitivity analysis once with respect to the state variables and parameters,
- A and g_z are regular,
- The initial values $y(t_0)$ and $z(t_0)$ must be consistent, i.e. $g(t_0, y(t_0), z(t_0), p) = 0$.

The code DAESOL is based on Backward Differentiation Formulae (BDF) method. The principal idea is to approximate the derivative $\dot{y}$ by a polynomial $\dot{P}(t_{n+1}; y_{n+1}, y_n, ..., y_{n-k})$ interpolating the actual unknown value y_{n+1} in step $n+1$ and the last already computed values of y:

$$\begin{aligned} A(t_{n+1}, y_{n+1}, z_{n+1}, p)\, \dot{P}(t_{n+1}; y_{n+1}, y_n, ..., y_{n-k}) &= f(t_{n+1}, y_{n+1}, z_{n+1}, p) \\ 0 &= g(t_{n+1}, y_{n+1}, z_{n+1}, p), \end{aligned}$$

Applying (3.34) into (3.35) gives

$$\begin{aligned} A(t_{n+1}, y_{n+1}, z_{n+1}, p) \cdot \frac{1}{h} \sum_{i=0}^{k} \alpha_i y_{n+1-i} &= f(t_{n+1}, y_{n+1}, z_{n+1}, p) \\ g(t_{n+1}, y_{n+1}, z_{n+1}, p) &= 0\,. \end{aligned}$$

or in more compact form:

$$\begin{aligned} A_{n+1} \left(\alpha_0 \cdot y_{n+1} + \sum_{i=1}^{k+1} \alpha_i \cdot y_{n+1-i} \right) - h \cdot f_{n+1} &= 0 \\ g_{n+1} &= 0, \end{aligned}$$

with

$$A_{n+1} = A(t_{n+1}, y_{n+1}, z_{n+1}, p), \qquad f_{n+1} = f(t_{n+1}, y_{n+1}, z_{n+1}, p), \qquad g_{n+1} = g(t_{n+1}, y_{n+1}, z_{n+1}, p).$$

This defines a nonlinear system of equations in the unknowns $x_{n+1} = (y_{n+1}, z_{n+1})$ which is solved by a Newton-like method:

1. Given estimates $x_{n+1}^{(0)} = (y_{n+1}^{(0)}, z_{n+1}^{(0)})$ for the unknowns (y_{n+1}, z_{n+1}) - here given by a polynomial, extrapolating the last already computed values x_n (Predictor), $x_{n-1}, ..., x_{n-k}$.

2. A Newton-iteration is defined by

$$x_{n+1}^{(m+1)} := x_{n+1}^{(m)} + \Delta x_{n+1}^{(m)},$$

with the increment (Corrector)

$$\Delta x_{n+1}^{(m)} = J^{-1} \cdot \begin{pmatrix} A_{n+1}^{(m)} \cdot (\alpha_0 y_{n+1}^{(m)} + \sum_{i=1}^{k} \alpha_i y_{n+1-i}) + h\, f_{n+1}^{(m)} \\ g_{n+1}^{(m)} \end{pmatrix}$$

and

$$J = \begin{pmatrix} \alpha_0 A + A_y\, (\alpha_0 y_{n+1}^{(m)} + \sum_{i=1}^{k} \alpha_i y_{n+1-i}) + h\, f_y & A_z\, (\alpha_0 y_{n+1}^{(m)} + \sum_{i=1}^{k} \alpha_i y_{n+1-i}) + h\, f_z \\ g_y & g_z \end{pmatrix}$$

DAESOL code uses a special monitoring strategy for minimizing the number of evaluations and decompositions of the Jacobians $\frac{\partial f}{\partial(y,z)}$, $\frac{\partial g}{\partial(y,z)}$, and $\frac{\partial A}{\partial(y,z)}$ in keeping them frozen as long as possible.

3.3.2.3 Step and Order Control

In a BDF method of order k, the truncation error can be estimated as follows

$$E_k(n) := \rho\,(t_{n+1}-t_n)^2(t_{n+1}-t_{n-1})\cdots(t_{n+1}-t_{n+1-k})\,\|y[t_{n+1},\ldots,t_{n-k}]\|$$

where $\rho < 1$ is independent of the step size.

For the next step $n+1$, the step size is computed as follows

$$h^{eq}_{k'} = \sqrt[k'+1]{\frac{\widehat{TOL}}{\rho\,k'!\,\|y[t_{n+1},\ldots,t_{n-k'}]\|}},\quad k' = k-1, k, k+1,\quad k' \leq 6,$$

where $\widehat{TOL} \leq TOL$, e.g. $\widehat{TOL} = \frac{1}{2}TOL$.

If the calculated step size is significantly bigger or smaller than the one from the last step, then we increase or decrease the order by one. Otherwise the order is retained.

With the newly computed step size, we compute the new truncation error for the new step $E_k(n+1)$. If

$$E_k(n+1) \leq TOL,$$

then the step size is accepted, otherwise it should be reduced.

Remark 3.3.13 *Step and order control allow DAESOL to control the truncation error in each step, i.e. the error in each time step is bounded. That is one significant advantage of this method in comparison with the fixed step methods which are commonly used for simulation of hydraulic systems in practice. The BDF method implemented in the solver DAESOL with step and order control function is an effective tool for simulation of the Saint-Venant equation.*

Chapter 4

Numerical Methods for Parameter Estimation

In this chapter, we discuss methods of parameter estimation for river systems. The problem is formulated in Section 4.1. This is a least-squares problem constrained by PDEs and can be solved by the Gauss-Newton methods, which have been introduced by Bock (1981 [10], 1983 [11], and 1987 [12]) and Schlöder (1987 [54]). The theoretical basis of these methods is presented in Sections 4.2 and 4.3. In Section 4.5 a statistical analysis for the solution of the parameter estimation problem is made. This shows how the statistical reliability, i.e. variance-covariance matrix or confidence intervals of the solution of the parameter estimation problem solved by Generalized Gauss-Newton method can be evaluated. And finally, Section 4.5 is devoted to a common summary of numerical approaches for solution of the simulation and parameter estimation problems for the Red River system.

4.1 Problem Formulation

4.1.1 Optimization Problem

In practice, the situation is that the measurement data z_{ki} for one or more state variables $k \in M^w$ (M_w is a set of the state variables, whose measurements are used for the parameter estimation), namely the water level or the water discharge at the gauging stations, is given at the time t_i ($i = 1, .., n_m$). Here n_m is the number of the measurement points.

If we denote by $u^{(k)}(t_i, w, p)$ the model response for the measurement z_{ki} with $i = 1, \ldots, n_m$, then the measurements can be described as follows

$$z_{ki} = u^{(k)}(t_i, w, p) + \epsilon_{ki}, \tag{4.1}$$

where, $w \in I\!R^{2\times N}$ denotes the state variables of the river system, which is divided into N discretization nodes, p are the parameters (B_0, S_0, S_f, q,...), and ϵ_{ki} is an error that is assumed to follow a normal distribution $\epsilon_{ki} \sim N(0, \sigma_{ki}^2)$, here σ_{ki} denotes the standard deviation of the measurement z_{ki}.

The parameter estimation problem is to determine the unknown parameter vector p that fit the model to the experimental data

$$\min_{p,w} \|F(p)\|_2^2 := \min_{p,w} \sum_{k\in M_w} \sum_{i=1}^{n_m} \frac{(z_{ki} - u^{(k)}(t_i, w, p))^2}{\sigma_{ki}^2}, \tag{4.2}$$

such that

$$\dot{w}(t,p) = f(t,w,p) \qquad w(t_0) = w_0. \tag{4.3}$$

Here, (4.3) is the Saint-Venant equation written in form of ODEs, with $f : [t_0, t_e] \times I\!R^{n_w} \times I\!R^{n_p} \to I\!R^{n_w}$ and $n_w = 2 \times N$, where N is the number of spatial discretization nodes.

4.1.2 Problem Discretization

The problem (4.2)-(4.3) is a high-dimensional constrained parameter estimation problem, as we transformed the PDE to a large ODE system which consists of up to thousands equations. This is an infinite dimensional problem, because we have to optimize in the function space (for $k \in M_w$). Now we describe how it is transformed into a finite dimensional optimization problem and the resulting discretized system is presented.

The simplest method of discretization is the single shooting method [61]. It treats the boundary problem as an initial value problem at the full integration interval, where the initial values of the integration are iteratively improved until the boundary conditions of the problem are satisfied. The disadvantages of the single shooting method is that for such problems, where the solution of the initial values problem is strongly sensitive *w.r.t.* variations of the initial values, it is very difficult to find a solution to the original initial-boundary value problem.

In order to reduce the impact of a high sensitive system, Bock (1981 [10], 1983 [11]) proposed the multiple shooting approach for the state discretization of parameter estimation problems. The idea behind this method is to split the long integration interval $[t_0, t_e]$ into m subintervals τ_j, τ_{j+1} ($j = 0, 1, \ldots, m-1$)

$$t_0 = \tau_0 < \tau_1 < \ldots < \tau_m = t_e \tag{4.4}$$

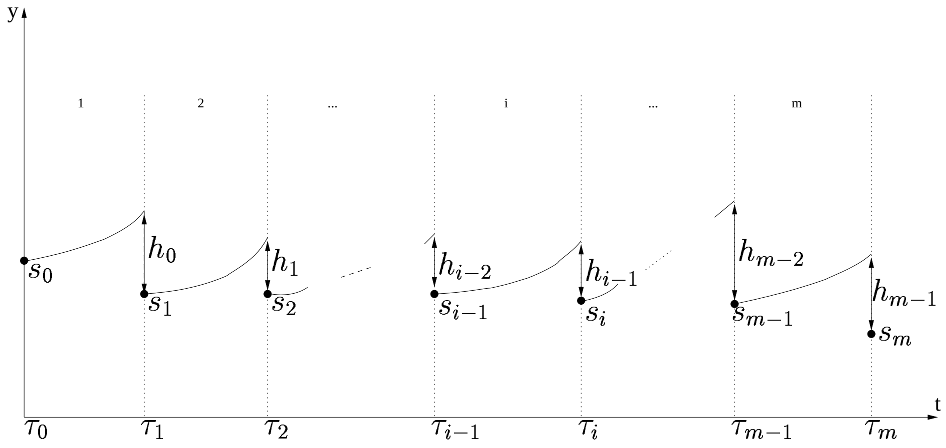


Figure 4.1: Multiple Shooting Discretization

With this approach the original initial-boundary value problem is transformed into a set of initial value problems. A new variable s_k at each multiple shooting node k is introduced as the initial value for the initial value problem formulated at this node,

$$\dot{y}(t) = f(t, y, p) \qquad y(\tau_k) = s_k, \qquad k = 0, ..., m-1 \tag{4.5}$$

To ensure continuity between the integration intervals, the following corresponding continuity conditions have to be satisfied

$$h_k(s_k, s_{k+1}, p) := y(\tau_{k+1}, s_k, p) - s_{k+1} = 0, \qquad k = 0, ..., m-1 \tag{4.6}$$

The scheme of the multiple shooting discretization is shown in Figure 4.1. This approach is especially suited for the parameter estimation problem for river systems for the reason that the multiple shooting method requires the continuity of the state functions and their derivatives only inside of multiple shooting subintervals. It is important because for real-life problems of parameter estimation for river flows, the input data for boundary conditions are usually measured discontinuously (normally these data are given in a table format). We can smooth them by e.g. spline interpolation to obtain piecewise continuously differentiable input for boundary conditions.

Finally, the following discretized nonlinear least-squares problem is obtained

$$\min_x \|r_1(x)\|_2^2 \tag{4.7}$$

$$r_c(x) = 0, \tag{4.8}$$

where $x = (s_0, \ldots, s_m, p)^T \in I\!R^n$, with $n = (m+1) \times n_y + n_p$, is the augmented vector, $r_1 \in C^3(I\!R^{n_y+n_p}, I\!R^{n_1})$ is the n_1 least-squares conditions, $r_c \in C^3(I\!R^{n_y+n_p}, I\!R^{n_2+m\times n_y+n_3})$ denotes the all equality constraints including n_2 initial conditions, n_3 possible equality conditions r_3 and m matching conditions (4.6).

For solution of this problem, the Reduced Gauss-Newton method introduced by Schlöder (1987 [54]) can be applied. In Section 4.2 an introduction to the Generalized Gauss-Newton method proposed by Bock (1981 [10], 1983 [11], 1987 [12], 2001 [13]) is made. It will be shown that for large scale problems like (4.7)-(4.8) the standard implementation of the Generalized Gauss-Newton method is not suitable. We are naturally led to the more specific strategy of the Reduced Gauss-Newton method, which is presented in Section 4.3. Finally, Section 4.5 gives a conclusion of this Chapter.

One important point we should note is that the reduced Gauss-Newton method introduced by Schlöder (1987 [54]) is a specific case of the Generalized Gauss-Newton method introduced by Bock (1981 [10], 1983 [11], 1987 [12], 2001 [13]).

4.2 Generalized Gauss-Newton Method

In this section we discuss the algorithm and the theoretical basis of the Generalized Gauss-Newton method introduced by Bock (1981 [10], 1983 [11], 1987 [12], 2001 [13]) and implemented in the software package for parameter estimation PARFIT at our research group *"Simulation and Optimization"*.

4.2.1 Basic Steps of the Generalized Gauss-Newton Method

For solution of nonlinear constrained least-squares problems of the type (4.7)-(4.8), Bock (1981 [10], 1983 [11], 1987 [12], 2001 [13]) proposed a Generalized Gauss-Newton method, the main steps of which are:

1. Starting from an initial guess x_0

2. Improving a given estimate x_k iteratively by

$$x_{k+1} = x_k + t_k \Delta x_k \tag{4.9}$$

   The increment Δx_k solves the following constrained linear problem

$$\min_{\Delta x} \|r_1(x_k) + J_1(x_k)\Delta x\|_2^2 \tag{4.10}$$

$$r_c(x_k) + J_c(x_k)\Delta x = 0, \tag{4.11}$$

   where $J_1(x) := \dfrac{\partial r_1}{\partial x}$, $J_c(x) := \dfrac{\partial r_c}{\partial x}$ and $t_k \in (0, 1]$ is a relaxation factor, also called the stepsize.

$$J := \begin{pmatrix} J_1 \\ J_c \end{pmatrix} = \begin{pmatrix} D_1^0 & D_1^1 & \dots & \dots & D_1^m & D_1^p \\ D_c^0 & 0 & \dots & \dots & 0 & D_c^p \\ G_0 & -I & & & & G_0^p \\ & G_1 & -I & & 0 & \vdots \\ & & \ddots & \ddots & & \vdots \\ & 0 & & G_{m-1} & -I & G_{m-1}^p \end{pmatrix} \qquad r := \begin{pmatrix} r_1 \\ r_c \\ h_0 \\ \vdots \\ h_{m-1} \end{pmatrix}, \quad (4.12)$$

with the abbreviations

$$\begin{array}{lll} D_i^j := \partial r_i(s_0, \dots, s_m, p)/\partial s_j, & D_i^p := \partial r_i(s_0, \dots, s_m, p)/\partial p, & i = 1, \dots, 3 \\ D_c^j := \begin{pmatrix} D_2^j \\ D_3^j \end{pmatrix}, & D_c^p := \begin{pmatrix} D_2^p \\ D_3^p \end{pmatrix} & \\ G_i := \partial y(\tau_{i+1}; s_i, p)/\partial s_i, & G_i^p := \partial y(\tau_{i+1}; s_i, p)/\partial p, & i = 0, \dots, m. \end{array}$$

and the dimensions

$$\begin{array}{lll} D_i^j \in I\!R^{n_i \times n_y}, & D_i^p \in I\!R^{n_i \times n_p} & i = 1, \dots, 3 \\ D_c^j \in I\!R^{(n_2+n_3) \times n_y}, & D_c^p \in I\!R^{(n_2+n_3) \times n_p}, & \\ G_i, I \in I\!R^{n_y \times n_y}, & G_i^p \in I\!R^{n_y \times n_p}, & i = 0, \dots, m-1. \end{array}$$

Remark 4.2.1 *The initial conditions r_2 depends only on s_0, therefore $D_2^j = 0^{(n_2 \times n_y)}$ for $j = 1, \dots, m$. Consequently, the matrix D_c^j has the following special structure*

$$D_c^j = \begin{pmatrix} 0 \\ D_3^j \end{pmatrix}$$

for $j = 1 \dots, m$.

4.2.2 Theoretical Background of the Generalized Gauss-Newton Method

Before continuing the discussion of the Generalized Gauss-Newton method we study some theoretical background of the method, i.e. the constraint qualification, the positive definiteness, the stationarity condition, the theorem of the existence of a generalized inverse, and the local convergence theorem. This theory is stated by Bock [10, 11].

4.2.2.1 Optimality Conditions

In this section we recall the nonlinear problem (4.7)-(4.8)

$$\min_x \|r_1(x)\|_2^2$$
$$r_c(x) = 0,$$

and the corresponding the linear problem (4.10)-(4.11)

$$\min_{\Delta x} \|r_1(x_k) + J_1(x_k)\Delta x\|_2^2$$
$$r_c(x_k) + J_c(x_k)\Delta x = 0$$

Definition 4.2.2 *(Lagrangian Function) The Lagrangian for the constrained nonlinear optimization problem (4.7), (4.8) is defined as*

$$L(x, \lambda) = \frac{1}{2}\|r_1(x)\|_2^2 - \lambda^T r_c(x), \tag{4.13}$$

where λ is the Lagrange multiplier

It is possible, however, that some column of the matrix J_c vanishes due to the algebraic representation of r_c, so that this does not play a role in the Lagrangian gradient. To ensure that such degenerate behavior does not occur we usually make an assumption called a constraint qualification [CQ]. One such CQ is defined as follows:

Definition 4.2.3 *(Constraint Qualification [CQ])*

Given the point $x \in D \subset I\!R^n$ and the constraint Jacobian J_c defined as

$$J_c := \begin{pmatrix} J_2 \\ J_3 \end{pmatrix},$$

we say that the [CQ] is satisfied if

$$Rg(J_c(x)) = n_c. \tag{4.14}$$

Definition 4.2.4 *(Regular Point)*

A feasible point $x \in D \subset I\!R^n$ which satisfies the condition (4.14) is said to be a regular point.

Definition 4.2.5 *(Positive Definiteness [PD])*

Given a point $x \in D \subset I\!R^n$ and the Jacobian J defined by (4.12).

We say that [PD] is satisfied if

$$Rg(J(x)) = n. \tag{4.15}$$

Lemma 4.2.6 *Let [PD] is satisfied. Then $J_1(x)^T J_1(x)$ is positive definite in the Kernel of $J_c(x)$.*

We state now the theorems for necessary conditions for solution of problem (4.7)-(4.8). The first order condition was derived by Karush (1939 [36]), Kuhn and Tucker (1951 [39]). The results for the second order necessary conditions have been developed by Fiacco and McCormick during 1960s [30].

Theorem 4.2.7 *(Necessary Optimality Conditions)*

Let $x^* \in D \subset I\!R^n$ be regular and a solution of problem (4.7)-(4.8). Then x^* is feasible, i.e.

$$r_c(x^*) = 0, \tag{4.16}$$

and the first order necessary condition holds: There exists a multiplier vector λ^* that satisfies the following conditions (Karush-Kuhn-Tucker conditions):

$$\frac{\partial}{\partial x} L(x^*, \lambda^*) = r_1(x^*)^T J_1(x^*) - \lambda^{*T} J_c(x^*) = 0. \tag{4.17}$$

Additionally, the second order necessary condition is satisfied: For all directions

$$\forall w \neq 0 \qquad J_c(x^*)w = 0$$

the Hessian matrix H of the Lagragian function L, which defined by

$$H(x, \lambda) := \frac{\partial^2}{\partial x^2} L(x, \lambda), \tag{4.18}$$

is positive semi-definite

$$w^T H(x^*, \lambda^*) w \geq 0. \tag{4.19}$$

Definition 4.2.8 *A vector (x^*, λ^*) which satisfies the feasibility condition (4.16) and the stationarity condition (4.17) is called a Karush-Kuhn-Tucker point (KKT point).*

Lemma 4.2.9 *Let [CQ] and [PD] be satisfied. Then the following equivalence holds*

(x^*, λ^*) is a KKT point of (4.7)-(4.8) $\iff$ $(0, \lambda^*)$ is a KKT point of (4.10)-(4.11).

In the Generalized Gauss-Newton method, the generalized inverse J^+ of the Jacobian J is required. The following theorem has been stated by Bock [10, 11, 12].

Theorem 4.2.10 *Let $J = (J_1^T, J_c^T)$ be the Jacobian matrix of the linear least-squares problem and satisfy the [CQ] and [PD] conditions. Then the following holds:*

1. *For any $r = (r_1^T, r_c^T) \in I\!R^{n_1+n_c}$ exists one KKT point $(\Delta x, \lambda)$ for (4.10)-(4.11), and Δx is a strict minimum.*

2. *There exists a linear mapping* $J^+ : \mathbb{R}^{n_1+n_c} \to \mathbb{R}^n$, *such that*

$$\Delta x = -J^+ R \tag{4.20}$$

is the solution of (4.10)-(4.11) for any $R \in \mathbb{R}^{n_1+n_c}$. *The solution operator* J^+ *is called generalized inverse and determined by*

$$J^+ = \begin{pmatrix} I & 0 \end{pmatrix} \begin{pmatrix} J_1^T J_1 & J_c^T \\ J_c & 0 \end{pmatrix}^{-1} \begin{pmatrix} J_1^T & 0 \\ 0 & I \end{pmatrix}.$$

3. *The generalized inverse* J^+ *satisfies the defining condition*

$$J^+ J J^+ = J^+. \tag{4.21}$$

4.2.2.2 Local Convergence

Theorem 4.2.11 *(Local Convergence Theorem)*

Let $J(x)^+$ *be the generalized inverse of the Jacobian* $J(x) = (J_1(x)^T, J_c(x)^T)^T$ *of the function* $r = (r_1^T, r_c^T) \in C^1(D, \mathbb{R}^{n_1+n_c})$ *in a nonlinear constrained least-squares problem. Assume further that the following Lipschitz conditions are satisfied:*

$$\|J(y)^+(J(x+t(y-x)) - J(x))(y-x)\| \le \omega t \|y-x\|^2, \qquad \omega < \infty, \tag{4.22}$$

$$\|(J(z)^+ - J(x)^+)\mathrm{Res}(x)\| \le \kappa(x)\|z-x\| \le \kappa\|z-x\|, \tag{4.23}$$

$$\mathrm{Res}(x) := R(x) - J(x)J(x)^+R(x) \qquad \text{(Residuum)} \qquad \kappa < 1$$

$$\forall t \in [0,1], \forall x,y,z \in D, x-y = J(x)^+R(x)$$

Then for all $x_0 \in D$ *with*

$$\delta_0 := \frac{\alpha_0 \omega}{2} + \kappa < 1, \qquad (\alpha_j := \|J(x_j)^+ R(x_j)\|), \tag{4.24}$$

$$D_0 := K\left(x_0, \frac{\alpha_0}{1-\delta_0}\right) \subset D, \tag{4.25}$$

the following holds:

1. *The iteration*

$$x_{j+1} = x_j + \Delta x_j, \qquad \Delta x_j = -J(x_j)^+ R(x_j) \tag{4.26}$$

is well-defined and remains in D_0.

2. *There exists* $x^* \in D$ *with* $J(x^*)^+R(x^*) = 0$ *and* $x_j \to x^* (j \to \infty)$.

3. *The following a priori error estimation holds*

$$\|x_j - x^*\| \leq \delta_0^j \frac{\alpha_0}{1-\delta_0}.$$

4. *The convergence is linear with*

$$\|\Delta x_{j+1}\| \leq \left(\frac{\alpha_j \omega}{2} + \kappa \right) \|\Delta x_j\| =: \delta_j \|\Delta x_j\|.$$

The following interpretations of the local convergence theorem can be made:

- The constant ω in (4.22) is a bound on the nonlinearity of the problem, and its inverse ω^{-1} charactizes the size of the region in which the linearized problem (4.10)-(4.11) is an acceptable approximation of the original problem (4.7)-(4.8). But normally, in practical applications of parameter estimation the initial guess x_0 is not sufficiently close to the solution, i.e. this point is out of the region, where the linear approximations is valid. In order to solve this problem, globalization strategies are applied. The idea of this is that in each iteration we relax the iteration (4.26) to

$$x_{k+1} = x_k + t_k \Delta x_k \qquad t_k \in]0, 1], \tag{4.27}$$

  where t_k is the relaxation factor (or stepsize), which is chosen such that the next step x_{k+1} is "better" than x_k. The stepsize can be determined by e.g. a line search method. More detailed material of globalization strategies can be found in Bock *et al.* (1987 [12], 2001 [13]).

- The coefficient κ in (4.23) characterizes the compatibility of the data with the model. If $\kappa < 1$, then a fixed point x^* is a local minimum, otherwise there may exist pertubations of the measurement data in the same order of magnitude as the measurements, such that the fixed point is stationary but not a minimum (see Bock [12] and Dieses [27]).

4.2.3 Solution of the Linear Problems

An important step in the algorithm of the Generalized Gauss-Newton method is to solve the linear system (4.10)-(4.11) for Δx. If the Jacobian of the system is as defined by (4.12), then the augmented vector Δx can be computed in principle by (4.20). From (4.12) we can note that the total Jacobian matrix of the problem (4.10)-(4.11) is large, but sparse. The matrix is of the size $(n_1 + n_2 + n_3 + m \times n_y) \cdot ((m+1) \times n_y + n_p)$, due to the augmented and the matching conditions, but has a special structure due to the explicit form of the linearized matching conditions. Base on this very useful property, Bock (1981 [10], 1987 [12]) proposed not to solve the original large system (4.10)-(4.11) directly, but eliminate extra variables $s_1, \ldots, s_m$ by e.g. Gauss elimination. The problem (4.10)-(4.11) is then transformed to the condensed problem, which depends only on Δp and Δs_0

$$\min_{\Delta s_0, \Delta p} \|E_1 \Delta s_0 + P_1 \Delta p + u_1\|_2^2 \tag{4.28}$$

$$E_c \Delta s_0 + P_c \Delta p + u_c = 0, \tag{4.29}$$

Here, the coefficient's matrices of system (4.28)-(4.29), i.e. E_1, P_1, and u_1 and E_c, P_c, and u_c can be computed as follows (see [12], [54]):

$$E_1 = D_1^0 + \sum_{i=1}^{m} D_1^i \prod_{j=1}^{i} G_{i-j} \tag{4.30}$$

$$E_c = D_c^0 + \sum_{i=1}^{m} D_c^i \prod_{j=1}^{i} G_{i-j} \tag{4.31}$$

$$P_1 = D_1^p + \sum_{i=1}^{m} D_1^i \left(\sum_{j=0}^{i-1} \left(\prod_{k=1}^{i-j-1} G_{i-k} \right) G_j^p \right) \tag{4.32}$$

$$P_c = D_c^p + \sum_{i=1}^{m} D_c^i \left(\sum_{j=0}^{i-1} \left(\prod_{k=1}^{i-j-1} G_{i-k} \right) G_j^p \right) \tag{4.33}$$

$$u_1 = r_1 + \sum_{i=1}^{m} D_1^i \left(\sum_{j=0}^{i-1} \left(\prod_{k=1}^{i-j-1} G_{i-k} \right) h_j \right), \tag{4.34}$$

$$u_c = r_c + \sum_{i=1}^{m} D_c^i \left(\sum_{j=0}^{i-1} \left(\prod_{k=1}^{i-j-1} G_{i-k} \right) h_j \right), \tag{4.35}$$

where the operator $\prod$ is defined as

$$\prod_{i=l}^{n} M_i := \begin{cases} M_l \cdot M_{l+1} \ldots M_n & \text{if} \quad l \leq n, \\ I, & \text{otherwise.} \end{cases}$$

Having solved system (4.28)-(4.29) for Δp and Δs_0, the increments of the variables $s_1, \ldots, s_m$ can be computed in the forward recursion

$$\Delta s_{j+1} = G_j \Delta s_j + G_j^p \Delta p + h_j, \qquad j = 0, \ldots, m-1. \tag{4.36}$$

In the following, the main steps of the algorithm implemented in PARFIT for solution of the condensed problem (4.28)-(4.29) are outlined (Bock 1981 [10], 1987 [12]). The scheme of this algorithm is shown in (4.37).

$$\begin{pmatrix} \bar{J}_c \\ \bar{J}_1 \end{pmatrix} \xrightarrow{(1)} \begin{pmatrix} R_{11} & R_{12} \\ 0 & B \end{pmatrix} \xrightarrow{(2)} \begin{pmatrix} R_{11} & R_{12} \\ 0 & R_{22} \\ 0 & 0 \end{pmatrix} \tag{4.37}$$

In step (1), the matrix $\bar{J}_c$ associated with the equality constraints is reduced to upper triangular form by a suitable method, e.g. orthogonal transformations or Gaussian elimination, and the first n_y variables are eliminated from the least-squares part.

In step (2), the remaining matrix B of the least-squares part is then triangularized by orthogonal transformations.

The above described procedure results in a equivalent triangular system, which can be easily solved for Δs_0 and Δp.

Remark 4.2.12 *We compute the augmented vector Δx the following steps:*

- *Deriving the condensed system (4.28)-(4.29) by (4.31)-(4.35),*
- *Solving (4.28)-(4.29) for Δs_0 and Δp by the scheme (4.37),*
- *Computing the other variables $\Delta s_1, \ldots, \Delta s_m$ by the forward recursion (4.36).*

Remark 4.2.13 *The condensed system (4.28)-(4.29) only has a size of $(n_1 + n_2 + n_3) \times (n_y + n_p)$ as in the case of single shooting. But to obtain the condensed problem (4.28)-(4.29), we need to compute and store all derivative matrices D_i^j, D_i^p, G_i^p and G_i, i.e. to store full Jacobian J. A single Jacobian storage is determined as follows (see Dieses (2000 [27]):*

Storage $= (n_1 + n_3) \times (n_y(m+1) + n_p) + n_y \times (n_y + n_p) \times m + n_2 \times (n_y + n_p)$ *memory cells.*

And as we have above mentioned, this procedure has to be repeated for each iteration. For the system derived from PDEs, the equation number is n_y normally is very large, e.g. for a river channel with the length of 500 *[Km], if the number of spatial discretization nodes is* 500 *(one node per Km), then the equation number $n_y = 1000$. Therefore, the needed memory to store the Jacobian is big.*

From the above two remarks we can see that to treat large scale problems, the standard implementation of the Generalized Gauss-Newton method is not efficient due to the high cost of computation. Hence, a specific strategy to reduce the computational effort is necessary. This reduced approach is presented in the next section.

4.3 Reduced Gauss-Newton Method

In this section we present the Reduced Gauss-Newton method which was developed and implemented in the code FIXFIT by Schlöder (1987 [54]). This is a version of the Generalized Gauss-Newton method specialized for parameter estimation problems in PDEs. The main idea of this method is to exploit equality conditions, e.g. initial conditions to reduce the computational effort for solution of the problem.

4.3.1 The Reduced Approach (Schlöder Trick)

As mentioned before, r_c consists of the initial conditions $r_2 \in I\!R^{n_2}$ and the equality constraints $r_3 \in I\!R^{n_3+m\times n_y}$. If we write $r_c = (r_2^T, r_3^T)^T$, and define $r_l^i(s_i, p)$ as the component part of r_l at the multiple shooting node i and its derivative matrix ${}^i\!D_l^p := dr_l^i(s_i,p)/dp$, where $i = 0, \ldots, m$, and $l = 1, 3$. Then, the following holds for $l = 1, 3$:

$$r_l = \sum_{i=0}^{m} r_l^i(s_i, p) \tag{4.38}$$

$$D_l^p = \frac{dr_l}{dp} = \sum \frac{dr_l^i(s_i,p)}{dp} =: \sum_{i=0}^{m} {}^i\!D_l^p \tag{4.39}$$

Due to the modification of the way to present the equality constraint r_c, the linear problem (4.7)-(4.8) and the corresponding linear problem (4.10)-(4.11) are formally led to the following forms

$$\min_x \|r_1(x)\|_2^2 \tag{4.40}$$

$$r_2(x) = 0, \tag{4.41}$$

$$r_3(x) = 0, \tag{4.42}$$

and

$$\min_{\Delta x} \|r_1(x_k) + J_1(x_k)\Delta x\|_2^2 \tag{4.43}$$

$$r_2(x_k) + J_2(x_k)\Delta x = 0, \tag{4.44}$$

$$r_3(x_k) + J_3(x_k)\Delta x = 0 \tag{4.45}$$

Here, as it has been mentioned in the last paragraph, $x = (s_0, \ldots, s_m, p)$.

The Jacobian J and the right hand side r of the system (4.43)-(4.45) are determined as follows,

$$J = \begin{pmatrix} J_1 \\ J_2 \\ J_3 \end{pmatrix} = \begin{pmatrix} D_1^0 & D_2^1 & \cdots & \cdots & D_1^m & D_1^p \\ D_2^0 & 0 & \cdots & \cdots & 0 & D_2^p \\ D_3^0 & D_3^1 & \cdots & \cdots & D_3^m & D_3^p \\ G_0 & -I & & & & G_0^p \\ & G_1 & -I & & 0 & \vdots \\ & & \ddots & \ddots & & \vdots \\ & 0 & & G_{m-1} & -I & G_{m-1}^p \end{pmatrix}; \quad r = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ h_0 \\ \vdots \\ h_{m-1} \end{pmatrix}, \tag{4.46}$$

As it has been discussed in Section 4.2.3, the Jacobian matrix J is large but sparse. Hence, we can transform it into the following condensed system by applying Gauss elimination to eliminate the variables $s_1, \ldots, s_m$:

$$\min_{\Delta s_0, \Delta p} \|E_1\Delta s_0 + P_1\Delta p + u_1\|_2^2 \tag{4.47}$$

$$E_2 \Delta s_0 + P_2 \Delta p + u_2 = 0, \quad (4.48)$$

$$E_3 \Delta s_0 + P_3 \Delta p + u_3 = 0, \quad (4.49)$$

where the coefficient's matrices are determined as (see [54, 27])

$$
\begin{aligned}
E_l &= D_l^0 + \sum_{i=1}^{m} D_l^i \prod_{j=1}^{i} G_{i-j}, \qquad l = 1,3 & (4.50)\\
E_2 &= D_2^0, & (4.51)\\
P_l &= {}^0D_l^p + \sum_{i=1}^{m} D_l^i \left(\sum_{j=0}^{i-1} \left(\prod_{k=1}^{i-j-1} G_{i-k} \right) G_j^p \right), \qquad l = 1,3, & (4.52)\\
P_2 &= D_2^p = {}^0D_2^p, & (4.53)\\
u_l &= r_l^0 + \sum_{i=1}^{m} \left\{ D_l^i \left[\sum_{j=0}^{i-1} \left(\prod_{k=1}^{i-j-1} G_{i-k} \right) h_j \right] \right\}, \qquad l = 1,3, & (4.54)\\
u_2 &= r_2 = r_2^0. & (4.55)
\end{aligned}
$$

Here, the operator $\prod$ is defined as

$$\prod_{i=l}^{n} M_i := \begin{cases} M_l \cdot M_{l+1} \ldots M_n & \text{if} \quad l \leq n, \\ I, & \text{otherwise.} \end{cases}$$

Assume that D_2^0 has full rank. In the our problem of parameter estimation for the Red River system, the initial condition s_0 is explicitly given, therefore $D_2^0 = I \in I\!R^{n_y \times n_y}$, i.e. the assumption is satisfied and consequently, there exists the inverse of D_2^0, namely I. Solving (4.48), (4.51) and (4.53) for s_0 gives

$$\Delta s_0 = -(D_2^0)^{-1}[{}^0D_2^p \Delta p + r_2^0] \quad (4.56)$$

Substituting (4.56) in problem (4.47)-(4.49) gives

$$\min_{||\Delta p} \tilde{P}_1 \Delta p + \tilde{u}_1\|_2^2 \quad (4.57)$$

$$\tilde{P}_3 \Delta p + \tilde{u}_3 = 0, \quad (4.58)$$

where ([54], [27])

$$
\begin{aligned}
\tilde{P}_l &= P_l + E_l[-(D_2^0)^{-1} \cdot {}^0D_2^p] \qquad l = 1,3\\
&= D_l^0[-(D_2^0)^{-1} \cdot {}^0D_2^p] + {}^0D_l^p + \\
&\quad \sum_{i=1}^{m} \{ {}^iD_l^p + D_l^i [\prod_{j=1}^{i} G_{i-j} [-(D_2^0)^{-1} \cdot {}^0D_2^p] + \sum_{j=0}^{i-1} \prod_{k=1}^{i-j-1} G_{i-k} G_j^p]\} & (4.59)\\
\tilde{u}_l &= u_l + E_l[-(D_2^0)^{-1} r_2^0] \qquad l = 1,3\\
&= D_l^0[-(D_2^0)^{-1} r_2^0] + r_l^0 + \\
&\quad \sum_{i=1}^{m} \{ r_l^i + D_l^i [\prod_{j=1}^{i} G_{i-j})(-(D_2^0)^{-1} r_2^0) + \sum_{j=0}^{i-1} \prod_{k=1}^{i-j-1} G_{i-k} h_j]\}. & (4.60)
\end{aligned}
$$

The problem (4.57)-(4.58) has only few degrees of freedom, i.e. n_p. In order to derive this problem, the matrices $\tilde{P}_l$ and $\tilde{u}_l$ need to be computed. It has been shown in the last section that in the standard procedure of the Generalized Gauss-Newton method, $\tilde{P}_l$ and $\tilde{u}_l$ are computed explicitly by (4.59)-(4.60), and this is hard on the computation of all derivative matrices, i.e. D_l^i, D_l^p, G_i, and *etc.*, which is very expensive, namely, the size of the matricies D_1^i and D_3^i is $(n_1 + n_3) \times (n_y \times (m+1) + n_p)$, the size of the matricies G_j^p and G_j is $m \times n_y \times (n_y + n_p)$, and the size of the matrix D_2 is $n_2 \times (n_y + n_p)$. In the next subsection, the efficient approach for computing the matrices $\tilde{P}_l$ and $\tilde{u}_l$ is outlined.

4.3.2 Generation of Derivatives

In order to reduce the computational effort which is very high for a large scale parameter estimation problems in PDEs, e.g. for river flows, Schlöder proposed to avoid the explicit computation and storage of D_l^i, G_i etc. by a successive evaluation of directional derivatives.

We define the following recursions

$$
\begin{aligned}
{}^{-1}G_p &:= -(D_2^0)^{-1} \cdot {}^0D_2^p &(4.61)\\
{}^{-1}G_R &:= -(D_2^0)^{-1} \cdot r_2^0 &(4.62)
\end{aligned}
$$

1. For $k = 0, \ldots, m-1$

$$
\begin{aligned}
{}^kG_p &:= G_k \cdot {}^{k-1}G_p + G_k^p &(4.63)\\
{}^kG_R &:= G_k \cdot {}^{k-1}G_R + h_k, &(4.64)
\end{aligned}
$$

2. For $i = 1, \ldots, m$ and $l = 1, 3$

$$
\begin{aligned}
\bar{P}_l^0 &:= D_l^0 \cdot {}^{-1}G_p + {}^0D_l^p \qquad \bar{P}_l^i := \bar{P}_l^{i-1} + D_l^i \cdot {}^{i-1}G_p + {}^iD_l^p, &(4.65)\\
\bar{u}_l^0 &:= D_l^0 \cdot {}^{-1}G_R + r_l^0 \qquad \bar{u}_l^i := \bar{u}_l^{i-1} + D_l^i \cdot {}^{i-1}G_R + r_l^i. &(4.66)
\end{aligned}
$$

Then, $\bar{P}_l$ and $\bar{u}_l$ are determined by

$$
\bar{P}_l = \bar{P}_l^m \qquad \bar{u}_l = \bar{u}_l^m. \tag{4.67}
$$

In the Schlöder approach it is proposed to evaluate $G_k \cdot {}^{k-1}G_p$ as n_p directional derivatives of y w.r.t. p instead of product of G_k with ${}^{k-1}G_p$, e.g. the jth column $({}^kG_p)_j$ is interpreted as

$$
({}^kG_p)_j = \frac{d}{d\epsilon} \; y\left(\tau_{k+1}; \bar{x}_k + \epsilon \begin{pmatrix} {}^{k-1}G_p \\ \hat{I} \end{pmatrix}_j \right) \Bigg|_{\epsilon=0} \tag{4.68}
$$

Analogously for the computation of the directional derivative $G_k \cdot {}^{k-1}G_R$.

In the software package FIXFIT (Schlöder, [54]) these directional derivatives are approximated by a difference quotient as follows

$$({}^{k}G_p)_j = \frac{y\left(\tau_{k+1}; \bar{x}_k + \epsilon \begin{pmatrix} {}^{k-1}G_p \\ \hat{I} \end{pmatrix}_j \right) - y(\tau_{k+1}; \bar{x}_k)}{\epsilon} + O(\epsilon) \tag{4.69}$$

The Schlöder approach for constrained least-squares problems in PDEs has made a very great progress for computational effort. Instead of computing $n_y + n_p$ derivatives in the standard Generalized Gauss-Newton method, in the Reduced Gauss-Newton method for the recursion (4.63)-(4.66) we need to compute only $n_p + 1$ (n_p for ${}^{k}G_p$ and 1 for ${}^{k}G_R$) directional derivatives. It is a great advantage because usually we have $n_y >> n_p$.

4.4 Statistical Analysis for the Solution

Parameters estimated by method discussed in the last sections are useful only if some estimate of their statistical reliability, i.e. variance-covariance matrix or confidence intervals is given. In the following we show how the covariance matrix and confidence intervals of the solution of parameter estimation can be evaluated in the Generalized Gauss-Newton method. The material for this discussion is taken from works of Bock (1981 [10], 1987 [12]), Schlöder (1987 [54]) and Dieses (2000 [27]).

As it has been assumed in Section 4.1, there is an error that follows a normal distribution in the measurements of data. Therefore, the right hand side of the least-squares problem r_1, and consequently the vector r and the solution Δx determined by

$$\Delta x := -J^{+} r \qquad r = \begin{pmatrix} r_1 \\ 0 \end{pmatrix}, \tag{4.70}$$

are random variables. Here, J is the Jacobian of the complete system (4.40)-(4.42).

The variance-covariance matrix for $x = (s_0, \ldots, s_{m-1}, p)$ is approximated by

$$\text{Cov}(x) = E(\Delta x \Delta x^T) = J^{+} E(rr^T) J^{+^T}, \tag{4.71}$$

On the other hand,

$$E(rr^T) = \beta^2 \begin{pmatrix} I_{n_1} & 0 \\ 0 & 0_{n_c} \end{pmatrix} =: \beta^2 \Lambda \tag{4.72}$$

Substituting (4.72) into (4.71) gives

$$\text{Cov}(x) = \beta^2 J^{+} \Lambda J^{+^T} =: \beta^2 P, \tag{4.73}$$

The works of Bock (1981 [10]), Schlöder (1987 [54]), Dieses (2000 [27]) show that the variance-covariance matrix for the parameters p, which are estimated by the Generalized Gauss-Newton method, can be easily approximated.

Let us consider the reduced condensed system (4.57)-(4.58) with the corresponding Jacobian $\tilde{J} = (\tilde{P}_1^T, \tilde{P}_3^T)^T$. In order to compute Δp this system is reduced to a triangular form using the equivalence transformations (4.37), which can be describe in more detail as follows,

$$\tilde{J} = \tilde{T} = \begin{pmatrix} T & 0 \\ L & Q \end{pmatrix} \begin{pmatrix} R_{11} & R_{12} \\ 0 & R_{22} \\ 0 & 0 \end{pmatrix} \quad \begin{matrix} \} n_3 \\ \Big\} n_1 \end{matrix} \tag{4.74}$$

The following steps are done in a triangularizing process (4.74):

- First, the part associated with equality conditions is reduced to an upper triangular form by a suitable transformation T, e.g. by Gauss elimination,
- Second, using the matrix L to eliminate the variables corresponding to the triangular matrix R_{11} from the least-squares part,
- Third, Using a suitable orthogonal transformation Q, e.g. Householder transformation, to triangularize the remaining least-squares part.

The variance-covariance matrix can then determined by

$$\mathrm{Cov}(p) = \beta^2 R^+ \bar{\Lambda} R^{+T} =: \beta^2 P, \tag{4.75}$$

where

$$R^+ = \begin{pmatrix} R_{11}^{-1} & -R_{11}^{-1} R_{12} R_{22}^{-1} & 0 \\ 0 & R_{22}^{-1} & 0 \end{pmatrix} \qquad \bar{\Lambda} = \begin{pmatrix} 0 & 0 \\ 0 & I_{n_1} \end{pmatrix} \tag{4.76}$$

The standard deviations of the parameter p are defined as

$$\sigma(p_i) = \beta P_{ii}^{\frac{1}{2}} \tag{4.77}$$

It can happen that the common factor β is unknown, then it can be independently estimated by

$$\beta^2 \approx \frac{\|r_1(s_0, \ldots, s_{m-1}, p)\|_2^2}{l_2}, \tag{4.78}$$

where $l_2 = n_1 - l_1$ and $l_1 = n_y + n_p - (n_2 + n_3)$

Approximations of the corresponding confidence intervals θ_i for the parameter i can be computed by

$$\theta_i = \beta(P_{ii} l_1 F_{l_1,l_2;1-\alpha})^{\frac{1}{2}} \qquad i = 1, \ldots, n_p, \tag{4.79}$$

where $F_{l_1,l_2,1-\alpha}$ denotes the quantile of the Fisher distribution on the $(1-\alpha)$ probability confidence level with the degrees of freedom l_1 and l_2.

4.5 Summary

This is served as a summary for Chapters 2-4. In these chapters, the following problems have been treated:

- The Saint-Venant equation system, which is specified for the Red River flows by neglecting weakly influential term, is chosen for modeling the Red River system with given initial and boundary conditions. This is a hyperbolic PDE system, and normally has no analytical solution. Therefore, a numerical approach has to be applied.
- The method of lines combined with the BDF method which is implemented in the solver DAESOL developed at the research group of Bock & Schlöder at the Interdisciplinary Center for Scientific Computing (IWR), Heidelberg, is used for solving the Saint-Venant equation system. The time step control strategy is applied to improve the stability of the numerical method and computing time.
- The parameter estimation problem for the Red River system is formulated. This is a large scale constrained least-squares problem, for solution of which the Reduced Gauss-Newton method developed and implemented in the code FIXFIT by Schlöder is described.

The numerical results presented in Chapter 5 show that the chosen numerical approach is fast, stable, and efficient for solution of simulation and parameter estimation problems for the Red River system.

Chapter 5

Numerical Results for Parameter Estimation and Simulation

In this chapter, the results for estimation of hydraulic parameters, and the modelling for fixed parameters are presented.

The first section is devoted to describe the Red River system and its specific behaviour. In Section 5.2 the numerical results of parameter estimation for the Red River system are shown. We insert those parameters into the model equation system for the Red River system and solve it by the method of lines combined with the BDF method which is introduced in Chapter 3 to obtain numerical results for simulation of the Red River system, which are given in Section 5.3. Section 5.4 presents a relaxed model, which is suitable for the optimal control of the Red River system. Finally, in Section 5.5 we summarize and discuss the results, which are presented in this chapter.

5.1 The Red River System

The network scheme of the Red River system is shown in Figure 2.4. It consists of 15 connected river channels with a total length of 477000 [m]. In this thesis we denote each channel by a number (see Figure 2.4), from 1 to 15 as in Table 5.1. Here, the letters, e.g. A, B, and C are used to denote the crosses between channels, where the names are not given or unknown. An important point, to which we should pay attention is that there exists the hydro-electric power plant Hoa Binh working in the Red River system. The water amount from the output of the hydro-electric power plant Hoa Binh is nearly 50% of the total amount of the Red River system, which is flowing through Ha Noi, and the volume of the reservoir Hoa Binh is very big, approximately 9×10^9 [m^3]. Therefore the working regime of this hydro-electric power plant plays a very important role in control of the level at Ha Noi.

Number	From	To	*Notation*	Length [m]
1	Hoa Binh	Trung Ha	1	58000
2	Phu Tho	Trung Ha	2	26000
3	Trung Ha	Son Tay	3	12000
4	Vu Quang	Son Tay	4	36000
5	Son Tay	Ha Noi	5	58000
6	Ha Noi	Thuong Cat	6	10000
7	Ha Noi	Hung Yen	7	78000
8	Hung Yen	A	8	9000
9	Hung Yen	Trieu Duong	9	8000
10	A	B	10	12000
11	A	Dinh Cu	11	60000
12	B	C	12	20000
13	B	Nam Dinh	13	8000
14	C	Phu Le	14	44000
15	C	Ba Lat	15	38000
Total				477000

Table 5.1: Notation of the Red River channels

In this chapter the Saint-Venant equation (2.24) with the parameterization of the hydraulic functions given in Section 2.3, is used as a model for the Red River system. The method of lines combined with the BDF method implemented in the solver DAESOL, introduced in Chapter 3 is used for numerical solution of the Saint-Venant equation. The following boundary conditions are needed for unique solution of the mathematical model of the considered Red River system:

- The upper boundaries of this system are the water discharge at Hoa Binh, the water discharge at Phu Tho, and the water discharge at Vu Quang
- The lower boundaries of this system are the water levels at Thuong Cat, at Trieu Duong, at Nam Dinh, at Phu Le, at Ba Lat, and the level at Dinh Cu.

The Red River system naturally can be splited into two part:

- **Part 1:** Domain of tidal non-influence
- **Part 2**: Domain of tidal influence

The first part is located from the highland to the gauging station Hung Yen, which is at about 70 km distance from the sea. In this station the influence of the tides is not noticeable. There are many gauging stations located in this area (see Figure 2.4), e.g. Hoa Binh, Phu Tho, Vu Quang, Trung Ha, Son Tay, Ha Noi, Thuong Cat, Hung Yen.

In the second part of the Red River system, tidal influences to the water level increase in the direction to the sea, i.e. down to the gauging stations Phu Le, Ba Lat, and Dinh Cu. Therfore the accuracy of the models at the gauging stations Phu Le, Ba Lat and Dinh Cu may be very low. In this thesis we focus in the river flows from Hoa Binh to Ha Noi. The model of the tidal influential part serves only for computing the lower boundary condition, i.e. the water level at the gauging station Hung Yen. The numerical results presented in the next sections show that this approach is acceptable as the hydrodynamic model of the flows in the first part of the Red River system is fitted well to the measurements.

In the following the numerical results of two problems are presented:

1. First, we present numerical results of the parameter estimation problem. The estimated values of unknown parameters are shown with their confidence intervals.
2. Second, we present numerical results for simulation of the Saint-Venant equation for the Red River system with estimated values of unknown parameters for a given period of time.

5.2 Numerical Results for Parameter Estimation

As mentioned in Section 2 the Manning friction coefficient C_n can not be arbitrarily measured but it can be modeled by the formulae (2.32), where the values of the unknown parameter p are the solution of the least-squares problem (4.2) constrained by (4.3). The values of the weighting coefficient in (4.2) are equal to the values of the corresponding measurement.

In this section we firstly show the values of the unknown parameters with their confidence intervals, and then a validation and a verification of those parameters are made.

5.2.1 Results of Parameter Estimation

In order to estimate unknown parameters of the Manning coefficients for the channels of the Red River system, the values of the water level at the gauging stations Hoa Binh, Phu Tho, Trung Ha, Vu Quang, Son Tay, Ha Noi, Hung Yen, and Tao Xuan in the flood season of the year 2000, i.e. from 1h00 am, July 15 to 1h00 am, August 15, 2000, are used as the measurement data. The water level at the gauging stations is measured every 6 hours. Initial guesses of the unknown parameters are taken from a research report of the Ha Noi

Institute for Meteorology and Hydrology (2003 [63]), and the geometrical data of the Red River system, which was measured in 1998-2000, is taken from the National Center of Hydrometeorological Forecasting.

As mentioned in Section 2.3 the number $n_p(i_{\text{chan}})$ of parameters for the channel i_{chan} in the parameter model (2.32) is determined by the algorithm which is given in paragraph 2.3.3. The main idea of this algorithm is to compute the residual for each case, e.g. for the case when $n_p = 2$ and for the case when $n_p = 3$. Based on the values of the residual we compute a test function F_{test} for linear hypotheses testing and compare it with the quantile of the Fisher distribution on some probality confidence level, say 0.95, with the corresponding degrees of freedom ([47]). This comparison is a criterion to decide if the case "$n_p = 3''$ is significantly better then the case $''n_p = 2''$. As a concrete example, in Table 5.2 the values of F_{test} and F_{n_p,n_m-n_p} of Channel 1 for the two following cases:

1. "$n_p = 2$" *vs.* "$n_p = 3$", and
2. "$n_p = 3$" *vs.* "$n_p = 4$",

are shown. In the case 1, it is shown that $F_{\text{test}} > F^{0.05}_{n_p,n_m-n_p}$, i.e. $n_p = 3$ is better than

Variables	Notation	Case 1	case 2
Number of measurements	n_m	121	121
Number of parameters	i	2	3
Residual for $n_p = i$	S_i	0.0084	0.0054
Residual for $n_p = i + 1$	S_{i+1}	0.0054	0.0048
$F_{\text{test}} = \frac{S_{i+1}-S_i}{s_i} \frac{n_m-n_p}{n_p}$		21.25	4.370
$F^{0.05}_{n_p,n_m-n_p}$		19.50	5.63

Table 5.2: Computation of F_{test} for Channel 1

$n_p = 2$. In contrast to that, for the case 2, $F_{\text{test}} < F^{0.05}_{n_p,n_m-n_p}$, i.e. $n_p = 4$ is not better than $n_p = 3$. It means that for Channel 1, the optimal number of parameters is $n_p = 3$. Here, n_m is the number of measurements and $F^{0.05}_{n_p,n_m-n_p}$ is the quantile of the Fisher distribution on the probality confidence level 0.95 with the degrees of freedom are n_p and $n_m - n_p$.

Analogously, the suitable numbers of the parameters for all the channels located in the first part of the Red River system, i.e. of the channels $1, \ldots, 7$ can be determined.

In the tidal influential domain, as a consequence of the tidal propagation the values of the water level in the channels oscillate. The values of the water level at the sea entrances Phu Le, Ba Lat and Dinh Cu can be either positive or negative, and therefore there exist possible backward flows. Then the sign of the water discharge can be changed, i.e. the derivative of the functional S_f determined by (2.31) can be discontinuous. This badly affects the stability of numerical methods for solution of the Saint-Venant equation and of the parameter estimation problem for the Red River system.

In order to avoid this problem we assume that the values of the water level at the sea entries Phu Le, Ba Lat and Dinh Cu are zero, and the values of the Manning coefficient of all channels located in the domain of tidal influence with the exception of the channel 9 are equal and independent of the values of the water discharge, i.e. the number of unknown parameters is 1. The second assumption is made due to the fact that there is only one gauging station, namely Tao Xuan located in this area, and therefore a detailed study of the processes in this domain is not available. The parameters for the channel 9 can be estimated using the measurements of the gauging station Hung Yen. However, in this thesis we focus on the first domain of the Red River system. The investigation of the second domain is used for computing the lower boundary for the Saint-Venant equation of the tidal non-influential domain, i.e. for computing the water level in Hung Yen. In the following the numerical results of the simulation show that the model response of the water level at the gauging stations Hoa Binh, Phu Tho, Trung Ha, Vu Quang, Son Tay, Ha Noi, Hung Yen and Tao Xuan is fitted well to the measurement data, i.e. the assumption made above is suitable.

In Table 5.3 the numerical results for the parameter estimation of the domain 1 are shown, namely the estimated values of the parameters for the channels $1, \dots, 7$ of the Red River system for the period of time from 1h00 am, July 15, 2000 to 1h00 am, August 15, 2000 with their confidence intervals. In this parameter estimation problem, we consider only the channels located in the domain 1 of the Red River system and our task is to estimate 17 unknown parameters of these channels (see Table 5.3). The following information is used as the input data for this parameter estimation problem:

- The values of the water discharge at the gauging stations Hoa Binh, Phu Tho, and Vu Quang in the investigated time period are used as the upper boundary conditions for the system,
- The values of the water level at the gauging stations Thuong Cat and Hung Yen in the investigated time period are used as the lower boundary conditions for the system,
- The values of the water discharge and the water level along all 7 considered channels at 1h00 am, July 15, 2000 are used as the initial conditions. In Section 5.3 a technique for computing initial conditions is discussed in more detail,
- The values of the water level at the gauging stations Hoa Binh, Phu Tho, Trung Ha, Vu Quang, Son Tay, and Ha Noi in the investigated time period are used as the measurement data for the parameter estimation problem,
- The initial guesses for the unknown parameters are given in Table 5.3.

This parameter estimation problem is solved in a computer P-IV, 2500 MHz, 2 G RAM. The total computing time is 51m0.31s.

Channel	Notation	Initial guess	Estimated
1	$p(1,0).10^2$	2.500	0.159 ± 0.064
	$p(1,1).10^2$	0.000	0.293 ± 0.035
	$p(1,2).10^1$	0.000	-0.402 ± 0.044
2	$p(2,0).10^2$	2.500	3.483 ± 0.093
	$p(2,1).10^2$	0.000	-0.113 ± 0.009
3	$p(3,0).10^2$	2.000	2.319 ± 0.133
	$p(3,1).10^2$	0.000	0.151 ± 0.093
	$p(3,2).10^1$	0.000	-0.218 ± 0.156
4	$p(4,0).10^2$	2.000	2.865 ± 0.054
	$p(4,1).10^2$	0.000	0.019 ± 0.011
	$p(4,2).10^1$	0.000	-0.020 ± 0.005
5	$p(5,0).10^2$	2.000	1.423 ± 0.082
	$p(5,1).10^2$	0.000	0.151 ± 0.078
	$p(5,2).10^1$	0.000	-0.472 ± 0.018
6	$p(6,0).10^2$	2.000	2.221 ± 0.152
7	$p(7,0).10^2$	2.000	1.976 ± 0.057
	$p(7,1).10^2$	0.000	0.142 ± 0.016

Table 5.3: Initial guess and estimated parameters for the domain 1 with data from the year 2000.

In Table 5.4 the numerical results for the parameter estimation of the domain 2 are shown, namely the estimated values of the parameters for the channels $8, \ldots, 15$ of the Red River system for the period of time from 1h00 am, July 15, 2000 to 1h00 am, August 15, 2000 with their confidence intervals. In this parameter estimation problem, we consider the model of the all 15 channels of the Red River system and our task is to estimate 2 unknown parameters of these channels (see Table 5.4). The following information is used as the input data for this parameter estimation problem:

- The values of the water discharge at the gauging stations Hoa Binh, Phu Tho, and Vu Quang in the investigated time period are used as the upper boundary conditions for the system,
- The values of the water level at the gauging stations Thuong Cat, Trieu Duong, Phu Le, Ba Lat, and Dinh Cu in the investigated time period are used as the lower boundary conditions for the system,
- The values of the water discharge and the water level along all 15 considered channels at 1h00 am, July 15, 2000 are used as the initial conditions. In Section 5.3 a technique for computing initial conditions is discussed in more detail,

- The values of the water level at the gauging stations Hung Yen and Tao Xuan in the investigated time period are used as the measurement data for the parameter estimation problem,
- The initial guesses for the unknown parameters are given in Table 5.4.

This parameter estimation problem is solved in a computer Intel P-IV, 2500 MHz, 2 G RAM. The total computing time is 51m30.44s.

Channel	Notation	Initial guess	Estimated
$i = 8, 10, \ldots, 15$	$p(i,0).10^2$	2.000	2.089 ± 0.043
9	$p(9,0).10^2$	2.000	1.743 ± 0.160

Table 5.4: Initial guess and estimated parameters for the domain 2 with data from the year 2000.

The Manning coefficients for every river channel can be computed by inserting the estimated parameter values into equation (2.32). Here the maximal water discharge is 20000 [m^3s^{-1}] for all channels. The results are illustrated in Figure 5.1.

5.2.2 Validation of the Estimated Parameters

Applying newly estimated values of Manning coefficients into the Saint-Venant equations which is coupled with corresponding initial and boundary conditions we can compute the values of the water level at the gauging stations Hoa Binh, Trung Ha, Vu Quang, Ha Noi, Hung Yen, etc. at any time. The computing results and the measurements from 1h00 am, Jyly 15 to 1h00 am August 15, 2000 are illustrated in Figure 5.2.

These show good coincidence between data and model response, especially for the domain tidal non-influence. In the gauging station Ha Noi, the model response is fitted is well to the measured data.

In order to qualify the model of the Red River system with the estimated parameters we recall the objective function (let be denoted by OBJ) of the least-squares problem (4.2) which can be written for the case of the water level at a gauging station as follows,

$$\text{OBJ} = \sum_{i=1}^{n_m} (1 - \frac{y_i}{z_i})^2,$$

where n_m is the number of measurements, z_i and y_i (with $i = 1, \ldots, n_m$) are the measurement data and the model response of the water level at this gauging station, respectively. The near OBJ to zero the better is model.

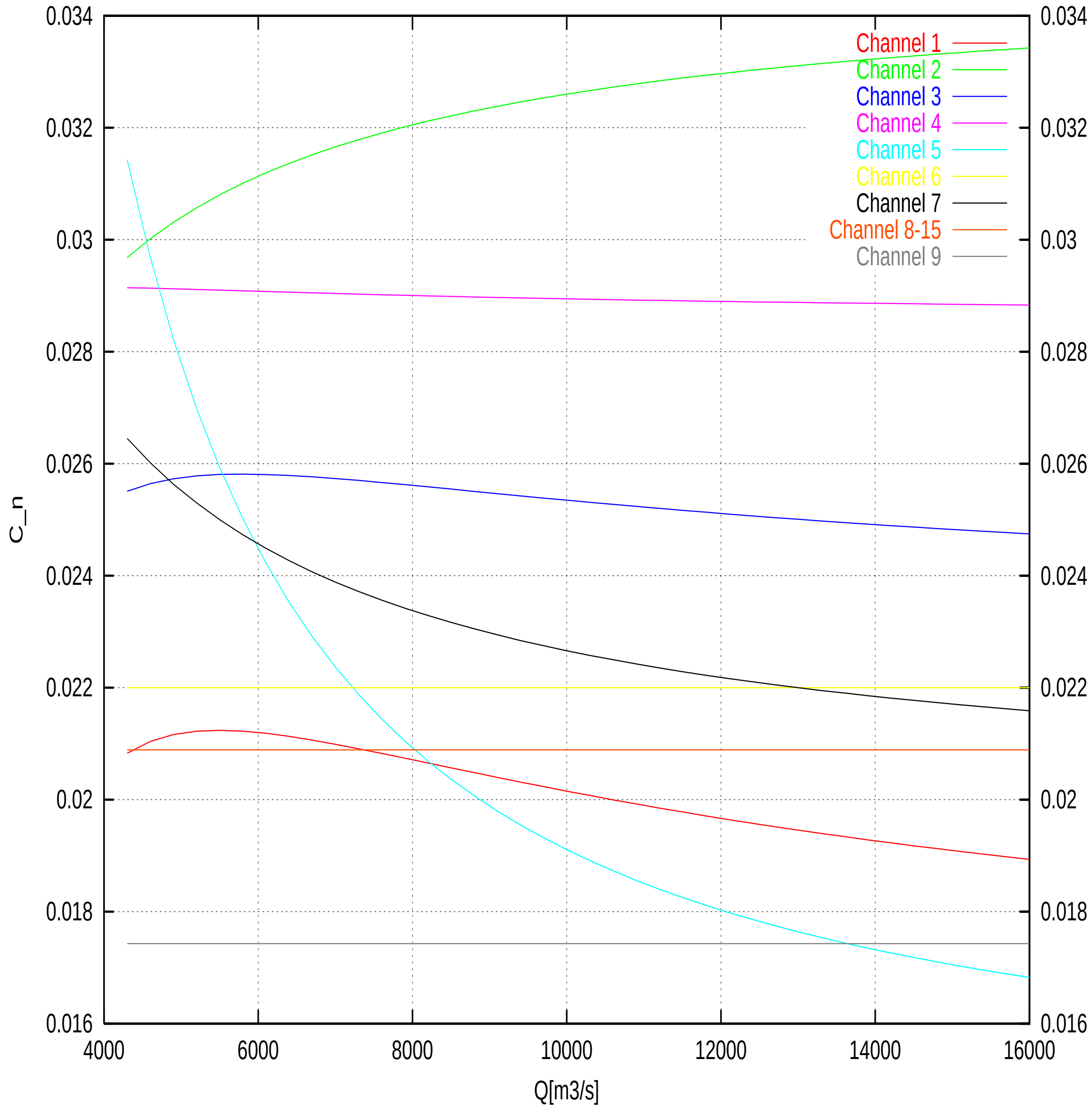
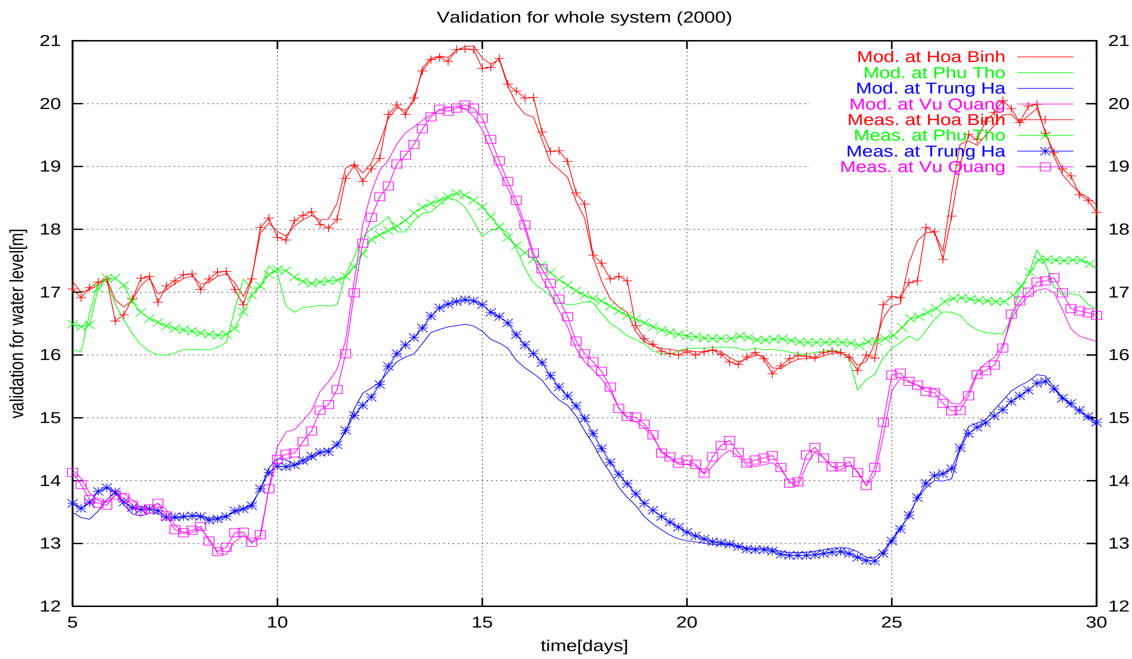


Figure 5.1: Estimated Manning Coefficients

Gauging station	OBJ	Gauging station	OBJ
Hoa Binh	$0.856 \cdot 10^{-2}$	Phu Tho	$3.780 \cdot 10^{-2}$
Trung Ha	$1.486 \cdot 10^{-2}$	Vu Quang	$1.001 \cdot 10^{-2}$
Son Tay	$1.132 \cdot 10^{-2}$	Ha Noi	$1.729 \cdot 10^{-2}$
Hung Yen	$6.500 \cdot 10^{-1}$	Tao Xuan	$6.404 \cdot 10^{-1}$

Table 5.5: Objective function for the water level in flood season 2000.



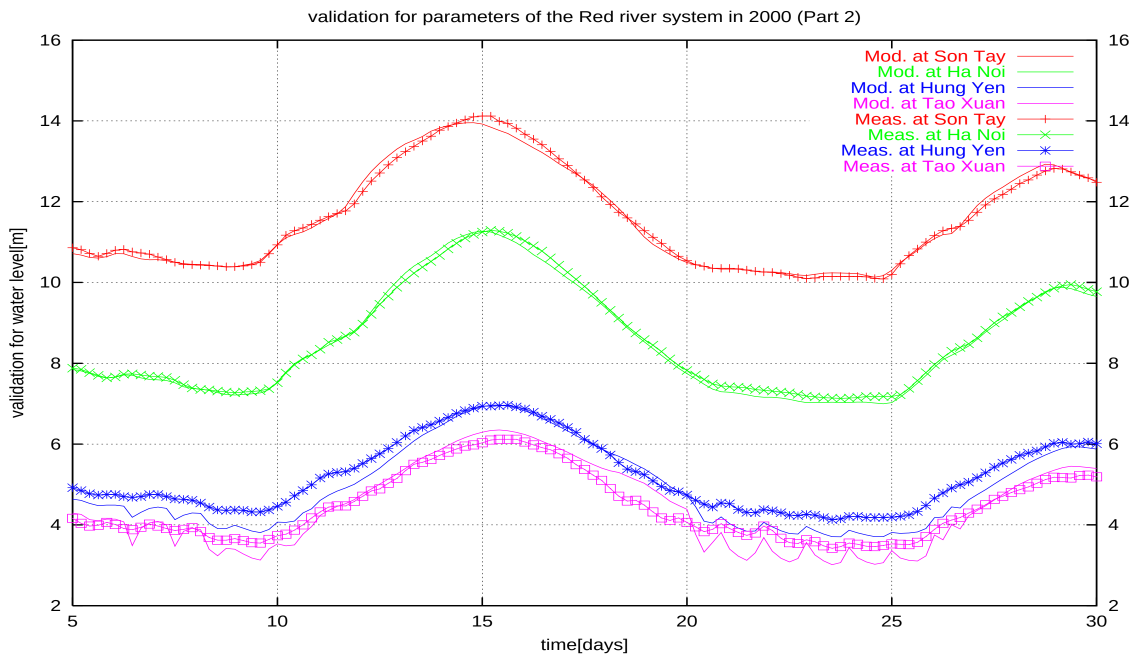


Figure 5.2: Validation of parameters for the Red River system in 2000

The values of the OBJ for the water level at the gauging stations are presented in Table 5.5.

The values of OBJ for the water level at all the gauging stations in the domain 1 are close to zero. In the gauging stations located in the domain 2 the values of the objective functions are much greater than the values of the objective functions of the water level at the gauging stations of the domain 1 due to the bad affect of the tidal propagation, but still acceptable, i.e. the estimated parameters can characterize the Red River system in the flood season of the year 2000, i.e. the time period, in which the parameter estimation has been realized. In order to test if these estimated parameters could characterize the Red River system for a large time interval in the following a verification is realized.

5.2.3 Verification for the Estimated Parameters

The idea of this verification for estimated parameters is to compare the model response and the measurements of the state variables of the system, e.g. the water level for some time interval which has not been used as measurement data for solution of the least-squares problem (4.2)-(4.3).

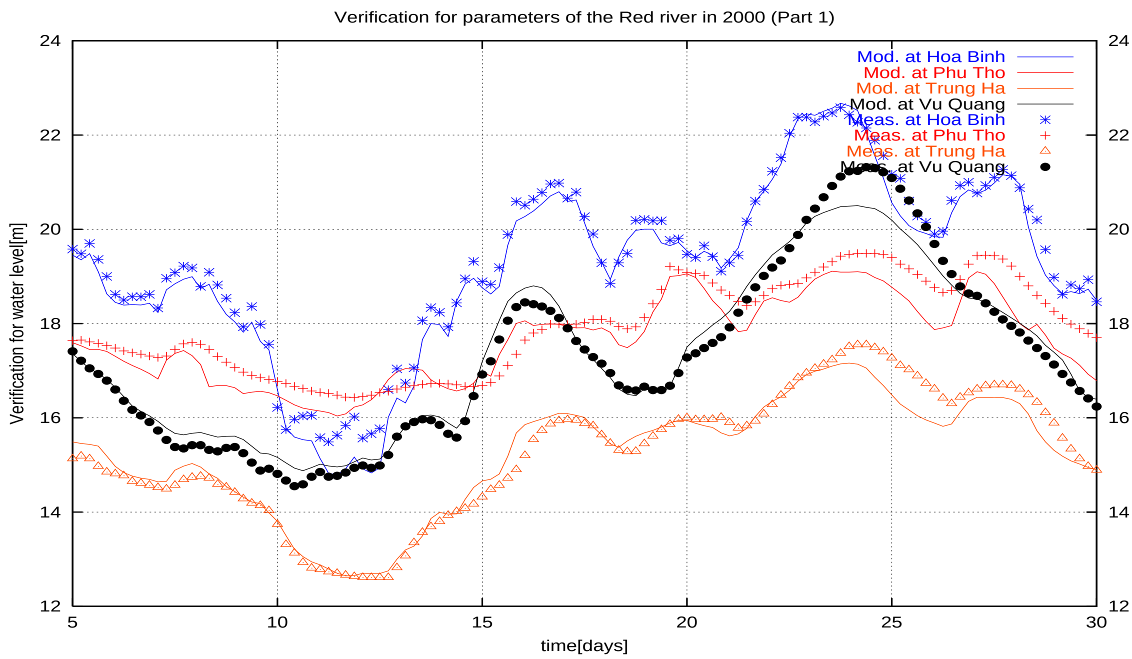
In this study we apply the estimated parameters from the previous section (2000) to compute the water level at the gauging stations Hoa Binh, Trung Ha, Phu Tho, Vu Quang, Son Tay, Ha Noi, Hung Yen, and Tao Xuan in the flood season of the year 1996, i.e. from August 01 to August 31, 1996. The results and the measurement data are illustrated in Figure 5.3.

As a criterion for the evaluation of the coincidence between data and model response the values of OBJ for the water level at the gauging stations are computed and presented in Table 5.6.

Gauging station	OBJ	Gauging station	OBJ
Hoa Binh	$3.952 \cdot 10^{-2}$	Phu Tho	$4.759 \cdot 10^{-2}$
Trung Ha	$3.943 \cdot 10^{-2}$	Vu Quang	$3.418 \cdot 10^{-2}$
Son Tay	$8.119 \cdot 10^{-2}$	Ha Noi	$3.900 \cdot 10^{-2}$
Hung Yen	$8.80 \cdot 10^{-2}$	Tao Xuan	$3.360 \cdot 10^{-2}$

Table 5.6: Objective function for the water level in flood season 1996

The coincidence is still good, e.g. for the water level in Ha Noi the value of OBJ is $3.90 \cdot 10^{-2}$, but it is clearly worse than in the previous validation. This can be explained by the fact that from August, 1996 to July, 2000 the Manning coefficients have been changed in the consequence of the deformation of the surface of the river bed. The practical solution to



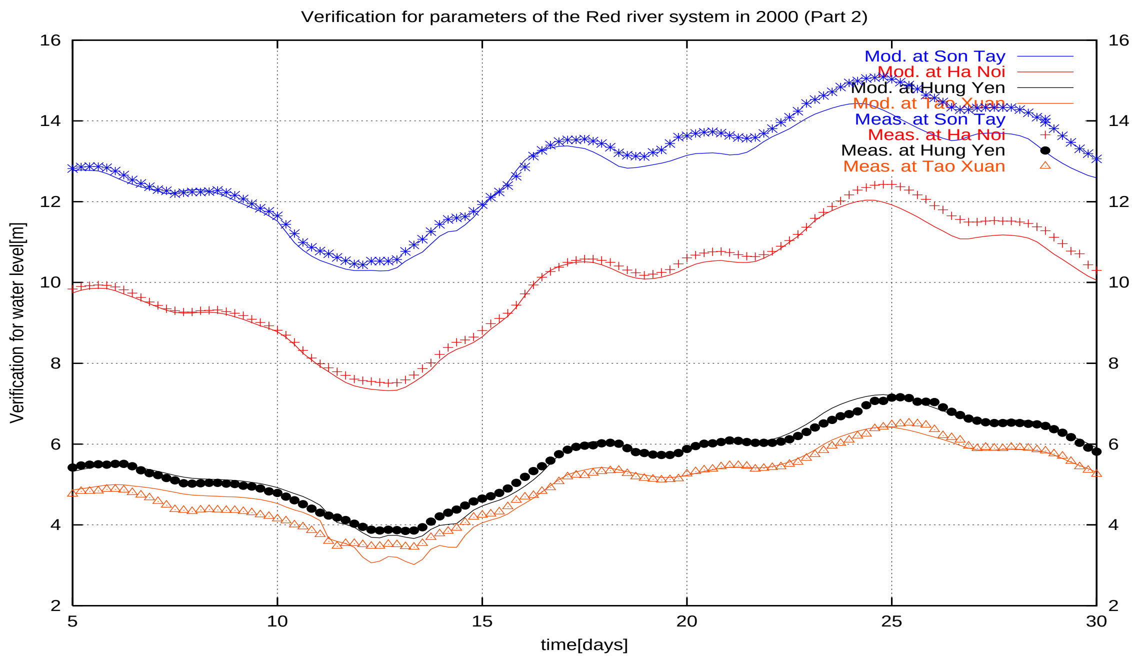


Figure 5.3: Verification of parameters in the year 1996

this problem would be to realize a periodical parameter estimation for the river system, say every year. However, in practical applications it can happen that not all needed measurement data are available. For instance, in this research as the measurement data for parameter estimation for the Red River system only the data in the flood seasons 1996 and 2000 years are available. In order to find out the parameters, which can characterize the system for the large time interval, say from August, 1996 to July, 2000 we are naturally led to the idea of multi-experimental parameter estimation.

5.2.4 Multi-Experimental Parameter Estimation

The idea of a multi-experimental parameter estimation is to find the values of the parameter, which simutaneously satisfy the least squares problem (4.2)-(4.3) for the data measured in both 1996 and 2000.

The computing results are presented in Table 5.7.

Channel	Notation	Initial guess	Estimated
	$p(1,0).10^2$	2.000	2.097 ± 0.039
1	$p(1,1).10^2$	0.000	0.044 ± 0.020
	$p(1,2).10^1$	0.000	-0.064 ± 0.024
	$p(2,0).10^2$	2.000	4.103 ± 0.090
2	$p(2,1).10^2$	0.000	-0.147 ± 0.01
	$p(3,0).10^2$	2.000	2.67 ± 0.097
3	$p(3,1).10^2$	0.000	-0.273 ± 0.071
	$p(3,2).10^1$	0.000	0.513 ± 0.122
	$p(4,0).10^2$	2.000	3.201 ± 0.062
4	$p(4,1).10^2$	0.000	-0.026 ± 0.014
	$p(4,2).10^1$	0.000	$-0.009 \pm 0.0.007$
5	$p(5,0).10^2$	2.000	1.484 ± 0.029
	$p(5,1).10^2$	0.000	0.265 ± 0.013
6	$p(6,0).10^2$	2.000	2.216 ± 0.091
	$p(7,0).10^2$	2.000	2.461 ± 0.043
7	$p(7,1).10^2$	0.000	0.028 ± 0.014

Table 5.7: Initial guess and estimated parameters for the domain 1 in 1996. and 2000.

The Manning coefficients for every river channel can be computed by inserting the estimated values parameters into equation (2.32). Here the maximal water discharge is 20000 [m^3s^{-1}]. The results are illustrated in Figure 5.4.

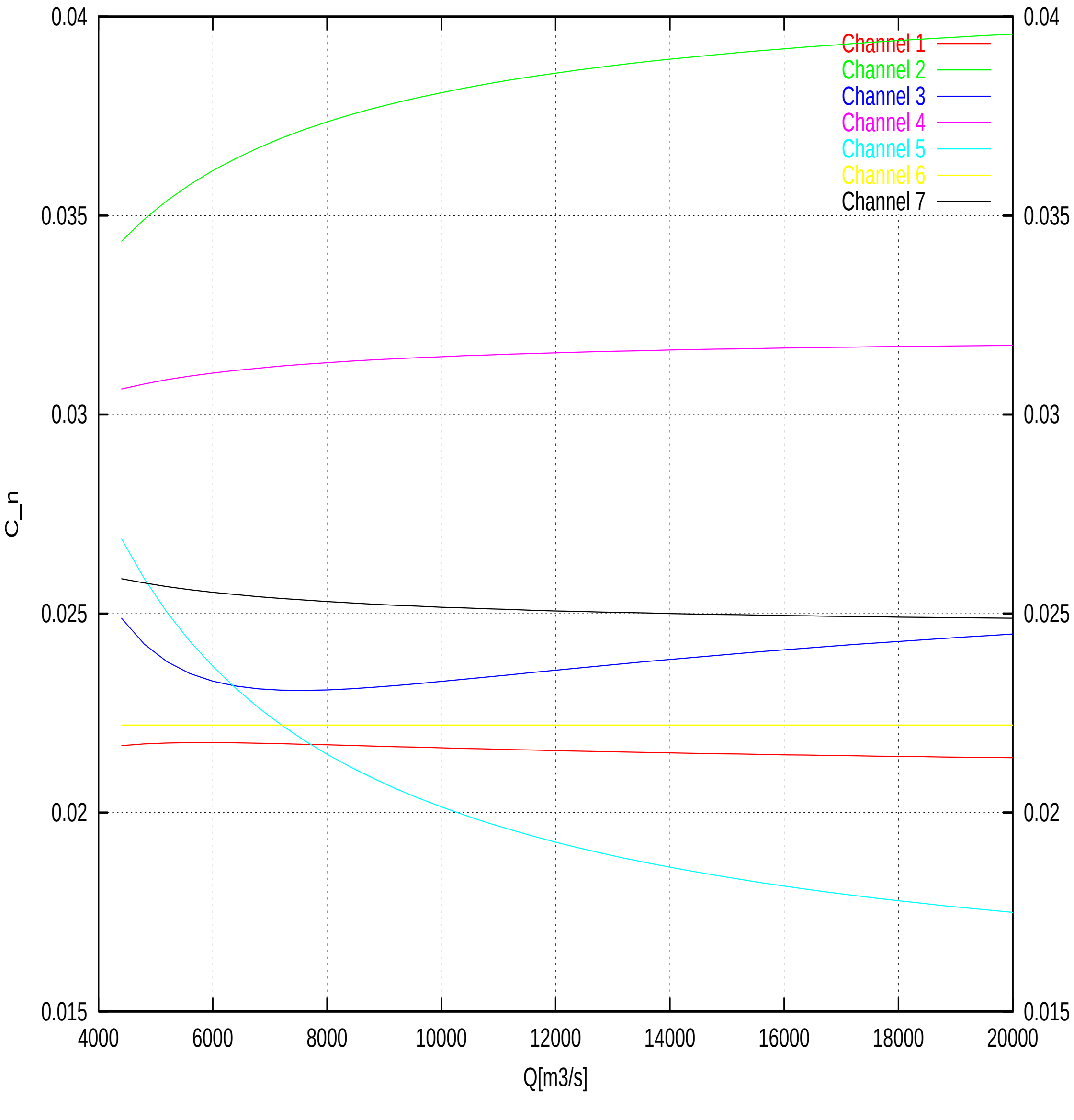


Figure 5.4: Estimated Manning Coefficients for 1996 and 2000

Figures 5.5 and 5.6 show the simulation of the water level at gauging stations with the parameters estimated by multi-experimental parameter estimation for two time intervals in 1996 and 2000. The good coincidence between measured data and response model is observed, and the objective functions of the water level at the gauging stations, which are small (Tables 5.8 and 5.9) show that the parameters presented in Table 5.7 are suitable for the Red River system.

Gauging station	OBJ	Gauging station	OBJ
Hoa Binh	$2.640 \cdot 10^{-2}$	Phu Tho	$4.247 \cdot 10^{-2}$
Trung Ha	$3.470 \cdot 10^{-2}$	Vu Quang	$5.826 \cdot 10^{-2}$
Son Tay	$4.929 \cdot 10^{-2}$	Ha Noi	$4.426 \cdot 10^{-2}$
Hung Yen	$1.372 \cdot 10^{-1}$	Tao Xuan	$3.190 \cdot 10^{-1}$

Table 5.8: Evaluation of multi-experimental parameter estimation in 1996

Gauging station	OBJ	Gauging station	OBJ
Hoa Binh	$2.667 \cdot 10^{-2}$	Phu Tho	$4.106 \cdot 10^{-2}$
Trung Ha	$1.019 \cdot 10^{-2}$	Vu Quang	$2.034 \cdot 10^{-2}$
Son Tay	$1.750 \cdot 10^{-2}$	Ha Noi	$3.734 \cdot 10^{-2}$
Hung Yen	$3.385 \cdot 10^{-1}$	Tao Xuan	$5.729 \cdot 10^{-1}$

Table 5.9: Evaluation of multi-experimental parameter estimation in 2000

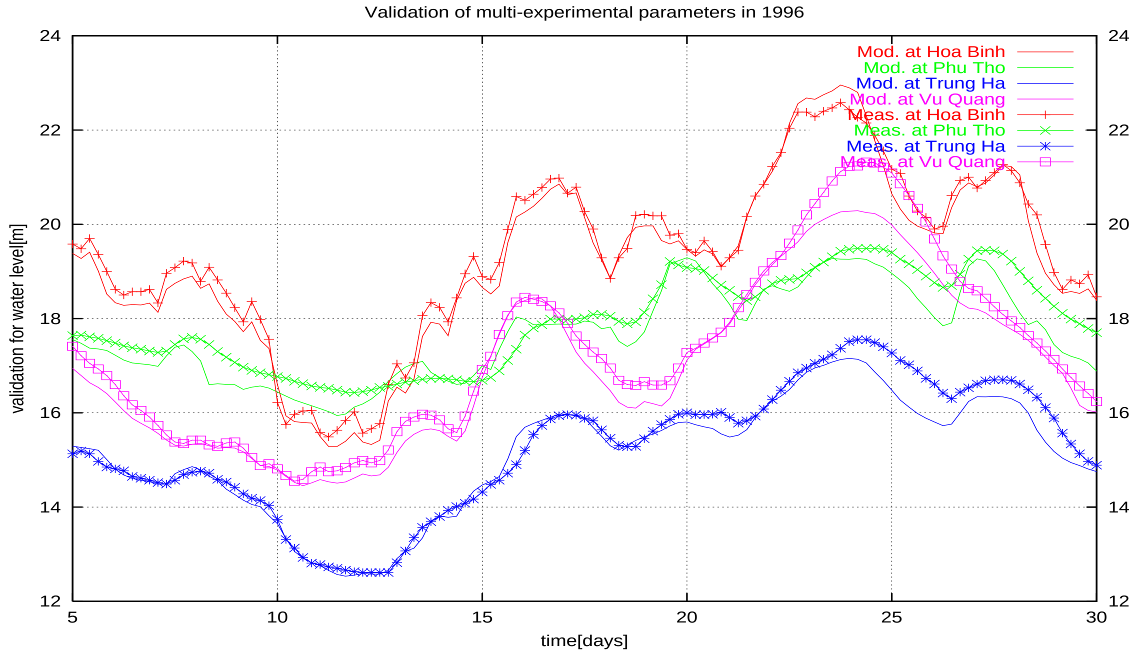
5.3 Numerical Results for Simulation of the Saint-Venant Equation for the Red River System

The Saint-Venant equation for the Red River system is completely determined if,

- the Manning coefficients of the channels are estimated as in the last section, and
- the geometrical data of the Red River system are given as mentioned in Chapter 2.

For an unique solution of this equation system, the corresponding initial and boundary conditions are required.

The boundary conditions are given as mentioned in Section 5.1.



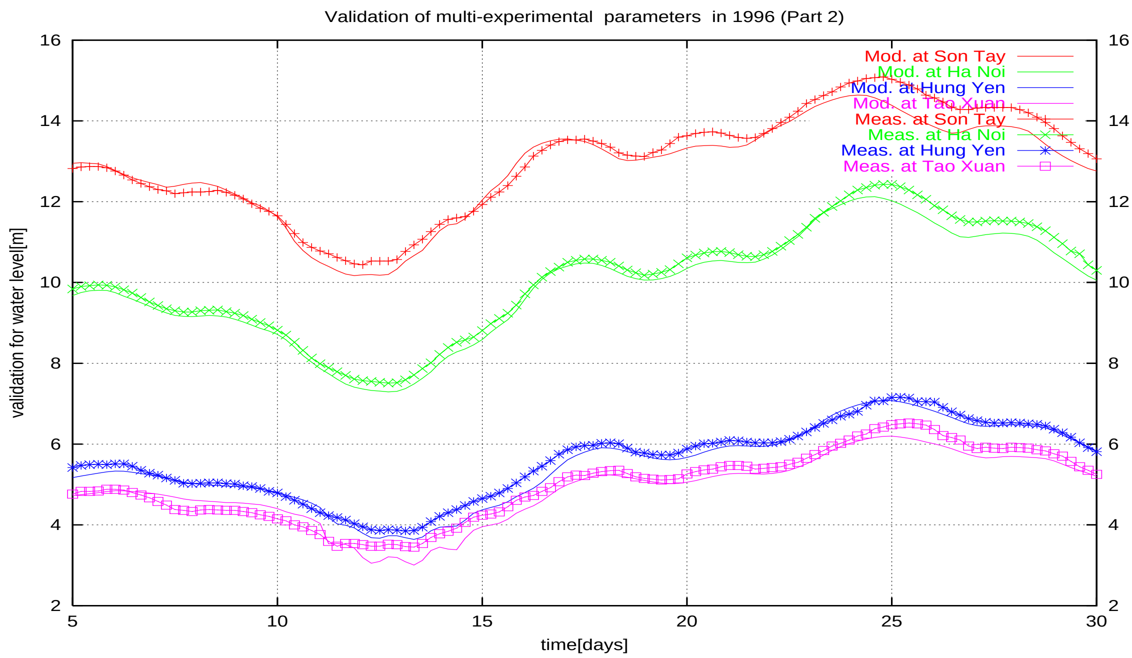
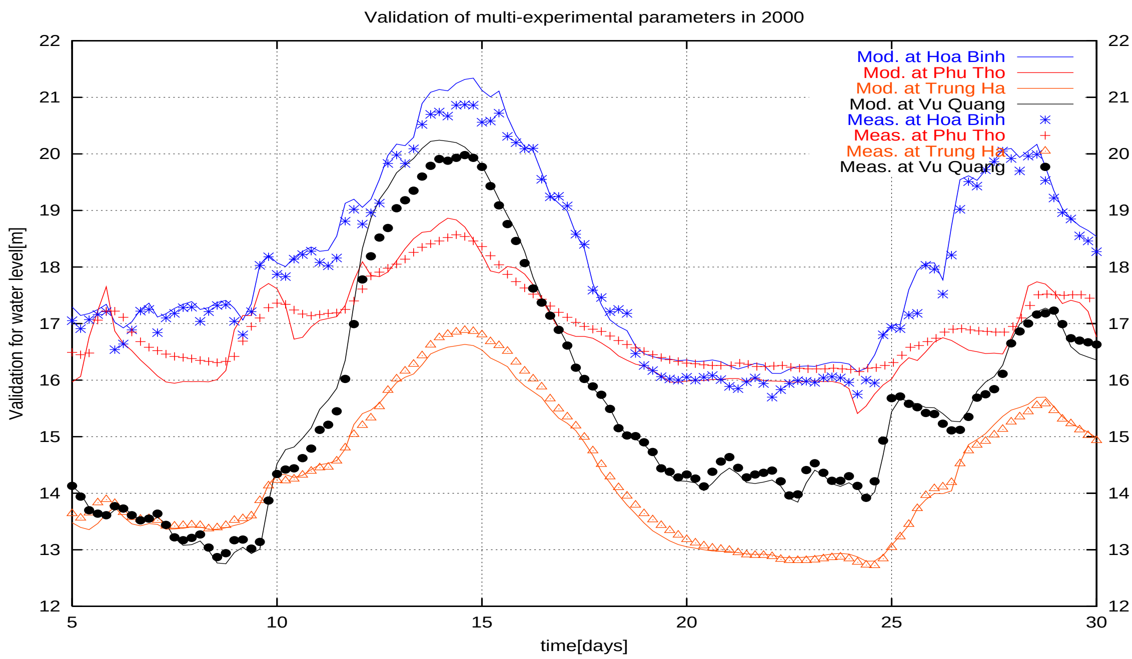


Figure 5.5: Verification of the multi-experimental parameters in 1996



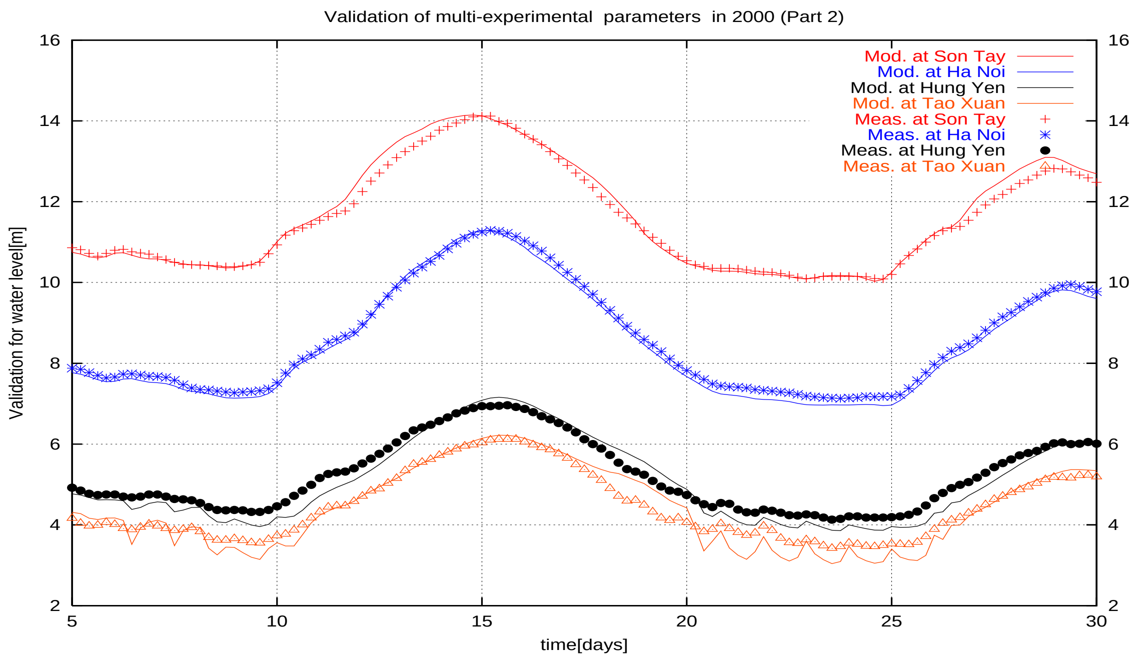


Figure 5.6: Verification of the multi-experimental parameters in 2000

The initial conditions mean all the values of the state variables, i.e. the water discharge Q and the water level y at all the spatial nodes at the first time moment t_0. But normally, this information is not available at the spatial nodes with the exception of gauging stations. Therefore, an approximation for the initial conditions must be made. One possible way is to assume that the processes are starting from a static position. Then, the initial conditions of the system are solution of the Saint-Venant equation in the static case, i.e. the Saint-Venant equation coupled with the following additional conditions:

$$\begin{cases} Q_t(x,0) = 0 \\ y_t(x,0) = 0 \end{cases} \tag{5.1}$$

Substituting (5.1) into (2.24) and rearranging give the following Initial Value Problem (IVP) in space,

$$\begin{aligned} Q_x(x,0) &= 0, \qquad Q(x_0,0) = Q_0 \\ y_x(x,0) &= \frac{gS_f}{\frac{Q^2(x,0)}{A^3}A_y - g}, \qquad y(x_f,0) = y_0 \end{aligned}$$

where, $x \in [x_0, x_f]$ is the space variable; $Q(x,0), y(x,0)$ and $Q_x(x,0), y_x(x,0)$ are the water discharge, the water level and their derivatives w.r.t. x at $t = 0$; A is the cross-sectional area at the location x and corresponding to the water level $y(x,0)$.

This IVP can be easily solved by a standard solver, e.g. the solver DAESOL. The obtained results are the initial conditions of the Red River system.

Figures 5.7-5.10 illustrate the water level and the water discharge at the discretization nodes of the Red River system depending on time. In this simulation, the Saint Venant equation (2.24) for the Red River system with the corresponding initial and boundary conditions is solved in the time interval from July 15 to August 15, 2000. The simultion is realized in a computer Intel P-IV-2500 MHz, 2 MB RAM, and the computing time is 37.66 seconds.

5.4 A Relaxed Model for the Optimal Control Problem of the Red River System

As mentioned in Chapter 3 for the unique solution of the Sant Venant equation for the Red River system, the neccessary upper and lower boundary conditions are required. In the simulation and the parameter estimation processes, the water discharge at upper boundaries, namely at the gauging stations Hoa Binh, Phu Tho, and Vu Quang, and the water level at the lower boundaries, namely at the gauging stations Thuong Cat, Trieu Duong, Nam Dinh, Phu Le, Ba Lat, and Dinh Cu, are given in the investigated time period as the boundary conditions for the Red River system. However, in Chapter 6 when using

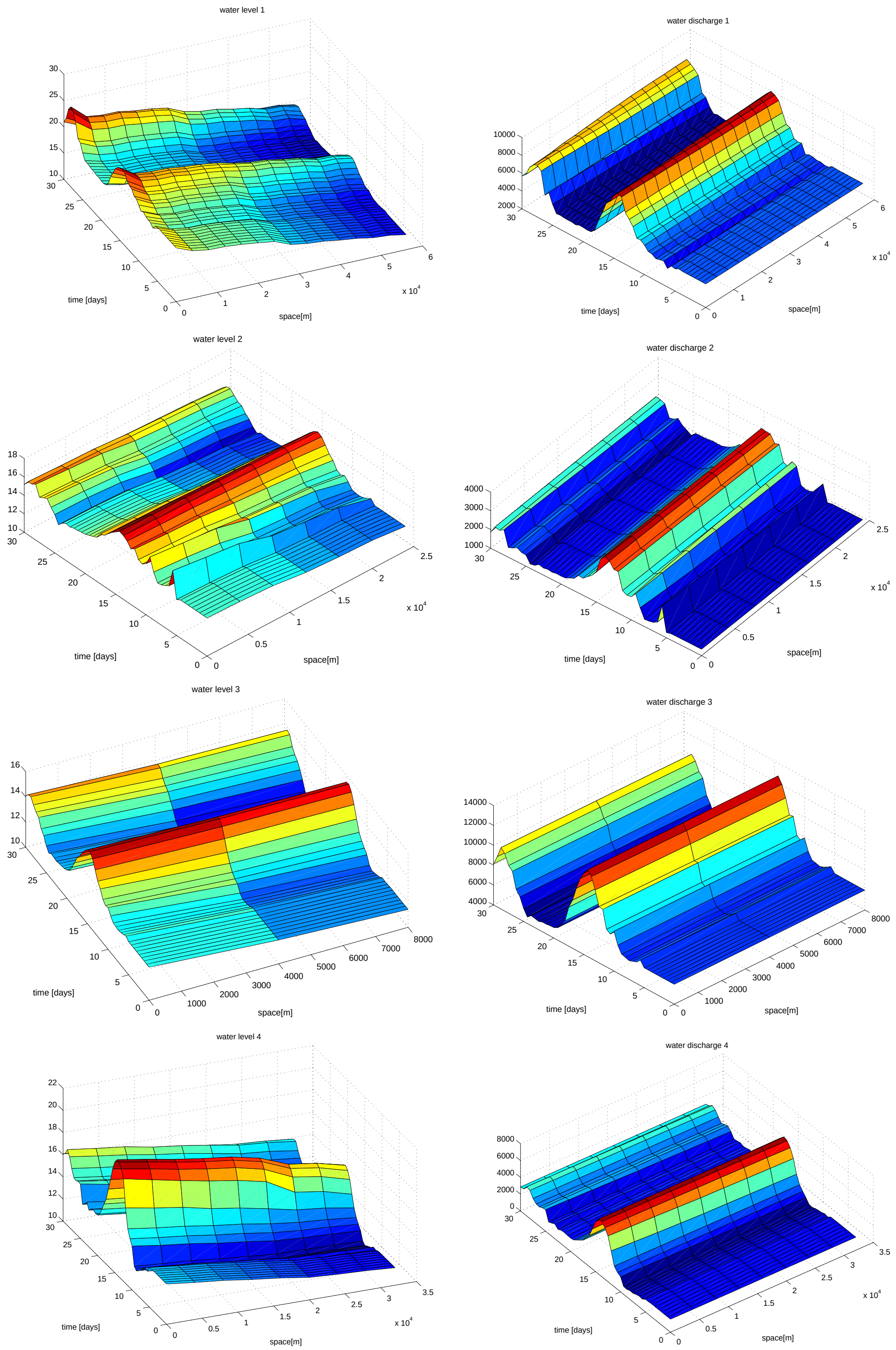


Figure 5.7: Water level [m] and water discharge [m^3s^{-1}] of Channels $1, \ldots, 4$

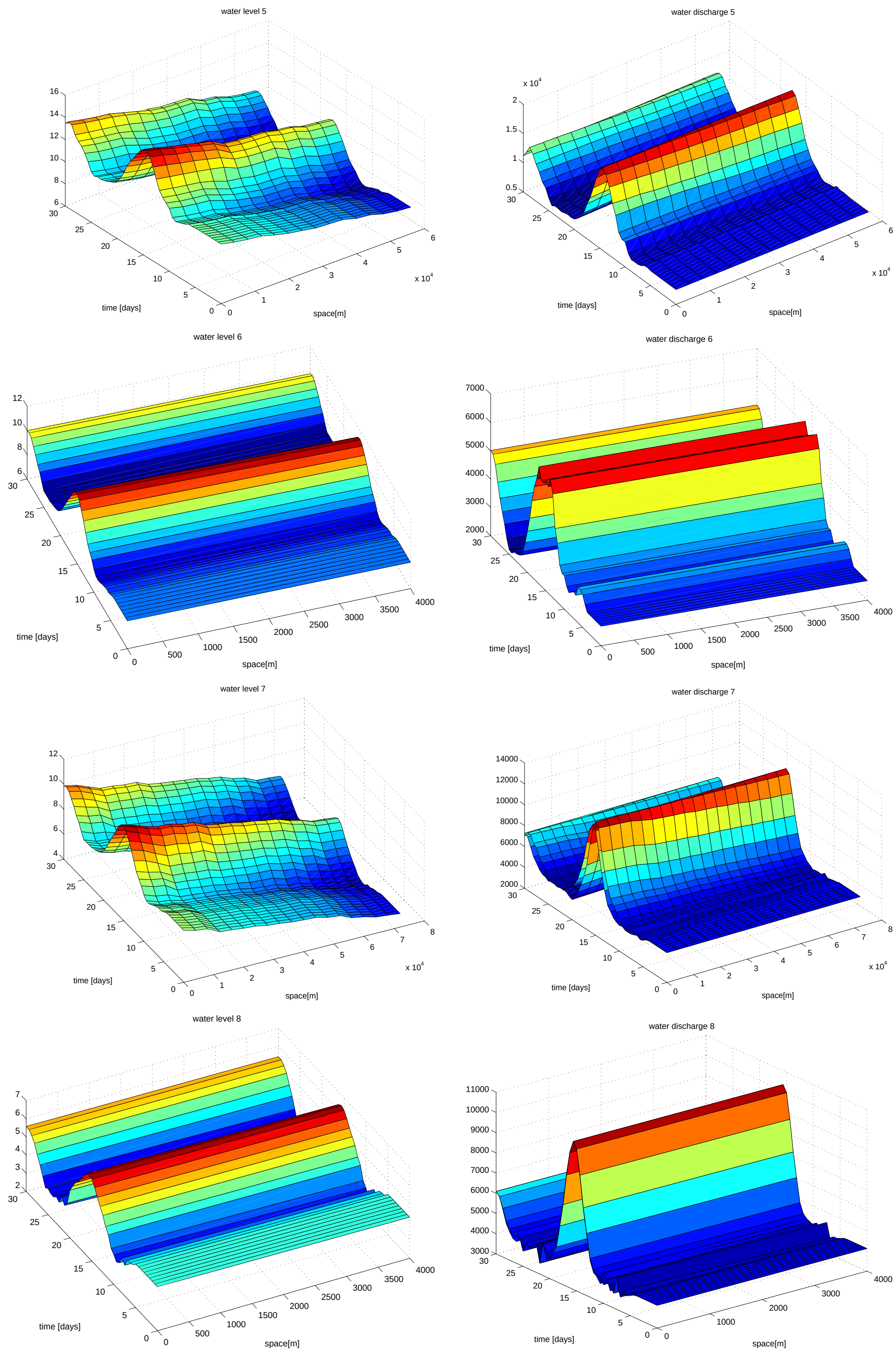


Figure 5.8: Water level [m] and water discharge [m^3s^{-1}] of Channels $7, \ldots, 8$

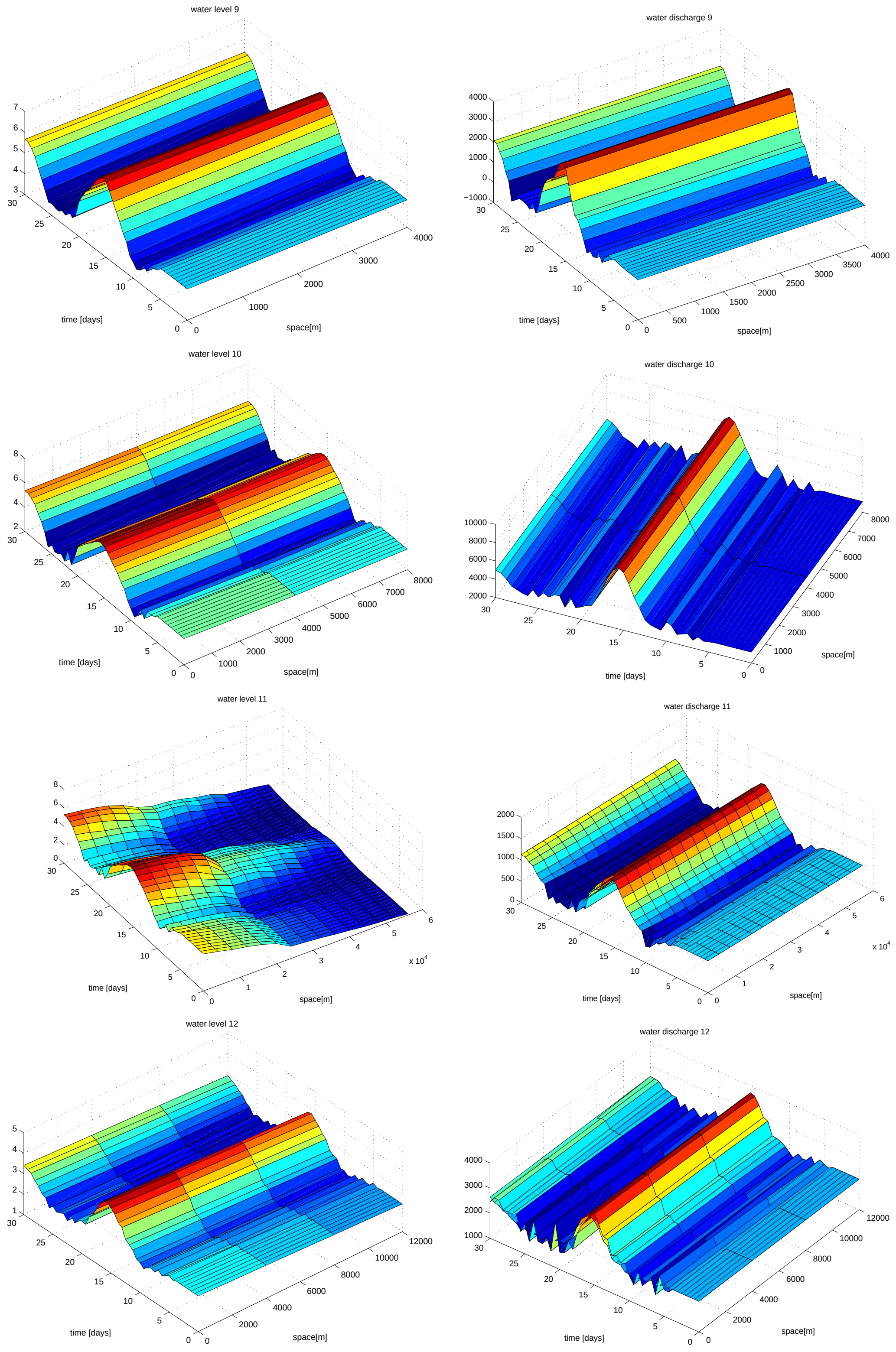


Figure 5.9: Water level [m] and water discharge [m^3s^{-1}] of Channels $9, \dots, 12$

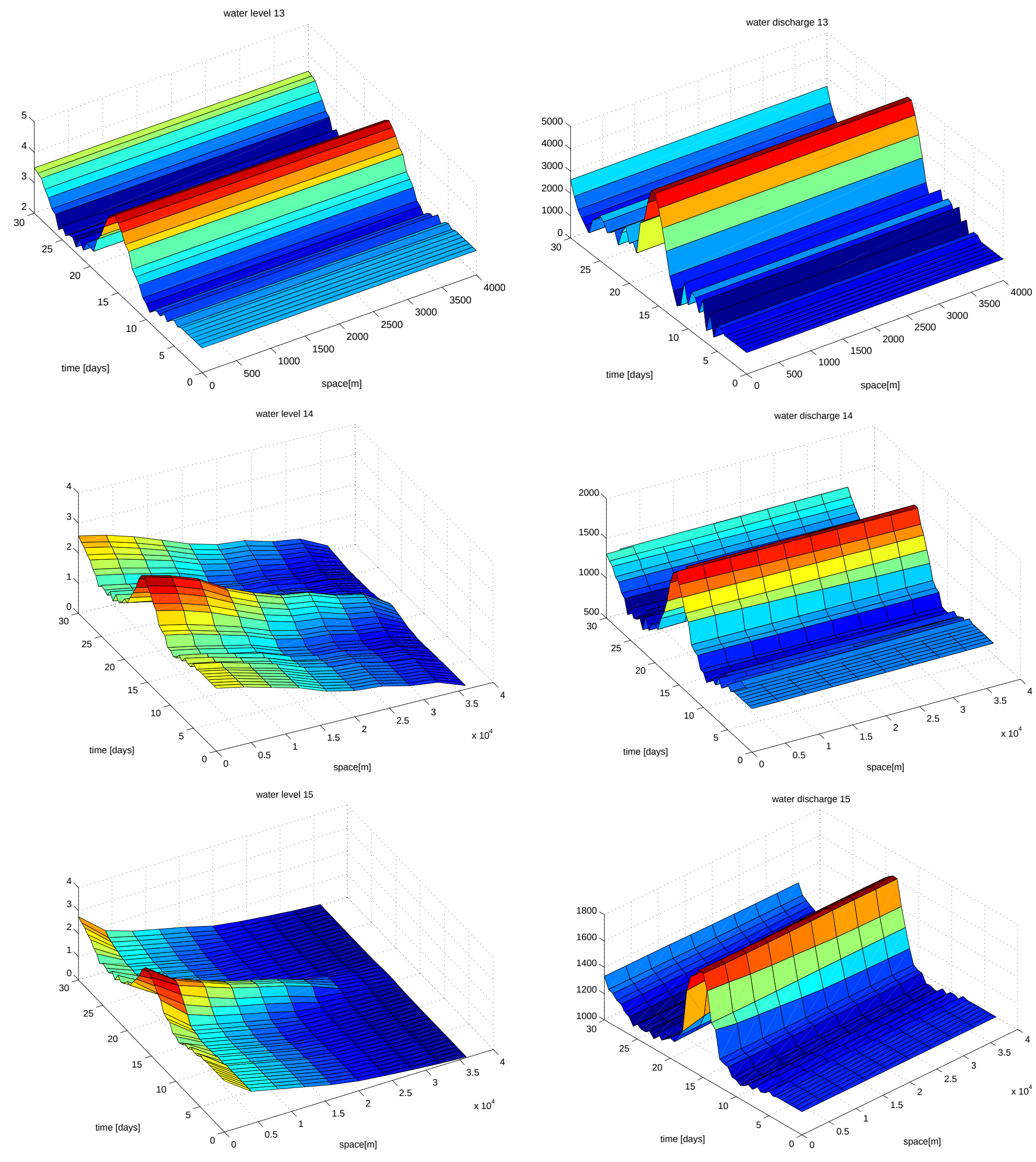


Figure 5.10: Water level [m] and water discharge [m^3s^{-1}] of Channels $13, \ldots, 15$

the model of the Red River system to find an optimal strategy for the control of the Red River system, a difficulity arose that any change of the control function, namely the water discharge from Hoa Binh, leads to a change of the water level in the gauging stations Thuong Cat, Trieu Duong, and Nam Dinh, i.e. the lower boundary conditions depend on the control function. This leads to a bad consequence that in a new iteration step of the optimization process with a new value of the control function, the lower boundary conditions of the Red River system are not defined. In order to avoid this problem and to come up with a good model of the Red River system, which is suitable for the optimal control problem, we relax the model of the Red River system by assuming that the water discharge at the input of the channel 6, 9 and 13 are functions of the water discharge at the output of the channel 5, 7 and 10 (see Fig. 2.4), respectively. We propose that the water discharge Q_{in} at the input of the channel i_{chan} with $i_{\text{chan}} = 6, 9, 13$ at the time t is defined by a polynomial as follows,

$$Q_{\text{in}}(i_{\text{chan}}, t) = \sum_{i=0}^{n_p(i_{\text{chan}})} p(i_{\text{chan}}, i) Q^i_{\text{out}}(i^+_{\text{chan}}, t), \tag{5.2}$$

where, $Q^i_{\text{out}}(i^+_{\text{chan}}, t)$ is the water discharge at the output of the coming river channel to the channel i_{chan}, namely of Channel 5, 7, and 10, respectively, and $n_p(i_{\text{chan}})$ is the number of the all parameters of the channel i_{chan}. The number $n_p(i_{\text{chan}})$ can be chosen by using F $-$ test for linear hypotheses testing as mentioned in Section 2.3.

In order to estimate the unknown parameters in (5.2) we have to solve the least-squares problem (4.2) for the time interval from July 15, 2000 to August 15, 2000. The initial and boundary conditions of the Red River system are given as mentioned in the last sections. As the measurement data, the values of the water level at the input of the channels 6, 9, and 13, which are computed from the simulation of the complete Red River system in the investigated time interval, are used. Our task is to estimate 5 unknown parameters as shown in Table 5.10. The initial guess of the parameter for the channel i_{chan} is based on the numerical results of the previous simulation of the complete Red River system with the assumption that the ratio $\frac{Q_{\text{in}}(i_{\text{chan}}, t)}{Q^i_{\text{out}}(i^+_{\text{chan}}, t)}$ is constant. The initial guess and the estimated parameters for the relaxed model are shown in Table 5.10.

Channel	Notation	Initial guess	Estimated
6	$p(6,0).10^{-4}$	0	-0.3648 ± 0.0450
	$p(6,1)$	0.1280	0.8880 ± 0.0801
	$p(6,2).10^{4}$	0	-0.1888 ± 0.0324
9	$p(9,1)$	0.3570	0.2068 ± 0.0052
13	$p(13,1)$	0.22	0.397 ± 0.0008

Table 5.10: Initial guess and estimated parameters for the relaxed model

Figure 5.11 shows the simulation of the water level at the input of the channels 6, 9, and 13 with the newly estimated parameters and the corresponding measurements. The good coincidence between measured data and response model is observed, and the objective functions of the least-squares problem for the water level at the investigated points, which are sufficiently small (Table 5.11), show that the relaxed model with the parameters presented in Table 5.10 can replace the model of the complete Red River system.

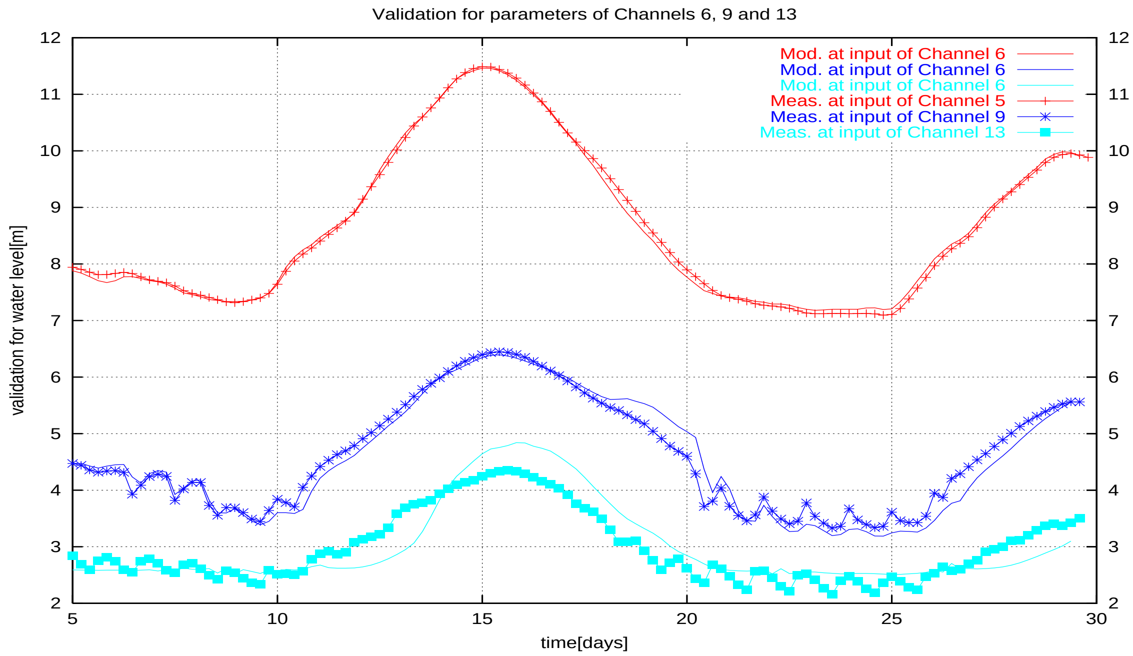


Figure 5.11: Validation of the parameters for the relaxed model

Channel	OBJ
6	$1.108 \cdot 10^{-2}$
9	$2.862 \cdot 10^{-1}$
13	1.077

Table 5.11: Evaluation of parameter estimation for the relaxed model in 2000

By doing the above relaxation we remove the channels 6, 9, and 13 with their lower boundary conditions, namely the water level at the gauging stations Thuong Cat, Trieu Duong, and Nam Dinh, from the model of the complete Red River system. As it has been mentioned in the last sections, the remained lower boundary conditions of the Red River system, namely the water level at the gauging stations Phu Le, Ba Lat, and Dinh Cu, are constant in the null level, therefore all the boundary conditions of the newly obtained (relaxed) model of the Red River system are now defined and independent of the control function. This model is suitable for the optimal control problem, which will be considered in the next section.

5.5 Summary

As a conclusion of this chapter we give some recommendation for future research in modelling of river systems:

- The Saint-Venant equation can be well solved by the method of lines combined with the BDF method which implemented in the solver DAESOL at the research group of Bock and Schlöder (IWR, Heidelberg). A stepsize and order control strategy is used in this solver and this improves the stability and computing time of the numerical methods.

- The unknown hydraulic, geometrical variables of a river system can be treated as unknown parameters, which can be estimated by means of optimization. The optimization problem of parameter estimation for a river system is a large scale least-squares problem, which can be solved effectively by the Generalized Gauss-Newton methods, which were developed by Bock (1981 [10], 1983 [11], and 1987 [12]) and Schlöder (1987 [54]). The software packages PARFIT and FIXFIT implemented research group of Bock and Schlöder are recommended tools for parameter estimation because of their stability and efficiency.

- In a data missing condition, where only some of the required measurements are available, a multi-experimental parameter estimation, as presented in 5.2.4 is recommended. However, more gauging stations should be built up. In order to determine an optimal number and suitable positions for the new gauging stations an optimal experimental design (see Fedorov [28, 29], Bauer [7], and Körkel [38]) is recommended to be considered.

Chapter 6

Optimal Control of the Red River System

The aim of this chapter is to find an optimal strategy for the control of the Red River system in order to prevent floods in the Red River lowland using the mathematical model of the Red River system, which has been discussed in Chapters 2-5.

In Section 6.1 the modelling of the control system of the Red River system is described, and then the optimization problem for preventing floods in the Red River lowland is formulated. This problem is solved by the SQP method combined with the multiple shooting technique which was developed and implemented in the software MUSCOD-II by Bock and Plitt (1984 [15]) and Leineweber (1999 [42]). In Section 6.2 an introduction to MUSCOD-II is made. Some scenarios for the optimal control of the Red River system are given in Section 6.3. Finally, Section 6.4 summarizes the results reported in this chapter and the outlook for future work.

6.1 Optimization Problem

6.1.1 Modelling of the Control Problem

The scheme of the Red River system is shown in Figure 6.1. The Red River system is controlled by the control of the water discharge at the output from the reservoir Hoa Binh, whose technical data [48] are given in Table 6.1.

The task of optimal control of the Red River system is to determine a strategy for control of the working regimes of the reservoir Hoa Binh for a given information about the current state of the reservoir Hoa Binh and the Red River system (feedback information), the

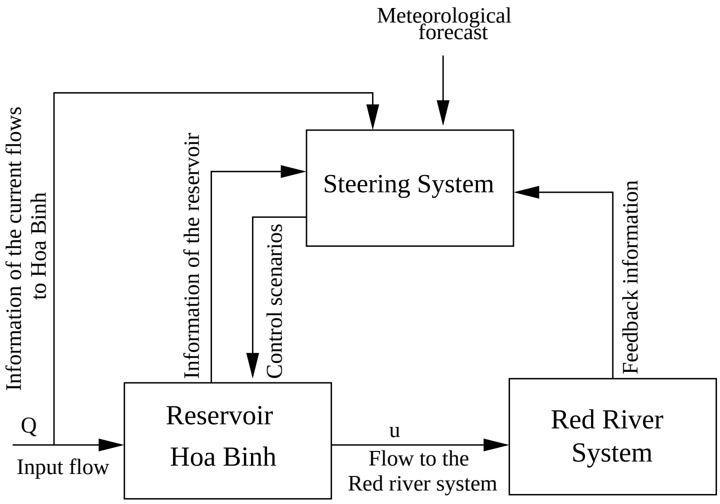


Figure 6.1: The control scheme of the Red River system

Number	Data	Notation	Values	Unit
1	Normal water level	H_{normal}	117	[m]
2	Minimal water level	H_{min}	80	[m]
3	Maximal water level	H_{max}	120	[m]
4	Flood waiting level	H_{wait}	88	[m]
5	Normal volume	V_{normal}	6.65×10^9	[m^3]
5	Minimal Volume	V_{min}	3.80×10^9	[m^3]
6	Maximal Volume	V_{max}	9.45×10^9	[m^3]
7	Number of turbines	n_{turbine}	8	[turbine]
8	Discharge of a turbine	Q_{turbine}	300	[m^3s^{-1}]
9	Number of upper tunnels	n_{upper}	6	[tunnel]
10	Discharge of an upper tunnel	Q_{upper}	2250	[m^3s^{-1}]
8	Number of lower tunnels	n_{lower}	12	[tunnel]
11	Discharge of a lower tunnel	Q_{lower}	1825	[m^3s^{-1}]
12	Maximal discharge in output	$Q_{\text{out}}^{\text{max}}$	37800	[m^3s^{-1}]

Table 6.1: Technical Data of Reservoir Hoa Binh

information of the current flows to the reservoir Hoa Binh and the forecast of the input flows to the system for some time interval in the future, such that some criteria are satisfied for this time interval.

There are two main criteria for the optimal control of the reservoir Hoa Binh:

1. to minimize floods in the Red River lowland, and
2. to maximize the production of electric energy of the Hydro-electric power plant Hoa Binh.

In this thesis, we are especially interested in the search for optimal controls of the reservoir Hoa Binh to minimize floods in the Red River lowland.

In the following the modelling of the control system of the Red River system including the Red River, the reservoir Hoa Binh, and the control function are described.

The Red River System

The modelling of the Red River system is shown in Chapters 2-5. It is shown that the processes in the Red River system can be modeled by the following ODE system,

$$\dot{y}(t) = \bar{f}(y(t), u(t), p) \tag{6.1}$$

$$y(t_0) = y_0. \tag{6.2}$$

Here, $t \in [t_0, t_f]$ is the time variable, $y \in I\!R^{n_y}$ denote the differential variables, $u \in I\!R^{n_u}$ is the control function, and p is the vector of the parameters such as hydraulic or morphometric parameters. The number of the differential state variables n_y is determined by the number of the ODEs obtained from the discretization of the Saint-Venant equations.

Reservoir Hoa Binh

Let us denote Q as the input discharge to the reservoir Hoa Binh, and the control function u is the water discharge from Hoa Binh to the Red River system, and V is the water volume in the reservoir Hoa Binh. We should note that Q, u and V are functions of the time t, and V is a function of Q and u, which is described by the continuity equation as follows

$$\dot{V}(Q(t), u(t)) = Q(t) - u(t) \tag{6.3}$$

with the natural constraints that

$$V_{\min} \le V \le V_{\max}, \tag{6.4}$$

where the values of $V_{\min}$ and $V_{\max}$ are given in Table 6.1

Control Function

Let $\theta_i \in [0, 1]$ denote the relative opening of the tunnel through the i-th turbine, and let u_i be the maximal flow through the i-turbine. Then the total water discharge of the output flow from the reservoir Hoa Binh to the Red River system is determined as,

$$u(t) = \sum_{i \in I_m} \theta_i(t) u_i,$$

where I_m is the index set of turbines and gates of the reservoir Hoa Binh, which are shown in Table 6.1. The control function u has to follow the following constraints,

$$u_{\min} \leq u(t) \leq u_{\max}, \tag{6.5}$$

where $u_{\min}$ and $u_{\max}$ are the minimal and the maximal water discharge from the reservoir Hoa Binh, respectively. From Table 6.1, it is obvious that $u_{\min} = 0$ (all the tunnels are closed) and $u_{\max} = 37800$ [$\mathrm{m}^3\,\mathrm{s}^{-1}$] (all the tunnels are opened).

For ease of presentation we define a new vector $x \in I\!R^{n_y+1}$ of the state variables for the Red River system as follows,

$$x = (y^T, V)^T \tag{6.6}$$

Then the modelling of the Red River system including the reservoir Hoa Binh is defined as system (6.1)- (6.2) coupled with the equation 6.3. This system can be written in a form of a DAE as follows,

$$\dot{x}(t) = f(x(t), u(t), p) \tag{6.7}$$

$$x(t_0) = x_0. \tag{6.8}$$

The ODE system (6.7-6.8) can be solved effectively by the BDF method as it has been discussed in Chapters 2-5.

6.1.2 Constraints

The state and control trajectories are required to satisfy so called *path constraints*

$$h(x(t), u(t), p) \geq 0, \qquad t \in [t_0, t_f].$$

This constraint type includes minimum or maximum values for the controls, safety restrictions on the system state, e.g. the constraints given by (6.4) or (6.5).

The initial conditions of the state variables of the system also may be treated as a constraint, which can be written in a general form as follows

$$r_0(x(t_0)) = 0.$$

6.1.3 Optimization Criteria

The Red River lowland is a very large area, and to formulate an optimal control problem for preventing floods at the whole system is an impossible task. In order to relax this problem we choose some important spatial nodes of the system, e.g. big cities, political, financial, or cultural centers, *etc.* and minimize floods at these places. In this thesis we focus on preventing floods in Ha Noi, the capital of Vietnam.

Let $H(x(t))$ denote the water level in Hanoi, and let $[t_0, t_f]$ be the time interval considered. Then the optimization criteria for the prevention of flood at Ha Noi can be given by e.g.

1. minimizing the average value of the water level at Ha Noi in the interval $[t_0, t_f]$, i.e.

$$\text{minimize} \qquad \int_{t_0}^{t_f} H(x(t))\, dt \tag{6.9}$$

2. minimizing the maximal water level at Ha Noi, i.e.

$$\text{minimize} \qquad \max_{t \in [t_0, t_f]} H(x(t)), \tag{6.10}$$

   This objective is nonsmooth. In order to reformulate it we introduce a global parameter $p[0] \in p$. Then the following problem is equivalent to (6.10):

$$\text{minimize} \qquad p[0], \tag{6.11}$$

   such that

$$H(x(t)) \leq p[0], \qquad \forall t \in [t_0, t_f]. \tag{6.12}$$

3. minimizing the water volume in the reservoir Hoa Binh at $t = t_f$ in order to prevent the forth-coming floods, i.e.

$$\text{minimize} \qquad V(Q(t_f), u(t_f)) \tag{6.13}$$

4. In addition, the following criteria

$$\text{minimize} \qquad \int_{t_0}^{t_f} (u(t) - Q(t))^2 dt, \tag{6.14}$$

   may be impossed to keep the work of the control system in the interval $[0, T]$ as less as possible.

All together the objective functional of the problem of preventing floods in Ha Noi is formulated as a sum of criteria (6.11), (6.9), (6.13) and (6.14) as follows,

$$\int_{t_0}^{t_f} (\alpha_1 H(x(t)) + \alpha_4 (u(t) - Q(t))^2)\, dt + \alpha_2 p + \alpha_3 V(Q(t_f), u(t_f)).$$

Here, α_i $(i = 1, \dots, 4)$ are the weighting coefficient and $T = [t_0, t_f]$.

The term $L = \alpha_1 H(x(t)) + \alpha_4 (u(t) - Q(t))^2$ is called the Lagrange term, and the term

$$E = \alpha_2 p + \alpha_3 V(Q(t_f), u(t_f))$$

is the Mayer term of the objective.

6.1.4 Problem Formulation

We can now formulate an optimal control problem for preventing floods in Ha Noi

$$\min_{\substack{x(\cdot), z(\cdot),\\ u(\cdot), p}} \int_{t_0}^{t_f} L(x(t), u(t), p)\, dt + E(x(t_f), p). \tag{6.15}$$

subject to

$$\dot{x}(t) - f(x(t), u(t), p) = 0 \tag{6.16}$$

$$h(x(t), u(t), p) \geq 0, \qquad t \in [t_0, t_f] \tag{6.17}$$

$$r(x(t_0)) = 0. \tag{6.18}$$

Solving the optimal control problem (6.15)-(6.17) we obtain optimal trajectories $x^*(t)$ and an optimal control function $u^*(t)$ for $t \in [t_0, t_f]$.

6.2 MUSCOD-II – a Software Package for Optimization

Problem (6.15)-(6.17) represents an infinite-dimensional optimization problem. This can be solved by direct multiple shooting in connection with a recursive quadratic programming technique which was developed and implemented in the software package MUSCOD-II by Bock and Plitt (1984 [15]) and Leineweber (1999 [42]). In this section, we first describe how Problem (6.15)-(6.17) is transformed into a finite-dimensional optimization problem by discretization of the control functions as well as the state variables. Then, the quadratic programming method for solution of the resulting discretized system is introduced. In the following we briefly sketch the algorithm. For details see e.g. Leineweber [41, 43, 42], where also multi-stage optimization is described.

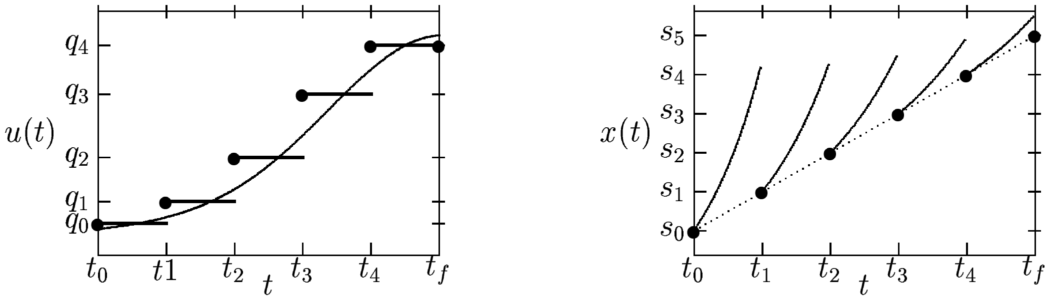


Figure 6.2: Control and state parameterization ($m = 5$).

6.2.1 Parametrization

In the software package MUSCOD the infinite-dimensional optimal control problem is discretized by means of multiple shooting technique (see e.g. Bulirsch [16], Deuflhard [23], Stoer [61], Bock [15]). In the following it is shown how the control function, the state variables and the path constraints are discretized by the multiple shooting method.

6.2.1.1 Control Discretization

In the direct multiple shooting method (as in all direct solution approaches) the infinitely many degrees of freedom $u(t)$ for $t \in [t_0, t_f]$ are approximated by a finite control representation. For that, first, we subdivide the internal $[t_0, t_f]$ into m subintervals as follows

$$t_0 < t_1, \ldots, t_{m-1} < t_m = t_f$$

One special feature of the direct multiple shooting method introduced by Bock and Plitt [15] is to use control functions that have only local support, like piecewise constant or linear functions on the control grid $\{t_0, t_1, \ldots, t_m\}$, i.e. the control functions are approximated by using given basis functions:

$$u(t) := \phi_i(t, q_i) \text{ for } t \in [t_i, t_{i+1}), \quad i = 0, 1, \ldots m - 1. \tag{6.19}$$

Here, q_i are local control parameters.

This approach has the advantage that the resulting discretized problem is a structured optimization problem.

Where continuity of the controls is desired, the control can conceptually be treated as an additional differential system whose time derivative can be controlled.

6.2.1.2 State Discretization

The basic concept of the multiple shooting method is to transform the boundary values problem in the interval $[t_0, t_f]$ into a system of m independent initial values problems. For this purpose $(m+1)$ additional vectors $s_0^x, s_1^x, \ldots, s_m^x$ of the same dimensions n_x as differential states are introduced, which we will denote differential *node values.*

All but the last node value serve as initial values for m independent *relaxed* initial value problems on the intervals $[t_i, t_{i+1}]$:

$$\dot{x}_i(t) = f(x_i(t), \phi_i(t, q_i), p_i) \tag{6.20}$$

$$x_i(t_i) = s_i^x. \tag{6.21}$$

Here, p_i is the parameter in the interval $[t_i, t_{i+1}]$. The continuity of the parameter p is formulated as

$$p_{i+1} = p_i, \qquad i = 0, \ldots, m-1$$

By substituting the independent trajectories $x_i(t)$ into the Lagrangian term L in Eq. (6.15) we can simultaneously calculate the integral objective contributions $L_i(s_i, q_i)$ that are given by

$$L_i(s_i, q_i, p_i) := \int_{t_i}^{t_{i+1}} L(x_i(t), q_i))\; dt. \tag{6.22}$$

The continuity of the state trajectory, i.e. of the solution of the $m-1$ independent initial values problem, is formulated by the following m matching conditions:

$$s_{i+1}^x = x_i(t_{i+1}; s_i, q_i, p_i), \qquad i = 0, \ldots, m-1$$

The initial conditions of the system now are required to be satisfied the following

$$r(s_0) = 0$$

6.2.1.3 Discretization of Path Constraints

Using the multiple shooting grid t_0, ..., t_m, the infinite dimensional path inequality constraints (6.17) are transformed into $m+1$ vector inequality constraints

$$h(s_i^x, \phi(t, q_i), p_i) \geq 0, \quad i = 0, 1, \ldots, m.$$

Note that it would be equally possible to use a finer grid for the discretization of the path constraints.

6.2.1.4 Discretized Optimization Problem

By discretizing the optimal problem (6.15)-(6.17) by the multiple shooting method we obtain the following finite dimensional nonlinear programming problem (NLP):

$$\min_{\substack{q_0,\ldots,q_{m-1},\\ s_0,\ldots,s_m}} \quad \sum_{i=0}^{m-1} L_i(s_i^x, s_i^z, q_i, p) + E(s_m^x, s_m^z, p) \tag{6.23}$$

subject to

$$p_{i+1} = p_i, \qquad i = 0,\ldots,m-1 \tag{6.24}$$

$$s_{i+1}^x - x_i(t_{i+1}; s_i, q_i, p_i) = 0, \qquad i = 0,\ldots,m-1 \tag{6.25}$$

$$r(s_0) = 0 \tag{6.26}$$

$$h(s_i^x, \phi_i(t, q_i), p_i) \geq 0, \quad i = 0,1,\ldots,m. \tag{6.27}$$

The advantage is that the NLP has a sparse structure, due to the fact that all constraint functions and the additive terms of the objective function each depend only on a small number of variables, and conversely, each variable appears only in a few problem functions.

For the ease of presentation we write the NLP (6.23) - (6.27) in a compact form by introducing the following vectors

$$q := \begin{pmatrix} q_0 \\ \vdots \\ q_{m-1} \end{pmatrix} \in \mathbb{R}^{n_q}, \quad s := \begin{pmatrix} s_0 \\ \vdots \\ s_m \end{pmatrix} \in \mathbb{R}^{n_s}, \quad \text{and} \quad w := \begin{pmatrix} q \\ s \end{pmatrix} \in \mathbb{R}^{n_w}$$

with $n_q := mn_u$, $n_s := (m+1)(n_x + n_z)$, and $n_w = n_q + n_s$, and define $F_1(w) := \sum_{i=0}^{m-1} L_i(s_i, q_i, p) + E(s_m, p)$ and summarize all equality constraints in a function $F_2 : \mathbb{R}^{n_w} \to \mathbb{R}^{n_2}$ and all inequality constraints in a function $F_3 : \mathbb{R}^{n_w} \to \mathbb{R}^{n_3}$. The NLP can then be summarized as

$$\min_{w \in \mathbb{R}^{n_w}} F_1(w) \quad \text{subject to} \quad \begin{cases} F_2(w) = 0, \\ F_3(w) \geq 0. \end{cases} \tag{6.28}$$

6.2.2 Solution of the NLP

In MUSCOD, the NLP (6.28) is efficiently solved by a tailored sequential quadratic programming (SQP) method that exploits the special sparse structure of the problem due to the local influence of the variables. SQP is an iterative method in which the NLP at each iterative step is approximated by the following quadratic problem (QP):

$$\min_{\Delta w} \quad \frac{1}{2}\Delta w^T B_k \Delta w + \nabla F_1(w_k)\Delta w \tag{6.29}$$

$$F_2(w_k) + \nabla F_2(w_k)\Delta w = 0 \tag{6.30}$$

$$F_3(w_k) + \nabla F_3(w_k)\Delta w \geq 0, \tag{6.31}$$

where B_k is an approximation of the Hessian of the Lagrangian function L of the problem (6.28), which is defined as

$$L = F_1 - \lambda_1^T F_2 - \lambda_2^T F_3.$$

The solution Δw_k of QP (6.29)-(6.31) is the new search direction for the optimum , i.e. at the value of w at step $k+1$ is determined by

$$w_{k+1} = w_k + \alpha \Delta w_k.$$

Here α is called the step length and is determined by a line search. This determines the trust region where the quadratic approximation (6.29)-(6.31) of the NLP is valid. A detailed description of SQP methods can be found in the optimization textbooks, e.g. Gill [33], Fletcher [31]. In the direct multiple shooting methods described in this chapter the QP has a block-sparse structure. Such problems can efficiently be solved by the reduced SQP methods developed by Bock (1984 [15]). In these methods instead of directly solving the QP, the problem first is condensed by eliminating the additional variables $s_1, \ldots, s_m$ introduced by the multiple shooting method, and then solve the resulting dense QP by a standard solver. The values of the variables $s_1, \ldots, s_m$ are computed by a forward recursion. For a more detailed description of this recursion formulae see Bock et al. [15] or Leineweber [42].

6.3 Selected Results for Optimal Control of the Red River System

6.3.1 Optimal Control of the Red River System

In order to find an optimal control for the Red River system to prevent flood in Ha Noi, we solve the optimal control problem (6.23) - (6.27) constrained by the Saint-Venant equation of the relaxed model of the Red River system, which was introduced in the last chapter, with the corresponding upper and lower boundary conditions of the system. In practice, the values of the boundary conditions of the (relaxed) Red River system are taken from the meteorological forecast. Let us now apply the numerical method for solution of optimal control problems, which is described above, to an example: to prevent the peak of the flood in the flood season 2000. The duration of the highest peak of the flood is 18 days (432 hours), starting from 1h00, July 15, 2000. We assume that the forecasting information is available in this time interval. Then based on it we find an optimal control for the Red River system in the flooding time, i.e. 432 hours.

In this flood season, in the case without any control, i.e. we let all the coming water to the reservoir Hoa Binh go through down to the Red River lowland, the water level at Ha Noi increased up to 11.3 [m] as illustrated in Figure 6.3.

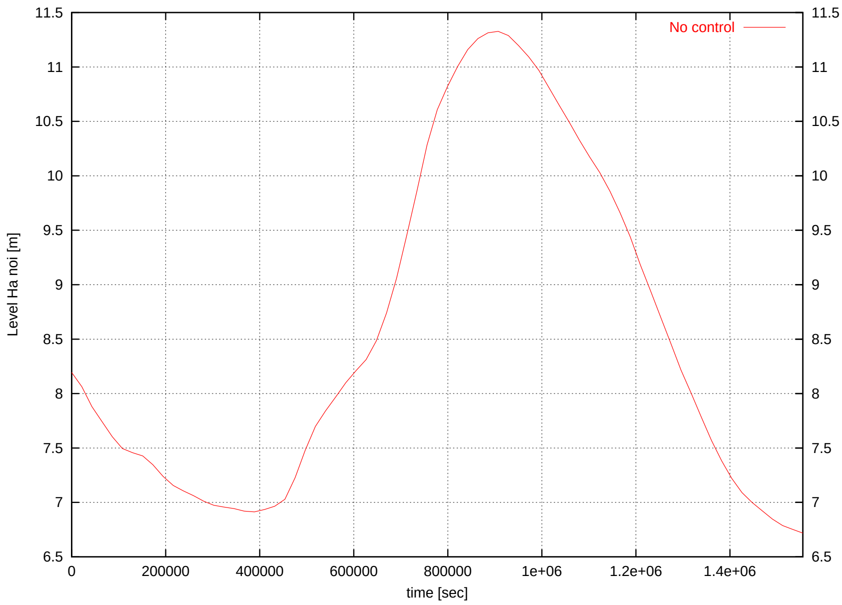


Figure 6.3: The Flood at Ha Noi in 2000

As it is shown in Table 6.1 there are

- 8 turbines with a total discharge of 2400 [m^3s^{-1}]
- 12 lower tunnels with a total discharge of 21900 [m^3s^{-1}]
- 6 upper tunnels with a total discharge of 13500 [m^3s^{-1}],

which can be used as the means of control function for preventing floods in the Red River lowland. However, the upper tunnels are used only for very urgent situations, when the safety of the reservoir is under dangers and the reservoir can be destroyed. Normally, only the lower tunnels and the turbines are used as a means for control of the Red River system.

At the beginning of the flood season in the year 2000, two lower tunnels are open and three turbines are working. The total water discharge from the output of the reservoir Hoa Binh then is 4550 [m^3s^{-1}]. In this test we assume that as means for control we can change the number of the openning lower tunnels from 0 to 5, i.e. If $Q(t)$ is the water discharge at the input of the reservoir Hoa Binh and $u(t)$ is the water at output of the reservoir to the Red River system, then $u(t) \in [900, 10025]$ [m^3s^{-1}]. By changing values of $u(t)$ we can control the water discharge at the output of the reservoir Hoa Binh, and consequently control the floods in the Red River lowland.

The aim of the optimal control is to minimize the maximal water level in Ha Noi in the time interval $[t_0, t_f]$ and the water volume in the reservoir at $t = t_f$. As above mentioned the objective functional is then

$$F_1(u(t)) = p[0],$$

where $p[0]$ is the global parameter that satisfies (6.12).

The values of $V_{\min}$ and $V_{\max}$ in the constraint (6.4) are given in Table 6.1. Because of the security reason the water volume in the reservoir Hoa Binh should not reach the maximal value, and it either should not be decreased down to the minimal value due to necessaries of water for the electric products and the transportation in the Red River lowland. Hence, we set $V_{\min} = 5 \times 10^9$ [m^3] and $V_{\max} = 8 \times 10^9$ [m^3]. At the beginning of the flood season the water volume of the reservoir Hoa Binh is 6×10^9 [m^3].

The above described optimal problem is solved with the software package MUSCOD-II developed at the research group Bock & Schlöder (IWR, Heidelberg). The initial values of the state variables are taken from the simulation of the Red River system, which has been described in the last chapters. The numerical setup of this problem is shown in Table 6.2.

Name	Values	Unit
Time	$1.5552 \cdot 10^6$	s
# multiple shooting nodes	72	-
# state variable	497	-
# inequality constraints	5	-
# controls	1	-

Table 6.2: Numerical setup of the offline optimal control problem

As a solution of the optimal problem for the Red River system the scenario for the optimal control of the reservoir Hoa Binh and the corresponding values of the water level in Ha Noi are given. Figure 6.4 illustrates the scenarios of optimal control of the reservoir Hoa Binh for the flood season 2000. This shows that the optimal control strategy could decrease the

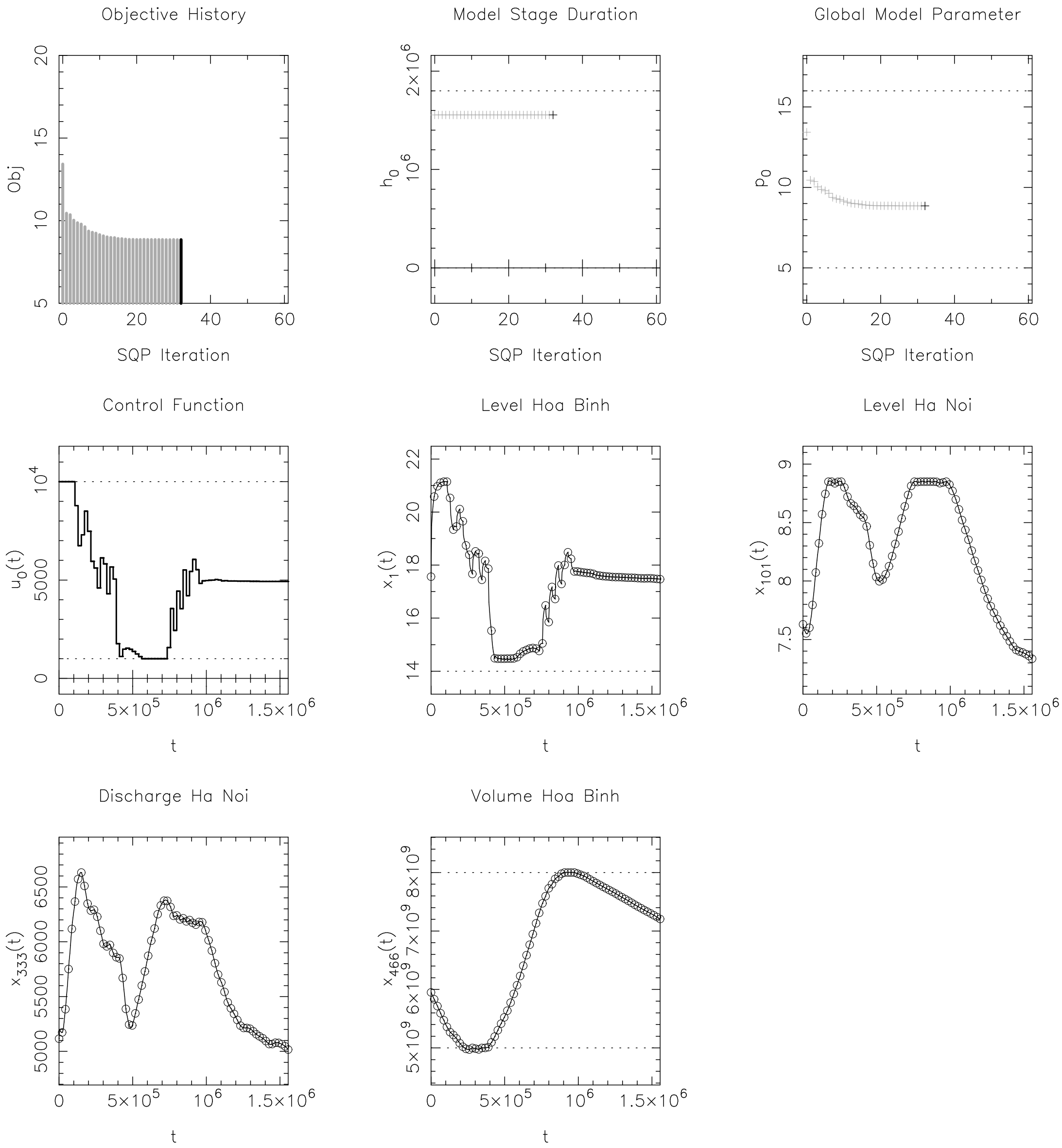


Figure 6.4: Scenario for Optimal Control of the Red River

peak of the water level in Ha Noi from 11.3 to under 8.9 m. The control strategy is that when the flood is still not coming, we let the water volume in the reservoir Hoa Binh go to minimum. Hence, when the peak of the flood is coming, a big free volume, namely 3.10^9 m^3, is available to accumulate water in order to keep the water level in Ha Noi low.

6.3.2 Online Control Approach for the Red River System

However, in practice a general meteorological forecast is normally available only 96 hours in advance, and an sufficiently exact meteorological forecast is normally available only 48 hours in advance. Therefore we can find the solution for optimal control of the Red River system only for a time interval $T = 96$ hours. In order to find an optimal control of the Red River system for a long time interval, say for the whole flood season, we propose to apply an online control technique, namely Nonlinear Model Predictive Control (NMPC). The process of NMPC reads:

1. At $t = t_0$ we find the optimal control of the Red River system for the time interval $[t_0, t_0 + T]$ with given information of the Red River system in this interval, e.g. the boundary conditions of the Red River system, the current water volume of the reservoir Hoa Binh, and the current water level in Ha Noi.
2. Apply the scenario obtained from Step 1 to control the Red River system.
3. At $t = t_0 + \Delta t$ we update new information of the Red River system, set $t_0 = t_0 + \Delta t$ and repeat Step 1. Here, $\Delta t < T$ is the time interval to update new forcasting information.

We apply NMPC algorithm to the problem, described in the last paragraph, i.e. to minimize the water level in Ha Noi in the flood season 2000 with $T = 96$ hours or $3.456 \cdot 10^5$ s, and $\Delta t = 48$ hours or $1.728 \cdot 10^5$ s. In each interval $[t_0, t_0 + T]$ the optimal control problem is solved by MUSCOD-II with the numerical setup shown in Table 6.3 Figures 6.5 and 6.6

Name	Values	Unit
Time	$3.456 \cdot 10^5$	s
# multiple shooting nodes	16	-
# state variable	497	-
# inequality constraints	5	-
# controls	1	-

Table 6.3: Numerical setup of the online optimal control problem

illustrate the control function, namely the water discharge from Hoa Binh, in the different

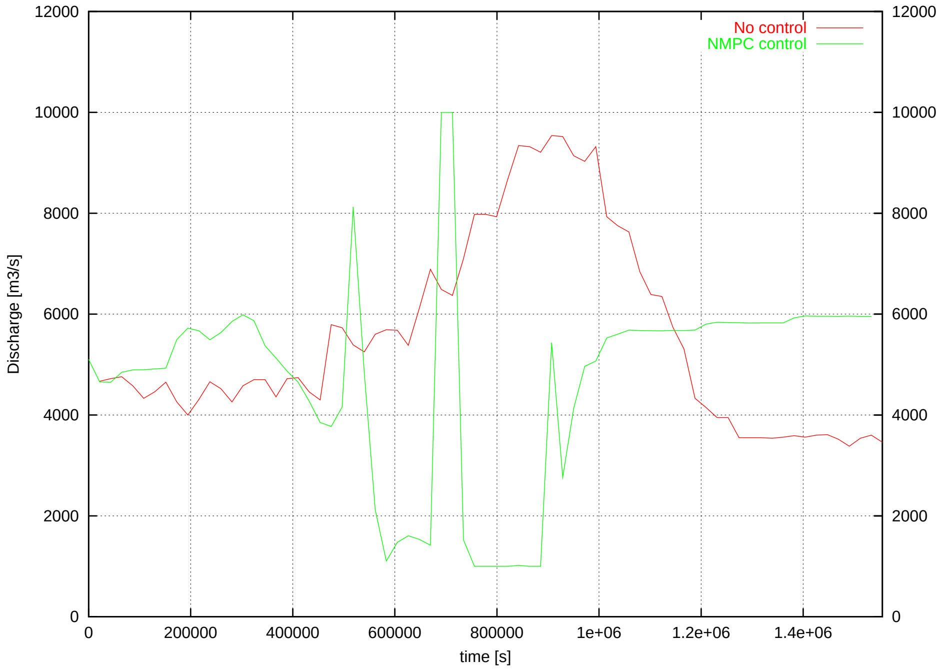


Figure 6.5: Water discharge from Hoa Binh in the flood season 2000.

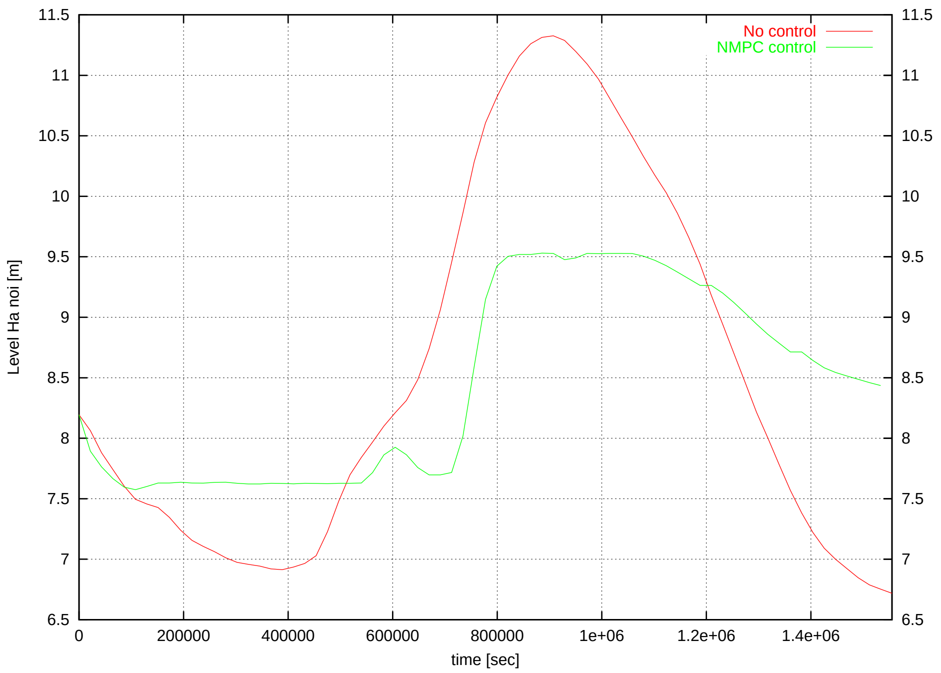


Figure 6.6: Water level in Ha Noi in the flood season 2000

scenarios: without control and with the NMPC, and the corresponding water level in Ha Noi. This show that by applying NMPC we can decrease the maximum water level in Ha Noi from 11.3 m (no control) to 9.6, i.e. the online algorithm, which we have introduced, can effectively reduce the maximum water level in Ha Noi.

Remark 6.3.1 *In the mentioned NMPC algorithm for the optimal control of the Red River system we have implicitly assumed that the forcast is exact. However, in practical applications it happens that the real process differs from the predictive process, e.g. the real water input in Hoa Binh differs from its forcast. In this case an adaptive strategy have to be considered.*

6.4 Summary

In this chapter the following work is done:

- Formulate the optimal control probem for preventing floods in the Red River lowland with the suitable objective functional.
- Use the direct multiple shooting in connection with the recursive quadratic programming technique within MUSCOD-II, the software for optimization, to find solution for the optimal control problem of the Red River system.
- Propose an online control approach for preventing floods in the Red River lowland and apply this approach to a concrete test problem, namely to prevent the flood in the year 2000.

Chapter 7

Conclusions and Outlook

Conclusions

The objective of this thesis was to investigate numerical methods for solution of simulation, parameter estimation and optimal control problems of river flows and their application to the Red River system in Vietnam. The ultimate aim is to explore the possibility of better control of the Red River system. The developed and validated model of the Red River shows excellent corresponce with reality and promises good prediction potential. Within this thesis, we have presented all necessary steps for development of a good model of a river system and its final use for control:

- **Dynamical Modeling:** Based on the specific properties of the Red River system and the necessity of explicit dependence of the state variables on the control functions we have chosen the one-dimensional Saint-Venant equation system to describe the processes in the Red River system. This is a pair of two nonlinear hyperbolic PDEs. Because several river channels are considered, several of these PDEs are coupled with each other.

- **Numerical Simulation Methods:** For the solution of the Saint-Venant equation system we have proposed to use the method of lines to transform the PDEs into a large system of ODEs, which can be solved by e.g. the BDF method. A stepsize and order control strategy is used in this solver, which improves the stability and computational cost of the numerical methods compared to fixed stepsize methods, which are implemented in most currently used software packages for simulation of river flows.

- **Parameter Estimation Problem:** In the past the unknown geometrical and hydraulic variables which can not be measured, e.g. the friction coefficients, river bed slope, *etc.* have been manually estimated. However, this way of estimating unknowns is not efficient due to the fact that the number of these parameters is high and they are strongly correlated with each other. In this thesis we have proposed to treat all the unknown variables as unknown parameters and estimate them by means of optimization. For this purpose we have formulated the optimization problem for parameter estimation for a river system. This is a least-squares problem constrained by a large system of ODEs. Numerical methods for solution of this problem have been discussed and based on this discussion we have chosen the Reduced Gauss-Newton method which was developed and implemented by Schlöder (see [54]) for solving the parameter estimation problem for the Red River system. A detailed description of this method was made.

- **Parameter Estimation and Validation for the Red River:** We have applied the optimization methods to estimate unknown parameters of the Red River system, namely the functional form of the Manning Coefficients for all river channels. The validation of the estimated parameters shows excellent correspondence of the model response and the measurement data. To the best of the author's knowledge this is the first time that optimization based parameter estimation has been carried out for a complete river system.
- **Optimal Control:** Based on the validated model, we have formulated an optimal control problem for preventing floods in the Red River lowland. This is solved by the direct multiple shooting method within the software package MUSCOD-II. We have proposed an online optimization approach to reduce the maximum flood level at Ha Noi by controlling the water discharge at the output of the reservoir Hoa Binh and demonstrated its potential at an example problem.

Based on the software packages PARFIT and FIXFIT for simulation and parameter estimation as well as the software package MUSCOD-II for optimization we have built up a tool for solution of simulation, parameter estimation and optimal control problems for a river system. The obtained numerical results for the Red River system have shown that this tool is capable to considerably support the modelling process and opens a door to model based optimal control of real river systems.

Outlook

Based on the results of our investigation we would like to note the following promising directions for future research:

- **Experimental design for location of gauging stations:** In order to obtain better information of the Red River system more gauging stations should be built up. Techniques of experimental design (see Fedorov [28, 29], Bauer *et al.* [7], and Körkel [38]) can help us to determine the optimal number and suitable positions for new gauging stations.

- **Real-time State and Parameter Estimation:** In this thesis the unknown parameters have been well estimated for some time period. However, these parameters slowly vary in time, therefore a real-time parameter estimation is recommended to keep the model up to date. Because not all state variables can be measured it is also important to develop state estimation techniques (see e.g. Christopher *et al.* [18]) for better observation and control of the river system.

- **Real-time Control of the Red river system:** We have proposed an online control approach for the Red River system. The demonstrated example problem shows the potential of this approach. The following open problems should be investigated in the future research: fast optimal control algorithms for river systems, suitable objective functions for real-time control and the stability of the closed-loop system, and ways to apply the optimal control scenarios to a real river system. As a framework for this research the results from the work of Diehl *et al.* [26, 24, 25] and of Rawlings [49] can be taken.

- **Mixed Integer Optimization:** In this thesis we have assumed that the control function $u(t)$ can be chosen form a continuous set of values. This assumption may be acceptable if u is the water discharge at the output of a turbine. But in the case when the water level in the reservoir is too high not only turbines, but also the upper and the lower tunnels would be used to let out water from the reservoir in order to decrease its water level for safety. The problem is that for the upper and lower tunnels of the reservoir there are only two standing positions, namely opening and closing. This leads to a mixed integer dynamic optimization problem that should be addressed by tailored solution techniques (see e.g. Lee *et al.* [40], Rehbock *et al.* [50], and Stein *et al.* [58]).

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