Flood Discharge Estimation for Complex River Geometries by Inverse Numerical Modelling

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Abstract

A new approach to estimate flood discharges in complex river geometries is presented. Discharges are here determined through the combination of non-intrusive measurements of surface velocities and water levels with an inverse numerical model. This inverse numerical model consists of an inverse problem formulation, coupled with a Computational-Fluid-Dynamics (CFD) model. The CFD-model provides the connection between the flow field in the river section, where measurements are available, and the inflow of the modelled section, where the discharge is defined as boundary condition. Both a 2D CFD-model that computes a vertical section, or a full 3D CFD-model, were used. Both CFD-models solved the Reynolds averaged Navier-Stokes equations and applied the k-ε turbulence model for closure. The free surface was calculated with the Volume-of-Fluid method for the 3D computations and with an adaptive grid approach for the 2D computations. The inverse method uses the Levenberg-Marquardt minimizing algorithm to adjust the flow field to the measurements, by altering the discharge and eventually its distribution.

The inverse numerical model was applied to two different case-studies. One test-case was a straight rectangular channel with two sills allowing for computations with the 2D CFD-model, whereas the other case required a full 3D CFD-model because of a 90° bend in its geometry. For both cases, laboratory measurements were available for flood situations with Froude numbers $Fr \geq 0.89$ to verify the CFD-models. The forward results of both case-studies showed acceptable agreement between the computed free-surface flow and the measurements (i.e., the average relative error in water depths was between 6 and 11% for the 2D-computations, and 6.2% for the 3D-computations). The CFD-models used were able to capture complex flows with separation zones. A sensitivity analysis was performed for different roughness values. However, the influence of different realistic roughness values on water level and surface velocity was negligible in the cases analyzed.

The inverse method was validated regarding uniqueness and stability using synthetically generated series-of-measurements. The discharge could be estimated uniquely, if the inflow velocity distribution and the river bed geometry were assumed to be known. One measurement was enough to predict the discharge with a high accuracy (i.e., within 2% for both case-studies), when no error in water level and surface velocity data was assumed. The sensitivity of water level data to discharge changes was small in the entire computed river section for both case-studies. It was even smaller for higher discharges. Therefore, the estimation of flood discharge should be combined with velocity data and not only be based on stage measurements.
The influence of random errors on the estimated discharge was reduced by increasing the number of measurement points. However, the improvement of the reliability of the discharge was small for more than 10 measurements in the two presented cases. The proposed non-intrusive Particle-Tracking-Velocity (PTV) technique provides water level and surface velocity data of several particles and is therefore particularly suited for the estimation of discharge.

The stability of the proposed method to estimate discharge depended considerably on the measurement location in the river section. The discharge estimation was more stable, when measurements were taken at locations where the sensitivity of the measurements to discharge changes was higher. By optimizing measurement locations, the relative discharge error was around 1.5 times the magnitude of the relative velocity data error. If the measurement locations were poorly selected, the relative discharge error exceeded the magnitude of the relative velocity error 4-6 fold in the 2D computations. River sections with complex flow fields may feature particularly sensitive locations, which can be computed since complex flow fields can be captured with the presented CFD-models. The information on suitable measurement locations can be obtained a priori.
Zusammenfassung


An zwei verschiedenen Fallbeispielen wurde das inverse numerische Modell getestet. Zum einen wurde mit dem 2D Programm ein gerader Kanal mit zwei Schwellen berechnet, und zum anderen erforderte ein weiteres Fallbeispiel mit einer \( 90^\circ \)-Kurve in der Gerinnegeometrie ein 3D Modell. Für beide Fallbeispiele standen Labormessungen für Hochwassersituationen mit Froudezahlen \( Fr \geq 0.89 \) zur Verfügung, um die Strömungsmodelle zu verifizieren. Die Vorwärtsresultate von beiden Fallbeispielen zeigten akzeptable Übereinstimmungen zwischen der berechneten freien Wasseroberfläche und den Messungen (d.h. der durchschnittliche, relative Fehler der Wassertiefe war zwischen 6 und 11% innerhalb der 2D Berechnungen und 6.2% innerhalb der 3D Berechnungen). Demzufolge sind die verwendeten Programme in der Lage, komplexe Strömungsverhältnisse mit Ablösezonen zu berechnen.

Die inverse Problemformulierung wurde hinsichtlich Eindeutigkeit und Stabilität validiert, wobei synthetisch generierte Messdaten verwendet wurden. Der Durchfluss konnte eindeutig bestimmt werden, falls die Geschwindigkeitsverteilung am Zuströmrand und die Gerinnebettgeometrie als bekannt angenommen wurden. Bereits eine Messung war ausreichend, um den Durchfluss mit einer hohen Genauigkeit zu bestimmen (d.h. auf 2% genau in beiden Fallbeispielen), wenn fehlerfreie Daten der Oberflächenlage und -geschwindigkeit angenommen wurden. Die Sensitivität der
Oberflächenlage auf Durchflussveränderungen war im gesamten simulierten Flussabschnitt für beide Fallbeispiele gering. Eine Durchflussbestimmung bei Hochwasser sollte daher mit Geschwindigkeitsmessungen kombiniert werden und nicht nur auf Messungen der Oberflächenlage basieren.


Die Stabilität der vorgeschlagenen Methode zur Durchflussbestimmung hängt stark von den Messstandorten im Flussabschnitt ab. Die Durchflussbestimmung war stabiler bei Berücksichtigung von Standorten mit einer höheren Sensitivität der Messvariablen auf Durchflussveränderungen. Bei einer optimalen Auswahl der Messstandorte pflanzt sich ein relativer Fehler der Oberflächengeschwindigkeiten mit dem Faktor 1.5 auf die Größenordnung des relativen Durchflussfehlers fort. Im Fall ungünstig gewählter Messpunkte kann der relative Fehler der Durchflussfehler die Größenordnung des relativen Geschwindigkeitsfehlers innerhalb der 2D Berechnungen um den Faktor 4-6 übersteigen. Eventuell weisen komplexe Flussabschnitte besonders sensitive Messstandorte auf, welche dann aufgrund der nachgewiesenen Anwendbarkeit auf komplexe Strömungsgebiete ausgenutzt werden können. Mittels der vorgestellten Berechnungen können optimale Messstandorte a priori bestimmt werden.
1 Introduction

Discharge measurements of flood events provide the basis for many hydrologic tasks such as calculating the magnitude and return period of a design flood. Because of the importance of accurate discharge estimations, a new method is developed, which is especially designed for flood events. The state-of-the-art in discharge estimation as well as possible uncertainties derived from the commonly employed method are described in section 1.1. Section 1.2 presents the proposed method and states the research objectives of this work.

1.1 Discharge Estimation

1.1.1 State of the Art

The discharge $Q$ is commonly determined as the cross-sectional integral of the flow velocity, which can be written as the product of the water body’s cross-sectional area $F$ and the mean velocity $v_m$.

$$Q = \int v \, dF = v_m \cdot F. \quad (1-1)$$

The first velocity measurements were based on drifting objects by taking their time to pass a certain distance (Jasmund 1911). Only surface velocities can be measured in this approach. Those are different from the required cross-sectional mean. Further improvement of velocity measurement was obtained by using a submerged, vertical pole, where the torque induced by the stream velocity is measured. This technique allows the determination of the mean velocity in vertical direction. The velocity measurement by propeller-current-meters is today’s most widely spread velocity measuring technique and was developed by Woltmann in 1790 (Sigrist 1988). This measuring technique can obtain the velocity at arbitrary positions in the water body, which allows subdivision of the cross section into smaller sections each with a velocity measurement. These measurements can be integrated over the cross-section, which leads to a more accurate discharge estimation as a non-uniform velocity field in a cross-section can be taken into account. In Switzerland, a cross section is divided up into up to 25 lateral sections with 5 sections in depth (Landeshydrologie 1982). A disadvantage is that one discharge measurement is very time and labor intensive. Thus, the discharge measurements cannot be obtained in a continuous manner, nor at flood situations with a rapidly variable discharge and high velocities and drift, which can disturb the velocity measurement with propeller-current-meters or might even be dangerous. Some
propeller-current-meters were replaced by electromagnetic-current-meters, but the devices still have to be submerged in the water body. Ultrasonic velocity measurements are increasingly used nowadays as the velocity can be obtained continuously, but a stabilized river bed has to be guaranteed because a reflector on the opposite channel side has to be installed, which restricts the applicability. ADCP (Acoustic Doppler Current Profiler) is another interesting velocity measuring technique, which was first developed in 1981 by RD Instruments\(^1\) and was applied by, e.g., Derecki and Quinn (1987), or Gordon (1989). However, the ultrasonic as well as the ADCP measurements are installed in less than 10% of the 200 gauging station run by the Swiss National Hydrological and Geological Survey (SNHGS) in Switzerland (Sigrist 2001). Thus, current-meters are still in use at more than 80% of all gauging stations.

In practice, a stage-discharge curve is usually derived from the available discharge measurements to handle the problem of a limited number of discharge measurements. The stage-discharge curve represents the discharge as a function of reference water depth. Thus, the stage is measured and the discharge is deduced from the stage-discharge curve. Stage measurements are much easier to obtain and supply continuous gauging records by, e.g., float- or bubbler-type gauges. Radar and echo-sounder measurements allow determination of the stage non-intrusively, with radar measurements being increasingly applied (Sigrist 2001).

### 1.1.2 Resulting Problems

The stage-discharge curve is often based on calibration measurements in the low and intermediate flow regime only. For large flood events, the curve is extrapolated, leading to major uncertainties in the estimation of the corresponding flood discharge and any further hydrologic calculations based on it, such as the calculation of magnitude and return period of a design flood.

The following three examples show possible uncertainties in flood discharge determination using a stage-discharge curve. The first example illustrates the error propagation of an error in gauging records and the second example shows possible difficulties arising from the use of an extrapolated stage-discharge curve. The third example illustrates the error propagation of a systematic error in the stage-discharge relation into the estimated design flood.

#### Error in Gauging Records

Figure 1.1 displays two stage-discharge curves derived from the SNHGS for the Saltina River (left) and the Dischma stream (right)\(^2\). The range, where calibration measurements were made is also shown in both diagrams. The example depicted here corresponds to an event with a return period of approximately 20-years in both cases. A 5% stage error (referring to the water depth) leads to a discharge error of 11% (Saltina river) or 15% (Dischma stream).

\(^1\) [http://www.rdinstruments.com](http://www.rdinstruments.com)

\(^2\) All stage-discharge relations derived from the SNHGS can be found under: [http://www.bwg.admin.ch/service/hydrolog/d/hyddaten.html](http://www.bwg.admin.ch/service/hydrolog/d/hyddaten.html)
These results exemplify how stage measurements get less sensitive for larger discharges as the stage-discharge curve is concave, leading to a larger uncertainty in the determination of discharge. Similar results can be expected for almost all gauging stations, since the energy dissipation due to bed roughness decreases for an increasing water depth and the channel width usually widens, both effects leading to a concave stage-discharge curve. The problem of extrapolating this curve, especially when special hydraulic phenomena appear, is stated in the next section.

**Extrapolated stage-discharge curve**

The gauging station at the Saltina River near Brig was built in 1965 and operated until the flood event of September 1993. It consisted of two sills, which were 5 meters apart (see figure 1.2). The stage measurement was taken with a floating gauge between the two steps. The relation between the stage data and the discharge was determined from flow velocity measurements, with 12.2 m$^3$s$^{-1}$ as the highest measured discharge. For higher flood events the stage-discharge curve was extrapolated.
Figure 1.3 shows the stage-discharge curve for the corresponding gauging station from the SNHGS. The curve from hydraulic experiments in a downscaled model (VAW 1994a), and the curve under additional considerations of hydrological aspects (VAW 1994b) are also shown in figure 1.3. The range where flow velocity measurements were obtained for calibrating the stage-discharge curve can be found on the x-axis. The design floods for a 20- and a 100-years return period are also indicated.

The two curves obtained by the Laboratory of Hydraulics, Hydrology and Glaciology (VAW) deviate clearly from the stage-discharge curve derived from the SNHGS. Furthermore these two curves show a sharp bend in a discharge range between 15 to 35 m³ s⁻¹, where the stage decreases with increasing discharge.

This bend occurred because a hydraulic jump between the two sills developed. The hydraulic jump then shifted downstream with rising discharge while the stage increased again. Generally, for a given stage a smaller discharge is read out from the stage-discharge curve obtained by the SNHGS. This measurement setup is quite common because backwater from downstream of the sills is prevented and the river bed is stabilized. But it is suited only for moderate flows at the Saltina River, as the flow characteristics mentioned above could not be obtained by extrapolating the calibrated range of the stage-discharge curve. Today, the gauging station is situated further downstream after the original station was destroyed during the flood event in 1993.

Similar problems in estimating the stage-discharge curve appeared at the Emme-Emmenmatt gauging station (SIGRIST 1996), where the measurements were also taken between two sills and the flow changed from sub- to supercritical for larger discharges at the gauging station. As a result, larger flood events are now measured further upstream whereas smaller and moderate flows are still measured between the two sills.

**Error Propagation in Design Flood Estimation**

The following example shows the influence of a systematic error in the measured annual maximal discharges due to an incorrect extrapolation of the stage-discharge curve on the design flood. A series of measurements for 27 years is available for the Saltina river near Brig (from 1966 until 1992; VAW 1994b), where the measured annual maximal discharges were either left unchanged or a relative error of 20% was added or subtracted. A flood frequency analysis was performed with the following statistical distributions: Gumbel, Log-Normal, General-Extreme-Value (GEV), Log-Pearson and Frechet-EV2, as shown in figure 1.4 (PFAUNDLER 2000).
The results reveal that a systematic error of 20% leads to an error of the same magnitude in the design flood for an event with a 20-years return period. A design flood with a 20-years return period corresponds to an event with a 10-years return period with 20% higher discharge measurements, whereas it corresponds to an event with a 50-years return period for 20% smaller discharge measurements. For larger flood events, the selection of the statistical distribution can have a much larger influence on the design flood than this measurement error.

The findings of these three examples indicate how the commonly used method to estimate the discharge based on a stage-discharge curve often fails in supplying reliable discharge estimations for flood events due to the following reasons:

- The stage is less sensitive to larger discharges, which leads to a larger uncertainty interval for larger discharges.
- Extrapolating a stage-discharge curve may lead to major uncertainties, especially when special hydraulic phenomena occur such as flow conditions changing from sub- to supercritical flow.
- The importance of reliable discharge estimation is also underlined by a Flood Frequency Analysis.

Uncertainties, which have not been mentioned in any of the examples above, but which may also lead to an inaccurate estimation of discharges, arise from not considering sediment transport resulting in an unknown river bed and its roughness. Another uncertainty in the estimation of the discharge may occur due to the hysteresis of the stage-discharge curve, i.e. the curve is not equal for a rising and for a falling water level.

The next section describes a new approach for estimating the discharge, which is subject of this study.
1.2 A new Approach for Discharge Estimation

1.2.1 Motivation

Section 1.1.2 has outlined why stage measurements are often not sufficient to estimate reliable discharges at flood events. Spreafico (1988) already mentioned that future research in hydro-metry should focus on developing more precise discharge estimation especially for flood events. He also proposed to measure velocities during flood events to derive a more reliable stage-discharge curve for larger discharges.

Making use of the rapid development in digital data acquisition and computer resources, a new technique is proposed for a more reliable discharge estimation.

1.2.2 Approach

Measurements

Non-intrusive measuring techniques should be used during flood events, because high velocities and turbulence as well as possible drift and sediment transport may damage submerged instruments.

Particle Tracking Velocimetry (PTV), an image processing method based on stereo video recordings, is a non-intrusive measuring technique. This measuring technique has already been investigated by, e.g., Maas (1992), Virant (1996) and Stürer (1999) who derived velocity fields in an entire 3D water body by using particles with the same density as water. Skripalle (1996) used the PTV technique to derive surface velocities for open channel flow by using drifts or air bubbles, a concept similar to the early velocity measurement (see section 1.1.1). Siedschlag (1998) combined the PTV measuring technique derived by Skripalle with a 2D CFD-model (Kolling 1994, see following section) to predict the discharge. Such an installation can be found at the sluice in Berlin-Mühldamm, which provides continuous discharge values.

In this work, measurements were assumed to be derived by the PTV technique as it has the advantage to measure a large number of velocity values, which can be used in a regressive way to damp out the influence of, e.g., local turbulent variations.

Inverse Numerical Model

A CFD-model provides the connection between the flow field that corresponds to the PTV measurements and the inflow to the section modelled. Thus, the flow field can be adjusted to the measurements by altering the discharge, defined at the inflow boundary. The procedure to minimize the deviations between measurements and corresponding computations by varying the discharge
1.2. A new approach for discharge estimation

is automatized by an inverse method. The best discharge value is obtained, when these deviations are minimal.

CFD-simulations are increasingly important in river hydraulics, with computer resources being no longer a limiting factor. 3D effects through turbulence and varying roughness are often not negligible in natural rivers at flood events, not even in straight river sections. The literature relating to 3D computation in natural rivers is accordingly diverse: SINHA ET AL. (1998) presented 3D computation in a natural river by using the k-ε turbulence model, but captured the free surface by measurements and did not compute its position. OLSEN (1996), WU ET AL. (1998) and GESSLER ET AL. (1999) computed 3D flow combined with a sediment transport model in a natural river. The idea of using CFD-models to predict more accurately the stage-discharge curve for larger flood events was mentioned by, e.g., HERMANN ET AL. (1996). VISCHER (1997) suggested the combination of PTV measurements and 3D computations for the estimation of more accurate flood discharges.

Kölling (KÖLLING 1994, KÖLLING AND VALENTIN 1995) developed a numerical model to estimate the discharge in sewers and open channels based on velocity measurements. This method considers a 2D cross section and is therefore limited to flows with negligible velocity gradients in the flow direction. The method also does not use an inverse formulation, instead a factor to calculate the mean velocity from the measured velocity at a given stage is deduced from the velocity distribution in the cross section where the measurement is taken. The method can be combined with ultrasonic or PTV measurements. It has already been successfully applied.

Inverse formulations are used for a wide range of applications, such as geophysics, hydrology and several optimization/control tasks (e.g., in process engineering). YEH (1986) gave a review of typical inverse solution techniques in geophysics. Yet the literature related to identification and estimation of parameters for open-channel flow is sparse. RAMESH ET AL. (2000) estimated the roughness in open-channel flow with an inverse problem formulation, using a 1D depth averaged CFD-model.

The inverse numerical model in this work combines the inverse formulation with a 3D CFD-model to carry out the objectives described in the following section.

1.2.3 Research Objectives

The goal of this research is to develop an inverse numerical model to estimate flood discharges using water level and surface velocity measurement data derived from PTV measurements. Thus, the following tasks are carried out to evaluate the feasibility of this method to estimate the discharge:

- Verifying the CFD-model for complex flow fields in rivers during flood situations. The necessity of using 3D models must be investigated, and suitable models have to be chosen for treating turbulence and the free water surface.
- Developing an inverse modelling tool to estimate the discharge from measurements. The cho-
The regression algorithm has the goal to estimate the discharge in a way that measurements are reproduced best by the computations.

- Evaluating uniqueness and stability for the discharge estimation, if measurements are only available at the water surface. Test runs have the goal to evaluate whether these measurements are sufficient to estimate the discharge uniquely and how robust the discharge estimation is concerning a data error.
- Providing recommendations for the measuring set-up. An a priori estimation can give information on the optimal positioning of cameras and the required number of particles.

Basically, this work has to show the feasibility and the limits of the inverse numerical method to better estimate the discharge in flood events without using a stage-discharge relationship. This alternative method could be applied in rivers with complex, non-uniform flow fields during flood events.
2 Hydrodynamic Equations

All physical relations which are needed in this work are stated briefly in this chapter. While sections 2.1 and 2.2 describe the Continuity resp. Reynolds Averaged Navier-Stokes equations, section 2.3 states the k-ε model used here as turbulence closure. The corresponding literature can be found in any fluid-dynamics textbook, e.g., SCHLICHTING (1965), LAMB (1993).

2.1 Continuity Equation

The continuity equation expresses the conservation of mass. By equating the mass entering and leaving an elemental volume, the non-steady flow of a compressible fluid is governed by,

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0,
\]

where \( \rho \) is the mass density and \( t \) represents the time, \( \mathbf{u} \) is the velocity vector. For an incompressible fluid, \( \rho = \text{constant} \), the continuity equation is reduced to,

\[
\nabla \cdot \mathbf{u} = 0.
\]

2.2 Reynolds Averaged Navier-Stokes Equations

The Navier-Stokes equations describe the conservation of momentum. For the purpose of this work we can limit the attention to isothermal flows of incompressible, Newtonian fluids.

Conservation of momentum is expressed as,

\[
\rho \frac{d \mathbf{u}}{dt} + \rho \mathbf{v} \cdot \mathbf{u} = -\nabla \rho + \rho \mathbf{g} + \nabla \tau,
\]

where \( t \) is the time, \( \rho \) is the pressure, and \( \mathbf{g} \) is the acceleration due to gravity. The viscous stresses \( \tau \) in
are expressed in terms of the fluid deformation rate as

\[ \tau_{ij} = \mu_e \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \]  

(2-5)

for a Newtonian fluid, with \( \mu_e \) the molecular viscosity.

Using (2-3) and (2-5) as well as the continuity equation (2-2) for incompressible fluids, the Navier-Stokes equations assuming constant viscosity are,

\[ \rho \frac{\partial \hat{\mathbf{u}}}{\partial t} + \rho \nabla \cdot \hat{\mathbf{u}} = -\nabla P + \rho \hat{\mathbf{g}} + \mu_e \Delta \hat{\mathbf{u}}. \]  

(2-6)

The Navier-Stokes equations can be used for both laminar and turbulent flows, as they describe all the details of turbulent motion (Rodi 1980). But Direct Numerical Simulation (DNS) is today still restricted to simple geometries and low Reynolds numbers, because all vortex structures have to be resolved, and the discretization requirements for high Reynolds number flows become excessive. In engineering applications usually only the mean flow is of relevance, whereas the turbulent fluctuations are of secondary interest. This is taken into account by statistically averaging the turbulent flow, leading to the Reynolds Averaged Navier-Stokes (RANS) equations.

All physical values \( \phi \) are split in an average value \( \Phi \) and a fluctuation term \( \phi' \) in a time interval \( T \),

\[ \phi(x, y, z, t) = \Phi(x, y, z, t) + \phi(x, y, z, t). \]  

(2-7)

With

\[ \Phi(x, y, z, t_t) = \frac{1}{T} \int_{t_t - T/2}^{t_t + T/2} \phi(x, y, z, t) \]  

(2-8)

and

\[ \frac{1}{T} \int_{t_t - T/2}^{t_t + T/2} \phi(x, y, z, t) = 0. \]  

(2-9)

The Reynolds Averaged Navier-Stokes (RANS) equations are then given by,

\[ \rho \frac{\partial \hat{\mathbf{u}}}{\partial t} + \rho \nabla \cdot \hat{\mathbf{u}} = -\nabla P + \rho \hat{\mathbf{g}} + \mu_e \Delta \hat{\mathbf{u}}. \]  

(2-10)

They have the same form as the original Navier-Stokes equations (2-6). The difference is that additional stresses (Reynolds stresses) appear, representing the exchange of momentum between fluid elements by turbulent motion. Because of the additional stresses the RANS equations can
only be solved with an additional turbulence model to close the system. The standard $k$-$\varepsilon$ turbulence model, which was used in this work, is described in the following section.

### 2.3 Standard $k$-$\varepsilon$ Model

The turbulence was modelled with the standard $k$-$\varepsilon$ model, as it is the most commonly used model in engineering tasks and it has been extensively tested.

This model is based on the eddy viscosity concept of Boussinesq, which sets the Reynolds stresses proportional to the velocity gradients (e.g., Rodi 1980),

$$-u'_i u'_j = \nu (\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}) - \frac{2}{3} \kappa \delta_{ij},$$  \hspace{1cm} (2-11)

with $U_i$ the Reynolds-averaged velocities in the spatial directions, $\delta$ the Kronecker Delta\(^1\) and $\nu$ the eddy viscosity, which can be set proportional to a velocity scale $\hat{V}$ and a length scale $L$ (Prandtl 1945),

$$\nu \propto \hat{V}L. \hspace{1cm} (2-12)$$

The $k$-$\varepsilon$ model uses the kinetic turbulent energy $k$ to describe the velocity scale $\hat{V}$ and the dissipation rate $\epsilon$ to describe the length scale $L$. The dissipation rate $\epsilon$ is the (dissipated) kinetic energy $k$ which is transformed into inner energy (heat) per unit time and mass. The following relations define the velocity scale $\hat{V}$ and the length scale $L$ (Prandtl 1945),

$$\hat{V} = \sqrt{k}, \hspace{1cm} (2-13)$$

$$L = c_\mu \frac{k^{3/2}}{\epsilon} \text{ with the proportionality constant } c_\mu. \hspace{1cm} (2-14)$$

The eddy viscosity $\nu$ is then defined by the relations (2-12), (2-13) and (2-14),

$$\nu = c_\mu \frac{k^2}{\epsilon}. \hspace{1cm} (2-15)$$

The transport equations for $k$ and $\varepsilon$ can be derived from the momentum equations under consideration of the eddy viscosity concept and additional model assumptions. For incompressible fluids the equations are (Lauder and Spalding 1974),

$$\frac{\partial k}{\partial t} + U_i \frac{\partial k}{\partial x_i} + U_j \frac{\partial k}{\partial x_j} + U_j \frac{\partial k}{\partial x_j} = \nu \left( \frac{\partial^2 k}{\partial x_1^2} + \frac{\partial^2 k}{\partial x_2^2} + \frac{\partial^2 k}{\partial x_3^2} \right) + \frac{\nu}{\kappa} - \epsilon \hspace{1cm} (2-16)$$

\(^1\) $\delta_{ij} = 1$ for $i = j$, and $\delta_{ij} = 0$ for $i \neq j$
\[
\frac{\partial e}{\partial t} + U_1 \frac{\partial e}{\partial x_1} + U_2 \frac{\partial e}{\partial x_2} + U_3 \frac{\partial e}{\partial x_3} = \frac{\nu}{\epsilon} \left( \frac{\partial^2 e}{\partial x_1^2} + \frac{\partial^2 e}{\partial x_2^2} + \frac{\partial^2 e}{\partial x_3^2} \right) + c_{1e} \epsilon \frac{\epsilon}{k} \cdot P_k - c_{2e} \epsilon^2 \frac{\epsilon^2}{k} \quad (2-17)
\]

with the production term \( P_k \)

\[
P_k = \sum_{i=1}^{3} \left[ \sum_{j=1}^{3} \left( \nu \left( \frac{\partial U_j}{\partial x_i} + \frac{\partial U_i}{\partial x_j} \right) \frac{\partial U_j}{\partial x_j} \right) \right]. \quad (2-18)
\]

The model can be closed with the following constants (Rodi 1980),

\[
c_\mu = 0.09, \quad \sigma_k = 1.0, \quad \sigma_e = 1.3, \quad c_{1e} = 1.44, \quad c_{2e} = 1.92. \quad (2-19)
\]

When modelling with the \( k-e \) model, deficits can appear for complex velocity fields, large anisotropy of the turbulence and special effects such as rotation etc., which cannot be considered within the eddy viscosity concept (Rodi 1998).
Chapter 3: CFD-Modelling

After selecting the mathematical model, one has to choose a suitable discretization method, i.e., a method of approximating the differential equations by a system of algebraic equations for the variables at some set of discrete locations in space and time. The Finite Element (FE) method was used for the 2D computations and the Finite Volume (FV) method for the 3D computations in this work. Section 3.1 gives a short description of the Finite Element method and section 3.2 depicts the Finite Volume method. The treatment of the free surface is described in section 3.3, and the boundary conditions used here are discussed in section 3.4.

3.1 Finite Element (FE) Method

3.1.1 Principle

This section describes the principle of the finite element method, as used in the 2D computations in this work. A more general description of the method is given in Taylor and Hughes (1981), or Zienkiewicz and Taylor (1989, 1991).

The solution domain in the finite element method is divided into a grid of elements, where the elements are composed of patterns of grid points (nodes). The variables and parameters of each differential equation are interpolated within the element by a polynomial \( N \), called shape function, where the shape function \( N_p \) for a certain node \( P \) is 1 at node \( P \) and 0 at all other nodes. The number of nodes of each elements is a function of its dimensionality, geometry and of the order of the shape function. I.e., a rectangular element has four nodes when using bilinear shape function, accordingly eight nodes are required when choosing a quadratic variation of the variable (see figure 3.1). In this work isoparametric bilinear or quadratic elements are used. The term isoparametric implies that both the element geometry and the variation in the variable across the element are described using the same type of shape function. Each variable \( \phi \) is then approximated by its discrete values \( \hat{\phi}_i \) at each node \( i \),

\[
\phi = \sum_{i=1}^{n} N_i \hat{\phi}_i.
\]  

Fig. 3.1 Unit element in local coordinate system.

-13-
where $N_j$ is the shape function for the variable $\phi_j$ at one of the $n$ discretization points $i$ in an element. A differentiated variable is discretized in the same way,

$$
\frac{\partial \phi}{\partial x} = \sum_{i=1}^{n} \frac{\partial N_j}{\partial x} \phi_i.
$$

(3-2)

An arbitrary Partial Differential Equation (PDE), $F(\phi) = 0$, is substituted by its discrete system $F(\phi) = 0$ by utilizing the approaches (3-1) and (3-2) for all variables at each node in the domain. The exact solution cannot be obtained with this discrete system, resulting in an error $\varepsilon = F(\phi) - F(\phi) = F(\phi)$.

The weighted residual method requires that the error $\varepsilon$, weighted with a weighting function $W_j$, $(j=1, \text{number of unknown variables in the entire system of equations})$ vanishes when integrating it over the entire domain $\Omega$.

$$
\int_\Omega W_j \varepsilon \, d\Omega = \int_\Omega W_j F(\phi) \, d\Omega = 0.
$$

(3-3)

The weighting function $W_j$ in equation (3-3) is chosen according to the standard Galerkin method, i.e. the weighting functions are set equal to the shape functions. By employing (3-1) and (3-2), equation (3-3) is written as,

$$
\int_\Omega N_j \left[ F \left( \sum_{i=1}^{n} N_j \phi_i \sum_{i=1}^{n} \frac{\partial N_j}{\partial x} \phi_i \ldots \right) \right] d\Omega.
$$

(3-4)

$F$ is any first order partial differential equation. Green’s formula is applied in the case of a second order partial differential equation (e.g., Bronstein, 1989),

$$
\int_\Omega \sum_{k=1}^{n} \frac{\partial^2 \phi}{\partial x_k^2} d\Omega \gamma n \left[ \sum_{i=1}^{n} \frac{\partial N_j}{\partial x_k} \phi_i \right] d\Omega = \int_{\Gamma} \sum_{k=1}^{n} \frac{\partial N_j}{\partial x_k} \phi_i d\Gamma - \int_{\Gamma} \sum_{k=1}^{n} \frac{\partial N_j}{\partial x_k} \phi_i d\Gamma
$$

(3-5)

with $\Gamma$ the boundary area of the domain $\Omega$. $\hat{n}$ is the normal direction out of the domain $\Omega$.

The numerical integration of function $F$ over a 2D element can be approximated by Gauss-Legendre quadrature. The integration points (Gauss points) lie within the element. The values of the integrated variables are calculated with the local coordinates of these Gauss points and weighted with the values $a_i$, $a_j$. In this work three Gauss points ($m=3$) were used.

Order of 3x3 Gauss point | Position and weighting factors of the Gaussian points
---|---
m | $i,j$ | $a_i,a_j$ | $\xi_i,\eta_i$
1 | 1,1 | 2 | 0
2 | 1,1 | -1/\sqrt{3}
2 | 2,1 | 1/\sqrt{3}
3 | 1,3 | 5/9 | -\sqrt{6}
3 | 2,3 | 5/9 | \sqrt{6}
3 | 3,3 | 0 | 0

Fig. 3.2 Gauss sampling points in a 2D unit element.
3.1. Finite Element (FE) Method

in each dimension (see figure 3.2). The integrated value $I$ over a 2D unit element is,

$$I = \sum_{i=1}^{m} \sum_{j=1}^{m} a_i \cdot a_j \cdot |J| \cdot F(\dot{\phi}),$$  \hspace{1cm} (3-6)

with $|J|$ the element area calculated from the determinant of the Jacobian matrix.

The unit element has to be transformed to global coordinates to build the equation system over the entire domain (figure 3.3). In the CFD-code FEMTOOL, which was used for the 2D computations (see section 3.5.1), quadrilateral unit elements are transformed into trilateral elements by letting two corner nodes coincide.

The contributions to common nodes of adjacent elements are assembled and a global element matrix $A$ with the dimension $I \times J$ ( $I=$ number of unknown variables in the entire domain) results,

$$
\begin{bmatrix}
A_{11} & \cdots & A_{1J} \\
\cdots & \cdots & \cdots \\
A_{IJ} & \cdots & A_{JJ}
\end{bmatrix}
\begin{bmatrix}
\phi_1 \\
\vdots \\
\phi_J
\end{bmatrix}
= 
\begin{bmatrix}
f_1 \\
\vdots \\
f_J
\end{bmatrix}
$$

(3-7)

Each line in the element matrix represents an equation for one discretized variable $\dot{\phi}_j$. The matrix is banded, sparse and non-symmetrical.

3.1.2 Temporal Discretization

The time-dependent equations must be discretized in both space and time. Temporal discretization involves the integration of every term in the differential equations over a time step $\Delta t$. Different approaches are available for time discretization. The method used for the 2D computations was the approximation by finite elements, similarly to the space discretization. With this finite element formulation for both space and time, the dimensionality is increased by one. Assuming a linear interpolation, only the previous $t-\Delta t$ and the actual time $t$ need to be considered (figure 3.4).

The time shape functions are completely independent of the space shape functions.
3.1.3 Continuity, RANS and \( k, \varepsilon \) Equations

In this section all governing finite element equations for the turbulent flow are written in the standard Galerkin formulation. The non-linear terms in the RANS, \( k \) and \( \varepsilon \) equations have to be linearized. The Picard iteration, Newton and quasi-Newton methods are the most frequently used methods for linearization. Cuvelier et al. (1986) give an overview of these methods. In this work, the Picard iteration is used to linearize the PDEs. The values taken from the last iteration step have been marked with a tilde: \( \tilde{\phi} \). The second-order derivatives of the diffusion terms in the RANS, \( k \)- and \( \varepsilon \)-equations have been treated by the Green formula (see equation 3-5).

**Continuity Equation**

with \( k = 1, 2, 3 \) for x-, y-, z-direction:

\[
\int_{\Omega} N_c \left( \sum_{k=1}^{n_{dim}} \sum_{i=1}^{n_u} \frac{\partial N^i_{nk}}{\partial x_k} U_{nk} \right) \, d\Omega = 0. \tag{3-8}
\]

**RANS Equations**

with \( h = 1, 2, 3 \) for x-, y-, z-momentum equations:

\[
\int_{\Omega} \left\{ \sum_{i=1}^{n_u} \sum_{k=1}^{n_{dim}} \frac{\partial N^i_{nk}}{\partial t} U_{nk} \right\} + \sum_{k=1}^{n_{dim}} \sum_{i=1}^{n_u} \left( N^i_{nk} \tilde{U}_{nk} \right) \sum_{i=1}^{n_u} \left( \frac{\partial N^i_{nk}}{\partial x_k} U_{nk} \right) + \sum_{i=1}^{n_u} \left( \frac{\partial N^i_{nk}}{\partial x_k} \right) P \right\} \, d\Omega \\
+ \sum_{i=1}^{n_u} \left( \frac{\partial N^i_{nk}}{\partial x_k} \right) \left( \frac{\partial N^i_{nk}}{\partial x_k} \right) \right\} \, d\Omega \\
- \int_{\Gamma} \sum_{i=1}^{n_u} \left( \frac{\partial N^i_{nk}}{\partial n} U_{nk} \right) \, d\Gamma = 0. \tag{3-9}
\]

The weighting function of the continuity equation \( N_c \) and the RANS equations \( N^m \), as well as the shape functions for the variables \( N^{\mu_1}, N^{\mu_2}, N^{\mu_3}, N^p \) and the number of element nodes \( n^{\mu_1}, n^{\mu_2}, n^{\mu_3} \) and \( n^p \) of the variables in the \( n^p \) elements are formulated generally in the equations (3-8) and (3-9). The Galerkin method stipulates: \( N_c = N^2 \) and \( N = N^{\mu_1} = N^{\mu_2} = N^{\mu_3} \). The shape functions of the three velocity components have to be of the same order \( (n^{\mu_1} = n^{\mu_2} = n^{\mu_3}) \).

The turbulent kinetic energy \( k \) appears as constant in (3-9), because of the decoupled determination of the turbulence variables (see equations 3-10 and 3-11). The distribution of \( k \) in an element
is also described with a shape function $N^k$.

The problem of pressure not appearing in the continuity equation can be faced with several methods. A common method applies a shape function for the pressure of one order lower than for the velocities (Cuvelier et al. 1986) to fulfill the Babuska-Brezzi criteria (Brezzi 1974). In this work, a linear shape function was chosen for the pressure and a quadratic one for the velocities, if the standard Galerkin method was applied. Correspondingly, a linear weighting function was chosen for the continuity equation and a quadratic one for the RANS equations.

Equations for Turbulence Variables $k$, $\varepsilon$

A modified version of the $k$-$\varepsilon$ turbulence model, the $q$-$r$ turbulence model according to Finnie and Jeppson (1991), was chosen for solving the turbulence model equations (2-16), (2-17). The $q$-$r$ model is derived from the $k$-$\varepsilon$ model through a variable substitution $q^2 = k$ and $r^2 = \varepsilon$, whereby the empirical parameters in equation (2-19) and the assumptions made are equal in both models. The advantage of the variable substitution is, avoiding negative values and having smaller intervals for $q$ and $r$, which improves the convergence behavior (Finnie 1994). The computations of the partial differential equations of $q$ and $r$ are decoupled from the continuity and RANS equations.

The turbulence model equations, written in the standard Galerkin method, are,

$$\int_{\Omega} \left( \frac{n^e}{\sigma_k} \sum_{k=1}^{n^q} \left( \sum_{j=1}^{n^q} \frac{\partial N^q_j q_i}{\partial x_k} \left( \sum_{i=1}^{n^u} \tilde{U}_i \sum_{j=1}^{n^q} N^q_j q_i \right) \right) \right) \, d\Omega = - \frac{2 c_{e_k}}{\sigma_k} \sum_{k=1}^{n} \left( \sum_{i=1}^{n^q} \frac{\partial N^q_i}{\partial x_k} \left( \sum_{i=1}^{n^q} N^q_i q_i \right) \right) \left( \sum_{j=1}^{n^q} \frac{\partial N^q_j q_i}{\partial x_k} \right) \right) \left\{ \sum_{i=1}^{n^q} N^q_i q_i \right\} \, d\Omega$$

$$\int_{\Gamma} \left( \frac{n^q}{\sigma_k} \sum_{i=1}^{n^q} \left( \sum_{j=1}^{n^q} \frac{\partial N^q_j q_i}{\partial n} \right) \right) \left( \sum_{j=1}^{n^q} N^q_j r_i \right) \, d\Gamma = 0$$

\[ (3-10) \]
\[ \int_{\Omega} N_j^f \rho \left( \sum_{i=1}^{n_x} N_j^i \frac{\partial N_j^i}{\partial t} + \sum_{k=1}^{n_x} \frac{\partial N_j^i}{\partial \mathbf{x}_k} \right) \, d\Omega \]

\[ -N_j^f c_{1t} \left( \sum_{i=1}^{n_x} N_j^i \hat{q}_i \right) \left( \sum_{i=1}^{n_x} \frac{\partial N_j^i}{\partial \mathbf{x}_k} \right) \left( \sum_{i=1}^{n_x} N_j^i \hat{q}_i \right) \]

\[ + \frac{2 c_{2t}}{\sigma_v} \sum_{k=1}^{\nu \Delta t} \left( \sum_{i=1}^{n_x} N_j^i \hat{q}_i \right) \left( \sum_{i=1}^{n_x} \frac{\partial N_j^i}{\partial \mathbf{x}_k} \right) \left( \sum_{i=1}^{n_x} N_j^i \hat{q}_i \right) \, d\Omega \]

\[ - \int_{\Gamma} N_j^f \left[ \frac{2 c_{2t}}{\sigma_v} \left( \sum_{i=1}^{n_x} N_j^i \hat{q}_i \right) \left( \sum_{i=1}^{n_x} \frac{\partial N_j^i}{\partial n} \hat{r}_i \right) \right] d\Gamma = 0 \]

where \( P^a \) is the production rate of turbulent kinetic energy (see also equation (2-18),

\[ P^a = \frac{1}{\nu} \sum_{i=1}^{3} \sum_{j=1}^{3} \left[ v_i \left( \frac{\partial U_j}{\partial x_i} + \frac{\partial U_i}{\partial x_j} \right) \frac{\partial U_j}{\partial x_j} \right] \]

which is calculated with the velocities of the last iteration/time step. The eddy viscosity \( \nu_t \), defined with the variables \( q \) and \( r \) is,

\[ \nu_t = \frac{c_t q^4}{r} \]

The empirical constants for the turbulence model, \( c_{1t}, c_{2t}, \sigma_v, \sigma_k, \sigma_e \) are specified in section 2.3, equation (2-19).

The weighting and shape functions of variables \( q \) and \( r \) are identical and are set equal to the order of the shape function for the velocities \( (N^{U1} = N^{U2} = N^{U3} = N^q = N^r) \). The number of discretization nodes is equal for all variables \( (n^{U1} = n^{U2} = n^{U3} = n^q = n^r) \).

### 3.1.4 Stabilization Techniques

It is well known that convective-diffusive transport equations are more difficult to solve numerically when convection dominates over diffusion. In this situation the Galerkin finite element solution usually exhibits numerical spatial oscillations. The numerical oscillations tend to be more severe as convection becomes more dominant. The ratio between convection (1. order terms) and diffusion (2. order terms) is characterized locally by the element Peclet Number \( Pe \),

\[ Pe = \frac{U h_e}{2 \nu} \]
3.1. Finite Element (FE) Method

Where $h_e$ is the characteristic element length, $U_i$ is the local velocity and $v = v_e + v_f$ is the sum of the kinematic and the eddy viscosity. Oscillations can occur for Peclet numbers $Pe > 1$ when using the Galerkin method.

Three different options are possible to prevent instabilities:

- A finer grid leads to smaller $Pe$-numbers, as the characteristic length $h_e$ gets smaller, but it leads to higher CPU times.
- A higher viscosity $v$ also reduces the Peclet-number, but it also changes the physical properties.
- The third possibility is to change the weighting function $W_j$ of the standard Galerkin method by adding an additional upwind weighting function $P$ (Zienkiewicz and Taylor 1991), which was used in this work:

Function $P$ can be defined by several approaches, which are described more generally in, e.g., Zienkiewicz and Taylor (1991). The Galerkin/Least-squares (GLS) method was used for the computations in this work (Hughes et al. 1989), where the weighting functions $W_j$ for the continuity, $W_j^C$, and RANS, $W_j^m$, equations are defined as,

$$W_j^C = N_j^C + \tau \left( \sum_{k=3}^{ndim} \frac{\partial N_k^C}{\partial x_k} \right)$$

$$W_j^m = N_j^m + \tau \left( \frac{\partial N_j^m}{\partial t} + \sum_{k=3}^{ndim} U_k \frac{\partial N_j^m}{\partial x_k} + \frac{1}{\rho} \sum_{k=3}^{ndim} \frac{\partial N_j^m}{\partial x_j} + \frac{\partial k}{\partial x_j} g_j \right)$$

The “upwind parameter” $\tau$ defines the weighting of the least-squares terms, which are added to the standard Galerkin formulation. It can be set to (Hughes et al. 1986a, Segal 1993),

$$\tau = \frac{\alpha h_e}{2|A_e|}$$

with

$$\alpha = \coth(Pe) - \frac{1}{Pe}$$

and $A_e$ the element area.

The GLS method has the advantage that it allows the same order of shape functions for the pressure and the velocities (Hughes et al. 1986b). Thus, only bilinear elements were used, which reduces the storage and the CPU-time. Applications of the GLS method and its mathematical proof of stability can be found in Hansbo and Szepessy (1990).
3.2 Finite Volume (FV) Method

3.2.1 Principle

In this section the principle of the FV method used in this work for the 3D computations is described. A more general description can be found in Ferziger and Peric (1999).

The solution domain is subdivided into a finite number of small control volumes (CV) by a grid which defines the control volume boundaries and not the computational nodes. In this work, the computational nodes were assigned to the centre of the CV. Figure 3.5 shows the notation used for the 3D case. The net flux through the CV boundary is the sum of integrals over the six CV faces,

\[
\int_{A} f dA = \sum_{k} \int_{A_k} f dA = \sum_{k} f_{k} A_{k},
\]  

(3-19)

where \( f \) is the component of the convective or diffusive flux and \( A_{k} \) is the surface area of cell face \( k \). There are a number of different discretization methods available for the finite volume approach. The difference is in how the values of \( \phi \) (velocity, concentration etc.) and its gradient normal to the cell face are interpolated from the cell mid points to obtain the convective and the diffusive fluxes at the mid point of a cell surface. Other schemes determine the values at the corner points too, for calculating the surface integral, but they are not discussed here. The theory can be found in, e.g., Ferziger and Peric (1999).

Some of the common methods for interpolating these values at the surfaces, are described briefly in the following with

\[
f = U \cdot A \cdot \phi + \Gamma \cdot A \frac{d\phi}{dx},
\]  

(3-20)

representing a convection-diffusion equation, where \( A \) is the surface area, \( U \) is the velocity normal to the surface, \( \Gamma \) is the turbulent diffusion coefficient at the surface and \( \phi \) is an arbitrary variable at the surface. \( \frac{d\phi}{dx} \) is the difference of \( \phi \) on each side of the surface, divided by the distance between the CV centers.

This equation (3-20) can be transformed to the following form to calculate the unknown variable value \( \phi_P \) in cell \( P \) (Ferziger and Peric 1999),

\[
\phi_P = \frac{\sum_{nb} a_{nb} \phi_{nb}}{a_P},
\]  

(3-21)
where the subscript \( \text{nb} \) refers to neighbor cells, and \( a_p \) and \( a_{\text{nb}} \) are the linearized coefficients for \( \phi_p \) and \( \phi_{\text{nb}} \), with \( a_p = \sum_{\text{nb}} a_{\text{nb}} \). These coefficients depend on the interpolation of the cell centered values to the values at the surfaces. The values \( \phi_{\text{nb}} \) might not be known either which is the implicit formulation. Then, the equations for each cell in the grid have to be solved simultaneously.

### First Order Upwind Scheme

In upwind schemes, the values of \( \phi \) on the cell surface are taken from the upstream cell. The first order method uses information in only one cell upstream of the cell surface. The value \( \phi_w \) on cell face \( w \) for example is equal to the value of cell \( W \), whereas value \( \phi_e \) is equal to the value of cell \( P \) if the main flow direction is from \( W \) to \( E \). The resulting fluxes and the coefficients for the above mentioned convection-diffusion equation (3-20) with a flow from \( T-N-W \) to \( B-S-E \) (see figure 3.5 for orientation) are,

\[
\begin{align*}
    f_w &= \frac{U_w A_w}{a_w} \phi_w + \frac{\Gamma_w A_w}{dx} (\phi_w - \phi_p) \\
    f_e &= \frac{U_e A_e}{a_p} \phi_p + \frac{\Gamma_e A_e}{dx} (\phi_p - \phi_e) \\
    f_n &= \frac{U_n A_n}{a_n} \phi_n + \frac{\Gamma_n A_n}{dy} (\phi_n - \phi_p) \\
    f_s &= \frac{U_s A_s}{a_p} \phi_p + \frac{\Gamma_s A_s}{dy} (\phi_p - \phi_s) \\
    f_t &= \frac{U_t A_t}{a_t} \phi_t + \frac{\Gamma_t A_t}{dz} (\phi_t - \phi_p) \\
    f_b &= \frac{U_b A_b}{a_p} \phi_p + \frac{\Gamma_b A_b}{dz} (\phi_p - \phi_b)
\end{align*}
\]  

(3-22)

### Second Order Upwind Scheme

The Second-Order-Upwind (SOU) scheme is based on a second-order accurate method to calculate the concentration on the cell surfaces. The SOU scheme uses the values in the neighboring cell (i.e. \( W \)) and also in one more cell further upstream (\( WW \)). The values are then extrapolated linearly from cell \( WW \) through cell \( W \) to the cell side \( w \) of control volume \( P \).

### QUICK Scheme

QUICK is an acronym for the Quadratic Upstream Scheme. Instead of using a straight line between cells \( W \) and \( WW \), a second order polynomial is used to fit a curve through points \( WW, W \) and \( P \).
3.2.2 Temporal Discretization

For the 3D computations, the time was discretized by a finite difference approach. When taking a generic expression for the time evolution of a variable $\phi$,

$$\frac{\partial \phi}{\partial t} = F(\phi),$$

(3-23)

where the function $F$ incorporates any spatial discretization, the first-order accurate temporal discretization is given by,

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = F(\phi).$$

(3-24)

And the second-order discretization is given by

$$\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\Delta t} = F(\phi),$$

(3-25)

where $\phi$ is a scalar quantity, $n$ is the current time level and $n+1/n-1$ is the next/previous time level.

Once the time derivative has been discretized, a choice remains for the evaluation of $F(\phi)$. I.e., at which time level the values $\phi$ should be used in evaluating $F$.

Implicit Time Integration

One method is to evaluate $F(\phi)$ at the future time level,

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = F(\phi^{n+1}).$$

(3-26)

The advantage of the fully implicit scheme is that it is unconditionally stable with respect to time step size.

Explicit Time Integration

This method evaluates $F(\phi)$ at the current time level,

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = F(\phi^n).$$

(3-27)

Here, the time step $\Delta t$ is restricted to the stability limit of the underlying solver (i.e., a time step corresponding to a Courant number $c = \frac{u\Delta t}{\Delta x}$ of smaller than 1).

3.2.3 Continuity and RANS Equations

The momentum and continuity equations were solved sequentially and pressure and velocity were both stored at the cell centers in this work. In this sequential procedure, the continuity equation was used as an equation for pressure. However, pressure does not appear explicitly for incom-
pressible flows. The SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) family of algorithms is used for introducing pressure into the continuity equation, which is described in the following (e.g., Olsen 1997). The main idea is to guess a value for the pressure and use the continuity defect to obtain an equation for the pressure-correction.

To derive the equations for the pressure-correction, the following notation is used. The initially calculated variables, which have not been corrected, are denoted with an index *. The correction of the variables is denoted with an index '. The variables after correction do not have an index,

\[ P = P^* + P', \quad (3-28) \]

\[ U_i = U_i^* + U_i', \quad (3-29) \]

where \( P \) is the pressure and \( U_i \) is the velocity with \( i = 1, 2, 3 \) for the spatial directions. Given guessed values for the pressure, the discretized version of the Navier-Stokes equations is,

\[ a_p U^*_p = \sum_{nb} a_{nb} U_{nb}^* + B - A \frac{\partial P^*}{\partial i}. \quad (3-30) \]

The linearized convective and diffusive terms have been discretized as described in section 3.2.1. The variable \( B \) contains the rest of the terms apart from the convective, the diffusive and the pressure term. The pressure term is given as \( A \frac{\partial P^*}{\partial i} \), with \( A \) the surface area of the CV normal to the pressure gradient. The pressure gradient can for example be evaluated as \( \frac{P_{i+1} - P_{i-1}}{2} \). The discretized version of the Navier-Stokes equations based on the corrected variables can be written as,

\[ a_p U_p = \sum_{nb} a_{nb} U_{nb} + B - A \frac{\partial P}{\partial i}. \quad (3-31) \]

If this equation is subtracted from equation (3-30), and the two equations (3-28) and (3-29) are used, the following equation emerges for the velocity correction,

\[ U'_p = \left( \frac{A}{a_p - \sum_{nb} a_{nb}} \frac{\partial P}{\partial i} \right)_p. \quad (3-32) \]

The SIMPLE method omits one term in the above equation and uses,

\[ U'_p = \left( \frac{A}{a_p} \frac{\partial P}{\partial i} \right)_p. \quad (3-33) \]

The above equation gives the velocity-corrections once the pressure-corrections are known. To obtain the pressure-corrections, the continuity equation is used,

\[ \sum_{nb} A_{i, nb} U'_{i, nb} = 0, \quad (3-34) \]
where equation (3-33) is inserted into equation (3-34). The result is an equation of the following form,

\[ a_P P' = \sum_{nb} a_{nb} P'_{nb} + b. \]  
(3-35)

The procedure is therefore:

1. Guess a pressure field, \( P^* \)
2. Calculate the velocity \( U^* \) by solving equation (3-30)
3. Solve equation (3-35) and obtain the pressure correction, \( P' \)
4. Correct the pressure by adding \( P' \) to \( P^* \)
5. Correct the velocities \( U^* \) with \( U' \) using equation (3-33)
6. Iterate from second point to convergence.

### 3.3 Free Water Surface

The position of the free surface is usually not known a priori and has to be determined for given boundary conditions, which requires a special treatment. The 2D computations were based on an adaptive grid approach where only the water phase was calculated (interface-tracking method), whereas the 3D computations were run on a rigid grid where the two phases water and air were considered (interface-capturing method). These two main categories in treating the free surface are explained in the following sections with focus on the methods used. A more detailed description can be found in, e.g., BÜRGISser (1999) for the interface-tracking methods or in HIRT AND NICOLS (1981) for the interface-capturing method.

#### 3.3.1 Interface-Tracking Method

The upper grid boundary is set equal to the position of the free surface for the interface-tracking method. Adaptive grids are therefore necessary to adjust the grid as the correct free surface is not known in advance or it changes in time. Boundary conditions have to be defined at the free water surface, where the following two conditions have to be fulfilled in steady-state:

- The pressure at the free water surface is equal to the atmospheric pressure \( (p = p_A) \)
- The normal component of the velocity vectors at the free water surface is equal to zero \( (U_n = 0) \)

By setting only one boundary condition, the other condition can be used to correct the free water surface. Thus, two possibilities emerge:
One possibility to adjust the grid is to set the boundary condition for the pressure ($p =$ atmospheric pressure) and correct the water surface with the normal components of the velocity vectors (see figure 3.6). This procedure of correcting the free water surface is called velocity-driven-grid-adaptation.

The other possibility is to define the tangential velocity vectors as boundary condition ($U_n = 0$) and correct the grid with the pressure deviations from the atmospheric pressure (see figure 3.7). This procedure is called pressure-driven-grid-adaptation.

The relaxation terms $\Delta C_u$ and $\Delta C_p$ are used to avoid oscillations of the solution. The calculated correction vector can either be in vertical direction or normal to the surface. If the surface is corrected in normal direction, the direction is calculated only with the upstream neighboring node in supercritical flow to increase the stability of the surface adjustment. A central scheme for the correction in normal-direction is appropriate for subcritical flow.

For transient computations it is necessary to distinguish between a stationary reference domain (*Eulerian description*) or a reference domain in motion (*Lagrangian, arbitrary Lagrangian-Eulerian (ALE) description*). The free surface can be determined in the same way as for the steady-state calculations, if Eulerian description is applied. If computing on a moving grid, the reference-domain velocity, $U_R$, has to be considered in the convective terms of the RANS equations (2-10), because these equations are stated in the Eulerian description. If the velocity of the reference domain is equal to the fluid velocity $U = U$ (*Lagrangian description*) the convective terms in equation (2-10) vanish. The ALE description allows the reference domain to move arbitrarily between a Eulerian or a Lagrangian description with the convective term in the RANS equation (2-10),

$$\rho (\vec{U} - \vec{U}_R) \cdot \nabla \vec{U}.$$ (3-36)

For further information on transient computations see Hughes et al. (1981), Bürgisser (1999), or Huerta & Liu (1988). All 2D computations were solved with the steady-state equations.

### 3.3.2 Interface-Capturing Method

The interface-capturing methods are applied on a fixed grid, which includes the water and air
phase. The shape of the free water surface is determined by cells which are partially filled by air and water. This is implemented by introducing either massless particles into the liquid phase near the free surface (e.g., Marker-and-Cell or MAC scheme, Harlow and Welch 1965), or a transport equation for the void fraction of the liquid phase (e.g., Volume-of-Fluid (VOF) scheme, Hirt and Nicols 1981). The VOF-scheme was used for the 3D computations and is explained in the following.

A transport equation for the void fraction \( c \) in addition to the conservation equations for mass and momentum is introduced and solved (e.g., \( c = 1 \) for CVs filled by water and \( c = 0 \) in CVs filled by air),

\[
\frac{\partial c}{\partial t} + \text{div}(c \mathbf{U}) = 0 . \tag{3-37}
\]

The critical issue in this type of method is the discretization of the convective term in equation (3-37). Low-order schemes (like first-order upwind) smear the interface and introduce artificial mixing of the two fluids, so higher-order schemes are preferred. Since \( c \) must satisfy the condition \( 0 \leq c \leq 1 \), one has to ensure that the method generates no overshoot or undershoot.

The interpolation near the interface can be treated by several schemes. In this work an implicit scheme was used for the steady-state computations and the more sophisticated geometric reconstruction scheme was applied to transient computations.

In the implicit interpolation method, a standard finite-difference interpolation scheme is used to obtain the face fluxes for all cells, including those near the surface,

\[
\frac{c^{n+1} - c^n}{\Delta t} V + \Delta t(U_f^{n+1} c_f^{n+1}) = 0 , \tag{3-38}
\]

with \( V \) the volume, \( U_f \) the volume flux through the face \( f \) and \( c_f \) the face value of the volume fraction, computed from the second-order upwind scheme.

The geometric reconstruction scheme assumes that the interface between two fluids has a linear slope within each cell, and uses this linear shape for calculation of the advection of fluid through the cell faces. The first step in this reconstruction scheme is calculating the position of the linear interface relative to the center of each partially-filled cell, based on the information about the volume fraction and its derivatives in the cell. The second step is calculating the advected amount of fluid through each face using the computed linear interface representation and information about the normal and tangential velocity distributions on the face. The third step is calculating the volume fraction in each cell using the balance of fluxes calculated during the previous step. A standard interpolation scheme is used to obtain the face fluxes, whenever a cell is completely filled with one phase or another (FLUENT 1998).

There are several variants of the VOF-approach. In the original VOF-method (Hirt and Nicols 1981), equation (3-37) is solved in the whole domain to find the location of the free surface. The
mass and momentum conservation equations are then solved for the liquid phase only. The method can calculate flows with overturning free surfaces, but the gas enclosed by the liquid phase will not feel buoyancy effects and will therefore behave in an unrealistic manner. The method used here (which is implemented in FLUENT) treats both fluids as a single fluid whose physical properties appearing in the transport equations are determined by the presence of the component phases in each control volume. If the phases are represented by the subscripts 1 and 2, the density in each cell is given by

\[ \rho = c \rho_1 + (1 - c) \rho_2. \]  

(3-39)

All other properties (e.g., viscosity) are computed in the same manner. The interface between the two fluids is treated as a discontinuity in fluid properties.

The VOF-approach can be applied to complex free surface shapes including breaking waves. However, the free surface contour is not sharply defined; it is usually smeared over one to three cells. Local grid refinement is important for accurate resolution of the free surface. The refinement criterion is simple: cells with \( 0 < c < 1 \) need to be refined (Ferziger and Peric 1999).

### 3.4 Boundary and Initial Conditions

#### 3.4.1 General Remarks

Due to the elliptic nature of the continuity (2-2), the RANS (2-10) and the turbulence model equations for \( k \) (2-16) and \( \varepsilon \) (2-17), boundary conditions must be specified for all variables. Additionally, all variables must be initialized in the domain to solve the transient equations. If a steady-state solution is searched, the variables have to be initialized within a convergence radius, because of the nonlinearity of the transport equations.

The RANS and the \( k \), \( \varepsilon \)-equations are Second Order PDEs. Boundary conditions can therefore be specified either for the variables \( \{ \mathbf{U}, P, k, \varepsilon; \} \) (Dirichlet Boundary Condition) or their normal gradients (Neuman Boundary Condition) or a linear combination thereof.

The continuity equation is a first order differential equation, which has to be fulfilled at each node in the flow field and on each boundary. The zero divergence condition on the solution is violated, at least locally, when a Dirichlet boundary condition for pressure is used.

#### 3.4.2 Solid Boundary

At the solid boundary non-slip condition exists, i.e., all velocity components vanish. If this condition is used in the simulation, a very fine discretization of the boundary layer is necessary in order to
compute the steep gradients with a sufficient accuracy. Furthermore, the flow field is dominated by viscous effects close to the wall. But the application of the standard $k-\varepsilon$ model is limited to flows with high Reynolds Numbers, because the viscous effects were neglected in its derivation (Rodi 1980). The standard $k-\varepsilon$ model can therefore not be used in this region. The exact simulation of the very thin boundary layer is generally only of secondary interest in complex flow fields or even not feasible in cases with high bed roughness.

Thus, the boundary layer is treated in a special way by using so called wall-functions. This leads to a significant reduction of the numerical effort. In this method the spatial discretization ends at a finite distance $Y$ from the solid boundary for the FE discretization. The FV grid is discretized up to the solid boundary, but its centre points are situated at a distance $Y$ from the wall. At this distance $Y$ the viscous shear stresses have already decreased rapidly, and the momentum transport is dominated by the Reynolds stresses. The turbulence structure is in a local equilibrium, i.e., production is equal to dissipation. The local Reynolds stresses $-\rho \overline{u_i u_j}$ correspond to the shear stresses $\tau_w$ (Rodi 1998). These assumptions allow to define the boundary conditions at the nodes/cells closest to the wall.

The logarithmic law-of-the-wall (figure 3.8) is applied to calculate the velocity boundary condition,

$$\frac{U_i}{u_*} = \frac{1}{k} \ln(Y^*) + AB,$$

(3-40)

with $U_i$ the tangential velocities and $u_*$ [ms$^{-1}$] the bed shear velocity,

$$u_* = \frac{\tau_w}{\rho},$$

(3-41)

where $\tau_w$ is the bed shear stress and $\kappa = 0.41$ is the Karman constant in equation (3-40). The dimensionless wall distance $Y^*$ is

$$Y^* = \frac{Y u_*}{v_e},$$

(3-42)

where $v_e$ is the kinematic viscosity and $Y$ [m] is the wall distance. The logarithmic law-of-the-wall has its validity in the region $30 < Y^* < 100$ (Rodi 1980). $AB$ is a roughness function of $k_s^+ = u_* k_s / v_e$ (with $k_s$ the equivalent roughness height) determined by CEBECI AND BRADSHAW (1977),

$$AB = \begin{cases} 
5.2, & k_s^+ < 2.25 \\
8.5 - \frac{1}{k} \ln k_s^+ \sin[0.4258 \ln(k_s^+ - 0.811)], & 2.25 \leq k_s^+ < 90 \\
8.5 - \frac{1}{k} \ln k_s^+, & k_s^+ \geq 90
\end{cases}$$

(3-43)
The tangential velocities $U_t$ were specified as Dirichlet boundary conditions for the 2D FE computations, where the shear stresses $\tau_w$ in equation (3-40) were calculated with the method of BE-NIM (1988), which has also been successfully tested by SCHRODER (1997):

Figure 3.9 shows an element close to the wall, where node 1 is a boundary node at a distance $Y_1$ from the wall and node 2 is in the flow domain. The grid has to be discretized such that both distances $Y_1$ and $Y_2$ lie within the validity of the law-of-the-wall to apply Benim's method. The shear stresses can then be determined by applying the law-of-the-wall at both grid points 1 and 2, resulting in the following relations,

\[
\tau_w = \begin{cases} 
\frac{\mu \cdot U_t}{Y_2} & \text{for } Y_2^+ < 11.6 \\
\frac{\kappa \cdot c_{u}^{1/4} \cdot \rho \cdot U_2 \cdot k_1^{1/2}}{\ln(Y_2^{+} / Y_2^{+} / k_u) + 5.2 \cdot \kappa} & \text{for } Y_2^+ \geq 11.6, \text{ hydraulically smooth} \\
\frac{\kappa \cdot c_{u}^{1/4} \cdot \rho \cdot U_2 \cdot k_1^{1/2}}{\ln(Y_2^{+} / k_u) - 8.5 \cdot \kappa} & \text{for } Y_2^+ \geq 11.6, \text{ hydraulically rough}
\end{cases}
\]  

(3-44)

The normal velocities were neglected. ($U_n = 0$, Dirichlet Boundary Condition).

For the 3D computations, the shear stresses $\tau_w$ in the law-of-the-wall were directly specified as Neuman boundary condition.

The turbulence variables $k$ and $\varepsilon$ at the solid boundary were specified by Dirichlet boundary condition for the 2D computations (Rodi 1980),

\[
k = \frac{\dot{u}_v^2}{\sqrt{c_{u}^e}},
\]

(3-45)

\[
\varepsilon = \frac{\dot{u}_v^2}{\kappa \cdot Y}.
\]

(3-46)

The 3D computations used the same boundary condition for the dissipation rate $\varepsilon$, but a Neuman boundary condition was defined for the turbulent kinetic energy $k$, with zero gradients normal to the boundary.

### 3.4.3 Upper Boundary

For the 2D computations, the upper boundary was equal to the free surface, with the boundary condition described in section 3.3.1. The velocity-driven-grid-adaption was used for all computations performed in chapter 6, with Dirichlet boundary conditions for pressure at the free water surface.

Zero fluxes of all quantities across the upper boundary were specified for the 3D computations,
with no convection nor diffusion across the plane, i.e.:

- Zero normal velocities and
- Zero normal gradients of all variables.

### 3.4.4 Inflow Boundary

The velocities in all spatial directions as well as the turbulence variables $k$ and $\varepsilon$ were specified by Dirichlet boundary conditions at the inflow boundary.

At a given discharge $Q$ the normal velocities were defined by a logarithmic profile (Jäggi 1995),

$$U_{i,j} = \frac{Q}{H} \cdot \frac{\ln \left( \frac{Z_i}{\delta_{w,H}} \right) + \rho_H}{\ln \left( \frac{H}{\delta_{w,H}} \right) + \rho_H - 1} \cdot \frac{\ln \left( \frac{B/2 - |Y_j|}{\delta_{w,B}} \right) + \rho_B}{B/2 \cdot \ln \left( \frac{B/2}{\delta_{w,B}} \right) + \rho_B - 1}$$

(3-47)

The parameters $\rho_B$ and $\rho_H$ are defined as $\rho_B = \rho_H = 3.4$ (Jäggi 1995). $\kappa$ is the Karman constant, $\delta_{w,B}$ and $\delta_{w,H}$ are the distances from the wall to the fully turbulent region. $H$ is the water depth, $B$ is the river width and $Y_j$, $Z_j$ are the corresponding distances along the coordinates (see figure 3.10).

The tangential velocities were set equal to zero.

The boundary conditions for $k$ and $\varepsilon$ were calculated as functions of the turbulence intensity $I$ (Libby 1996). The turbulence intensity, $I$, is defined as the ratio of the root-mean-square of the velocity fluctuations, $u'$, and mean flow velocity, $U_{avg}$. But at the core of a fully-developed duct flow, $I$ can be estimated from the following equation derived from an empirical correlation for pipe flows (FLUENT 1998),

$$I = \frac{U'}{U_{avg}} = 0.16 \cdot Re^{-1/6},$$

(3-48)

where $Re$ is the Reynolds number. A turbulence intensity of 1% or less is generally considered low and turbulence intensities greater than 10% are considered high.

The relation between the turbulent kinetic energy $k$, and the turbulence intensity, $I$, is

$$k = \frac{3}{2} (U_{avg} I)^2,$$

(3-49)

and the turbulent dissipation rate $\varepsilon$ is then calculated as,
\[ \varepsilon = C_{\mu}^{1/4} \frac{K^{2/3}}{e}, \]  
(3-50)

where \( \varepsilon = 0.07L \) is the turbulence length scale in fully-developed duct flows. The factor of 0.07 is based on the maximum value of the mixing length in fully-developed turbulent pipe flow, where \( L \) is the hydraulic diameter.

For the 3D computations, where both phases (water and air) were calculated, two inlet boundaries were defined: One for the air and one for the water phase. The boundary conditions for the water phase were set according to the above mentioned values. The inlet velocity for the air phase was set to a similar magnitude as the inlet water velocity at the water surface to avoid shear stresses. The turbulence parameters \( k \) and \( \varepsilon \) were set to zero for the air phase.

### 3.4.5 Outflow Boundary

The outflow boundary was chosen at (or close to) a region with uniform flow to allow a Neuman boundary condition equal to zero,

\[
\frac{\partial U_j}{\partial x_n} = \frac{\partial k}{\partial x_n} = \frac{\partial \varepsilon}{\partial x_n} = 0. \tag{3-51}
\]

At least one Dirichlet boundary condition for pressure has to be defined, which was fixed at a cell of the outflow boundary for the 3D computations.

### 3.5 CFD-Codes

#### 3.5.1 FEMTOOL

FEMTOOL (Finite Element Method TOOLbox) by Rutschmann (1993, 1994) was used for the 2D computations. This program is written in C and FORTRAN and solves steady-state or transient non-linear coupled PDEs. The specific problem is set up in an element-matrix routine. Two other routines allow for the implementation of initial conditions and time-dependent boundary conditions. In four other interfaces, additional user functions can be defined to influence the problem data, before or after each iteration step, or after an iteration or time step has converged. The entire source-code was available. The numerical integration of transient PDEs is also based on finite elements. Different shape functions for different variables and for space and time may be chosen to solve the problem. The order of shape function is not restricted. The SPARSE1.3-solver (Kundert and Sangiovanni-Vincentelli 1988) is used to solve the global element-matrix.

FEMTOOL has been successfully applied to the solution of 2D and 3D Navier-Stokes equations (NSE) with grid adaption using the Arbitrary Lagrangian Eulerian (ALE) method (Bürgisser
In this work NEGEFF (Net Generator For Femtool, BÜRGISSER 1998) was used to generate a triangular grid, allowing for local refinements. The 2D test cases were computed with the extended version of FEMTOOL developed by BÜRGISSER (1999), where the adaptation of the free surface as well as the $k$-$\varepsilon$ turbulence model were modified. The following figure 3.11 shows the schematic computation process for the turbulent free surface flow, where the turbulence model equations are solved decoupled from the continuity and RANS equations and the grid is adapted after each time step or after convergence is achieved, for the steady-state computations.

\begin{center}
\begin{tikzpicture}
  \node (init) {Initial conditions $\Omega^n_0, U^n_0, P^n_0, k^n_0, \varepsilon^n_0$};
  \node[below=of init] (flow) {solution of the flow equations $U^{k+1}_i, P^{k+1}_i$};
  \node[below=of flow] (turb) {solution of the turbulence equations $k^{k+1}, \varepsilon^{k+1}$};
  \node[below=of turb] (conv) {converged?};
  \node[below=of conv] (boundary) {boundary conditions $k^{n+1}, \varepsilon^{n+1}$};
  \node[below=of boundary] (grid) {grid correction};
  \node[below=of grid] (accept) {grid acceptable?};
  \node[below=of accept] (remesh) {remeshing};

  \draw[->] (init) -- (flow); \\
  \draw[->] (flow) -- (conv) node[above] {no}; \\
  \draw[->] (conv) -- (turb); \\
  \draw[->] (turb) -- (conv) node[above] {yes}; \\
  \draw[->] (conv) -- (boundary); \\
  \draw[->] (boundary) -- (grid); \\
  \draw[->] (grid) -- (accept); \\
  \draw[->] (accept) -- (remesh); \\
  \draw[->] (remesh) -- (grid) node[above] {yes}; \\
  \draw[->] (remesh) -- (conv) node[above] {no}; \\

  \node[below=of conv, yshift=2cm] {Converged?};
  \node[below=of conv, yshift=-2cm] {No};
  \node[below=of conv, yshift=-4cm] {Yes};

  \node at (current bounding box.center) {Fig. 3.11 Schematic solution process of turbulent free surface flow with FEMTOOL.}
\end{tikzpicture}
\end{center}
3.5.2 FLUENT

FLUENT (2000) is a commercial CFD package based on the Finite Volume method, which was used for the 3D computation in this work. Supported mesh types in FLUENT include 2D triangular/quadrilateral, 3D tetrahedral/hexahedral/pyramid/wedge, and mixed (hybrid) meshes. FLUENT also allows to refine or coarsen the grid based on the flow solution.

In this work a segregated solver was used, applying the \( k-\varepsilon \) turbulence model with standard wall-functions near the wall and refining/coarsening the grid to position the cell-centroids at a distance within the validity of the wall function. The free surface was calculated with the VOF method.
4 Inverse Formulation

The purpose of the inverse method is to determine the discharge \( Q \) and its distribution over the cross-section at the inflow boundary, such that measured water surface elevations and surface velocities in a channel section are reproduced best by simulated data. An objective function, which defines the agreement between measurements and model, is described in section 4.2. Section 4.3 describes the algorithms to minimize the objective function, followed by the definition of the standard deviation of parameters in section 4.4. Identifiability, Uniqueness and Stability of the solution are discussed in section 4.5.

4.1 Direct/Indirect Method

A common classification divides the inverse solution techniques into direct and indirect methods (e.g., Sun 1994). The direct method requires a dense distribution of observations. Nodal equations have to be rearranged such that the parameters are then considered as unknown variables while the state variables are substituted by their observations. In this work a standard indirect method is used, which solves the inverse problem indirectly through the repeated solution of the forward problem (e.g., Carrera and Neuman 1986a,b,c).

4.2 Objective Function

Given is a model that has \( M \) adjustable parameters \( p_i \, | \, i = 1, \ldots, M \). These parameters have to be optimized such that the computed variables \( y_i(p) \) at the measurement locations \( x_i \, | \, i = 1, \ldots, N \) correspond best to the measurements \( y_i^* \). The agreement between computed and measured variables is quantified by an objective function, which is conventionally arranged so that small values represent close agreement. The parameter vector \( p \) is then adjusted to achieve a minimum in the objective function, yielding best-fit parameters.

4.2.1 Least Squares as a Maximum Likelihood Estimator

The deviations between measured and computed values in the objective function were described by a least-squares formulation according to a maximum likelihood estimation in this work:

The Likelihood function, \( L(p,y^*) \), describes the probability to obtain the measurements \( y^* \) assuming that the parameters \( p \) are correct. The optimal set of parameters \( p \) maximizes the Likelihood.
function. While not leading to an exact reproduction of the measurements, this statistical approach allows the model to provide the set of parameters \( \mathbf{p} \), which reproduces the measurements with the highest probability.

Supposing that each measurement \( y_i^* \) has a measurement error that is independently random and normally (Gaussian) distributed around the “true” model \( y_i(\mathbf{p}) \), the probability of the measurement-set is then the product of the probabilities of each point,

\[
L(\mathbf{p}|y^*) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma_i} \cdot e^{-\frac{1}{2} \left( \frac{(y_i^* - y_i(\mathbf{p}))^2}{\sigma_i^2} \right)}.
\]

(4-1)

The maximum of the product in equation (4-1) is equal to the minimum of the sum of its negative logarithms,

\[
-\ln[L(\mathbf{p}|y^*)] = \sum_{i=1}^{N} \left[ \frac{(y_i^* - y_i(\mathbf{p}))^2}{2\sigma_i^2} \right] - \sum_{i=1}^{N} \ln\left( \frac{1}{\sqrt{2\pi}\sigma_i} \right).
\]

(4-2)

The last term in equation (4-2) can be neglected for the extreme value analysis, if the standard deviations are known. The objective function \( \zeta(\mathbf{p}) \) is then,

\[
\zeta(\mathbf{p}) = \sum_{i=1}^{N} \left[ \frac{(y_i^* - y_i(\mathbf{p}))^2}{\sigma_i^2} \right] = \sum_{i=1}^{N} f_i^2,
\]

(4-3)

which is a least-squares fitting, if the measurement errors are independent and normally distributed.

### 4.2.2 Objective Function in this Work

In this work the measurements \( y_i^* \) referred to the water level measurements \( h_i^* \) and surface velocities, given by their components \( U_{ij}^* \) (\( j = 1, \ldots, \text{number of spatial dimensions} \)) or by their magnitude \( |U_{ij}^*| \). The discharge \( Q \) and (for some calculations) a form parameter \( P_H \) for the velocity distribution at the inflow boundary were the model parameters \( \mathbf{p} \) to be optimized. The computed values \( y_i(\mathbf{p}) \) at a measurement location \( x_i \) for a certain parameter set \( \mathbf{p} \) were \( h_i(\mathbf{p}) \) and \( U_{ij}(\mathbf{p}) \), resp. \( |U_{ij}(\mathbf{p})| \). The objective functions \( \zeta_k(\mathbf{p}) \) for the different variable types \( k \) were defined as,

\[
1. \text{velocity-magnitude } |U| = \sqrt{U_1^2 + U_2^2 + U_3^2}
\]
4.3 Optimization

The nonlinearity of the objective function regarding the parameters $p$ leads to an iterative optimization process to find its minimum. If the objective function $\zeta(p)$ is second-order differentiable, the following conditions are necessary for $\dot{p}$ to be a local minimum of $\zeta(p)$:

- Gradient $\nabla \zeta(\dot{p}) = 0$ (defining an extreme value)
- Hessian $\nabla^2 \zeta(\dot{p})$ is a positive definite matrix (defining a minimum and not a maximum).

The following section 4.3.1 defines the gradient, Jacobian- and Hessian-matrix used in the mini-
mizing algorithms in section 4.3.3, focusing on the Levenberg Marquardt method used here. A more general overview of minimizing algorithms can be found in, e.g., FLETCHER (1987) or SUN (1994).

4.3.1 Gradient, Jacobian- and Hessian-Matrix

The gradient \( g_j \) of the objective function \( \zeta(p) \) (4-3) is its derivative with respect to the parameter \( p_j \):

\[
g_j = 2 \sum_{i=1}^{N} f_i \frac{\partial f_i}{\partial p_j} \tag{4-7}
\]

where \( f_i \) contains the deviations between the measured and calculated values at the measurement location \( x_i \), scaled with the standard deviation, \( f_i = 1/\sigma_i(y_i - \hat{y}_i(Q)) \).

By defining the Jacobian matrix \( J \) with the dimension \( N \times M \) (\( N = \) number of measurements and \( M = \) number of parameters to be optimized),

\[
J = 
\begin{bmatrix}
\frac{\partial f_1}{\partial p_1} & \ldots & \frac{\partial f_1}{\partial p_M} \\
\vdots & \ddots & \vdots \\
\frac{\partial f_N}{\partial p_1} & \ldots & \frac{\partial f_N}{\partial p_M}
\end{bmatrix},
\]

(4-8)

the gradient vector \( g(p) \) can be rewritten as,

\[
g(p) = 2J^T(p) \cdot f(p). \tag{4-9}
\]

The second partial derivative of the objective function, \( \nabla^2 \zeta(p) \), is called the Hessian matrix \( H \),

\[
H = 
\begin{bmatrix}
\frac{\partial^2 \zeta}{\partial p_1^2} & \ldots & \frac{\partial^2 \zeta}{\partial p_1 \partial p_M} \\
\vdots & \ddots & \vdots \\
\frac{\partial^2 \zeta}{\partial p_M \partial p_1} & \ldots & \frac{\partial^2 \zeta}{\partial p_M^2}
\end{bmatrix}. \tag{4-10}
\]

The individual terms of the Hessian matrix can be obtained by differentiating equation (4-7),

\[
H_{kj} = 2 \sum_{i=1}^{N} \left[ \frac{\partial f_i}{\partial p_k} \frac{\partial f_i}{\partial p_j} + f_i \frac{\partial^2 f_i}{\partial p_k \partial p_j} \right]. \tag{4-11}
\]

The complete Hessian matrix can be written as,

\[
H(p) = 2[J^T(p)J(p) + S(p)], \tag{4-12}
\]

with \( S(p) \) defined as,
4.3 Optimization

\[ S(p) = \sum_{i=1}^{N} f_i(p) \nabla^2 f_i(p). \]  
(4-13)

Thus, the gradient as well as the Hessian matrix are defined, if the Jacobian matrix is known. The determination of the Jacobian matrix in this work is described in the following section.

4.3.2 Calculation of Jacobian Matrix

The Jacobian matrix can be obtained by several approaches, e.g., the sensitivity equation method, the finite difference approach or the adjoint state method (Sun 1994). In this work the sensitivity equation or the finite difference approach were applied to calculate the Jacobian matrix, depending on whether the position of the free water surface was calculated or fixed. The adjoint state method has no advantage here, as only few parameters were optimized. (A description of this method can be found in Sun 1994).

The sensitivity equation method was used for the 2D computations with a fixed water surface. The transport equations (2-10) differentiated with respect to the optimization parameters were solved,

\[ U_j \frac{\partial U_j}{\partial x_j} + \sum_{i=1}^{N} \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial P}{\partial x_j} + \frac{u_j}{\rho} \frac{\partial^2 U_i}{\partial x_j^2} - \frac{\partial}{\partial x_j}(u_i u_j) + g_i, \]  
(4-14)

where \( U_j \) was taken from the last CFD-simulation of the flow field and \( U_i, P' \) are the differentiated variables. This equation was implemented in the CFD-model FEMTOOL (Rutschmann 1993, 1994), and can be solved similarly to the flow equation. The boundary conditions were differentiated with respect to the optimization parameters too. E.g., \( h_i'(Q) \) was obtained by differentiating equation (4-6) with respect to the discharge \( Q \),

\[ h_i'(Q) = \frac{\partial h_i(Q)}{\partial Q} = \frac{2|U_i, o(Q)|}{2g} \cdot \frac{\partial |U_i, o(Q)|}{\partial Q} \cos \alpha. \]  
(4-15)

The finite difference approach was used for the 2D computations on an adaptive grid and for the 3D computations. In these cases the partial derivatives of the water depth cannot be obtained from equations (4-14) and (4-15) as no normal velocity components exist at the free water surface. The position of the free water surface was determined for the discharges \( Q \pm \Delta Q \) and the finite differences were computed by subtracting the water levels at discharges \( Q + \Delta Q \) and \( Q - \Delta Q \) and dividing by \( 2\Delta Q \). The finite differences for the surface velocities were computed in the same way.

If further parameters were optimized, such as a form parameter \( p_H \) for the inflow velocity distribution, the procedure stated above was repeated:

- either by differentiating the transport equation with respect to the form parameter \( p_H \) when using the sensitivity equation method,
- or by computing the flow field with an inflow velocity distribution using a form parameter \( p_H \pm \Delta p_H \) when using the finite difference approach.
4.3.3 Minimizing Algorithms

The most common tool in the study of numerical optimization is the Taylor expansion of the objective function $\zeta(p)$ around a point $p_k$ (Sun 1994). It can be represented by the following matrix form,

$$
\zeta(p_k + \Delta p_k) = \zeta(p_k) + g(p_k)^T \Delta p_k + \frac{1}{2} (\Delta p_k)^T H(p_k) \cdot \Delta p_k + HOT,
$$

(4-16)

where gradient vector $g$ and Hessian matrix $H$ are evaluated at point $p_k$. HOT represents the third and higher order terms.

If $p_k$ is a point of search sequence, gradient $g(p_{k+1})$ can be expressed approximately by differentiation of (4-16),

$$
g(p_{k+1}) = g(p_k) + H(p_k) \cdot \Delta p_k.
$$

(4-17)

According to the necessary condition for a minimum on page 37, we expect that $g(p_{k+1}) = 0$, leading to,

$$
H(p_k) \cdot \Delta p_k = -g(p_k).
$$

(4-18)

With $f_k = f(p_k)$, $J_k = J(p_k)$ and $S_k = S(p_k)$ and the equations (4-9), (4-12) and (4-18), Newton’s method for minimizing the objective function is given by the equations,

$$(J_k^T J_k + S_k) \cdot \Delta p_k = -J_k^T f_k,$$

(4-19)

$$
p_{k+1} = p_k + \Delta p_k.
$$

(4-20)

If $\zeta(p)$ is a quadratic function, there is no error in equation (4-17). As a result, its minimum can be found directly by solving equation (4-19) only once. For the general case, however, an iteration procedure is necessary. If $\zeta(p)$ is close to a quadratic function it rapidly converges to a minimum, which is the major advantage of the Newton method. However, there are several disadvantages associated with this method. First, it is impractical to calculate matrix $S(p)$ and second, if $p_k$ is not close to the minimum, the Hessian matrix is not necessarily positive definite. As a result, there is no guarantee that $\zeta(p_{k+1}) < \zeta(p_k)$. Figure 4.1 shows the minimizing procedure with two parameters, where the lines of constant levels of the quadratic approximation of the objective function $\zeta$ are ellipsoids.

The Gauss-Newton method neglects matrix $S(p)$ in equation (4-19), which simplifies the optimiza-
4.3. Optimization

The optimization procedure, as no second order derivatives have to be determined. The optimizing equation is then,

\[
J_k^T J_k \Delta p_k = -J_k^T f_k.
\]  

(4-21)

This simplification is tolerable, because the term \( S(p) \) is approximately zero close to the minimum of \( \zeta(p) \) (resp. residuals \( f_i(p) = \text{small} \)). If large residuals occur - due to poorly initialized parameters \( p_k \) or strongly scattered measurements \( y^* \) - the step length \( \Delta p_k \) is generally too large, possibly not leading to convergence.

The Levenberg-Marquardt algorithm is a modification of the Gauss-Newton approach, which is designed to overcome this problem. Equation (4-21) is modified into

\[
(J_k^T J_k + \mu_k I) \Delta p_k = -J_k^T f_k,
\]  

(4-22)

with \( \mu_k > 0 \) the Levenberg parameter, and \( I \) the identity matrix. When \( \mu_k = 0 \), \( \Delta p_k \) reduces to the Gauss-Newton direction. On the other hand, when \( \mu_k \) tends to infinity, \( \Delta p_k \) turns to the steepest descent direction and the size of \( \Delta p_k \) tends to zero. Therefore, \( \zeta(p_{k+1}) < \zeta(p_k) \) can always be expected by increasing the value of \( \mu_k \).

There are several other optimization algorithms, such as the conjugate gradient method or the Quasi-Newton method, as well as search methods with no requirement of any derivatives of the objective function. These methods are generally less efficient (Sun 1994), especially when a large number of parameters is optimized. Several authors also suggest a combination of several optimization methods, such as using a robust method to come close to the minimum and then use an accurate and fast method for the last iterations. Yeh (1986) for example gives a broad literature review of the commonly used methods in hydrogeology.

The Levenberg-Marquardt method was used in this work, as it has been widely tested in practical optimizations and is known to be robust but also of a good convergence behavior.

The optimization procedure can now be described as following: One inverse cycle \( k \) includes one run of the forward model to determine \( f_k \). If \( f_k \) is smaller than \( f_{k-1} \), either two more runs of the forward CFD-model with discharges \( Q \pm \Delta Q \) or one run with the sensitivity equation (4-14) are needed to determine the Jacobian matrix. The discharge is then updated with equation (4-22) and (4-20) and the convergence criteria are checked. When no convergence is achieved and the maximum number of inverse iteration steps is not yet reached a new inverse iteration step is performed.
4.4 Standard Deviation of Parameters

The standard deviation $\hat{\sigma}_Q$ of the estimated discharge $Q$ can be calculated as

$$\hat{\sigma}_Q = \sqrt{\sum_{i=1}^{N} \left( \frac{\sigma_i}{J_i} \right)^2},$$  \hspace{1cm} (4-23)

where $\sigma_i$ is the standard deviation of measurement $i$, $J_i$ is the $i$-th element of the Jacobian matrix, and $N$ is the number of measurements. A more sophisticated method to determine the covariance matrix for more than one parameter is described, used and discussed in Carrera and Neuman (1986a).

4.5 Identifiability, Uniqueness and Stability

This section describes the problem of ill-posed optimizations by defining the phenomena identifiability, uniqueness and stability and by discussing how each of these phenomena affect the behavior of the inverse solution.

4.5.1 Definition

The terms identifiability, uniqueness and stability can be defined as (Carrera 1984):

- **Identifiability** is given, if a solution of the forward simulation can be obtained from only one single parameter set. If there exist two different parameter sets which lead to the same solution, then the parameters are unidentifiable.

- An inverse solution is **unique**, whenever the criterion to be minimized is convex, i.e., it has only one global minimum in the parameter space. This means, if different parameter sets may originate from given measurements (here, water levels and surface velocities) then the parameters are non-unique.

- **Stability** is given, if small errors in measurement do not result in large changes in the computed parameters. Instability is generally associated with a flat estimation criterion near the minimum so that most minimization algorithms converge slowly near this minimum.

The inverse problem is referred to as being ill-posed, if it may fail to satisfy one or more of these three requirements.

4.5.2 Discussion

The parameter set used here contains information on the inflow boundary, i.e., the discharge and (for some calculations) a form parameter for the inflow velocity distribution. The flow field comput-
ed with certain values of the parameter set can not be obtained with any other values. Thus, the parameters chosen here are always identifiable. Identifiability is necessary but not sufficient for uniqueness of the inverse solution as shown below.

A unique and stable solution is obtained if only one parameter set exists for a given series of measurements. Uniqueness and stability are also a function of the chosen measurements and their accuracy, as well as the chosen objective function. Uniqueness and stability may not be given in the problem of this work when optimizing the discharge and a form parameter, with surface measurements only. Generally, a better posed inverse problem is achieved with (CARRERA AND NEUMANN 1986b):

- more (independent) measurements,
- measurements more sensitive to changes of the optimizing parameter,
- smaller measurement errors,
- smaller dimensionality of the parameter space or
- reduced non-linearity in the objective function (e.g., taking the log-value).

### 4.6 Implementation

The INVERS-program consists of the FORTRAN-routines of the Levenberg-Marquardt algorithm, which were taken from the internet library NETLIB where it can be found in the sub-directory MINPACK\(^1\). The interface between these routines and the CFD-code is set up to estimate the discharge \(Q\) as well as a form parameter \(p_H\) for the velocity distribution at the inflow boundary. Flexibility is provided for measurement input, where only stage or velocity measurements or both measurement types can be considered. Velocity measurements can further be considered as velocity components in all computed dimensions or as the velocity magnitude. One can choose between CFD-computations on a fixed water surface that is linearly interpolated through the measured stages or computations involving the calculation of the position of the free water surface.

The variables \(y(p)\) can be computed with an arbitrary CFD-code in the same way as in forward computations. The partial derivatives \(\partial y(p)/\partial p\) with respect to the optimizing parameters \(p\) can either be computed by the sensitivity equation method (which has to be implemented in the CFD-code) or by the finite difference approach.

Four termination criteria were distinguished:

- The maximum number of iteration steps is reached (maxfev).
- The cosine of the angle between the objective function vector and any column in the Jacobian matrix is smaller than a tolerance (gtol).

---

1. [http://www.netlib.org/cgi-bin/netlibget.pl/minpack/lmder.f](http://www.netlib.org/cgi-bin/netlibget.pl/minpack/lmder.f)
4. INVERSE FORMULATION

- Relative error between two consecutive iterations is smaller than a tolerance (xtol).
- Actual and predicted reductions in the sum of squares are smaller than a tolerance (ftol).

The following figure 4.2 shows the structure of the inverse calculation procedure.

**INVERS-Programme**

**Minimizing Routine**

- Calculating $L_2$-Norm (objective func.):
  \[
  \sum_{i=1}^{N} f_i^2
  \]
- Calculating $L_2$-Norm (gradients).

  *If gradient-norm ≤ g-tolerance: end!*

- Calculating $\Delta p$ with Levenberg-Marquardt method.
- Calculating $L_2$-Norm ($p$).
- Calculating $L_2$-Norm (objective func.).

- Calculating ratio between actual and predicted reduction of the objective-function-norm.
  
  if ratio < 0.0001

- Updating the step length $\mu_k$ due to the ratio.
- Updating the parameter set $p$.

- Tests for convergence, resp. termination.

- If no termination

**First call of CFD-programme to compute $y(p)$.

calculating objective function**

**Call of CFD-programme to compute the partial derivatives, $\partial y(p)/\partial p$.**

**calculating Jacobian matrix**

**Further calls of CFD-programme to compute $y(p)$.

calculating objective function**

*Fig. 4.2* Program structure of the inverse calculation procedure.
5 Computations: General Remarks

This chapter gives an overview of the computations performed in the following two chapters. Additionally, possible error sources in estimating the discharge are discussed in section 5.2. Section 5.3 describes the concept of using synthetically generated series of measurements for all discharge estimations in this work. A feasibility study for the proposed method is described in section 5.4 and applied in the computations of the following chapters.

5.1 Overview

The following two chapters present the results of the inverse numerical simulations for two test cases. Measurements from laboratory experiments were available to verify the CFD-simulations. Both test cases represent flood situations in a river section with complex geometry.

The 2D computations in chapter 6 considered only a vertical cross section along the river axis, neglecting any secondary cross-stream flow. The Finite Element approach (section 3.1) was applied to determine the flow field, solving the continuity (2.1) and the RANS equations (2.2) combined with the \( k-\varepsilon \) turbulence model (2.3). The free surface was calculated by adapting the grid as described in section 3.3.1.

Chapter 7 presents the 3D computations solved with the Finite Volume method (section 3.2) on a rigid grid, where the free surface was calculated with the Volume-of-Fluid (VOF) method as described in section 3.3.2. Turbulence was taken into account using the \( k-\varepsilon \) model.

The same inverse formulation was used around the CFD-simulations for both cases, where the objective function is based on a least-squares formulation as defined in section 4.2.1. The objective function was minimized by the Levenberg-Marquardt algorithm (section 4.3.3).

Both studies provide information on the feasibility of the presented method to estimate discharge. They allow to draw conclusions for a wide range of applications as two generally different river geometries and CFD-codes have been considered.
5.2 Error Sources

The estimation of the discharge $Q$ is associated with uncertainties that occur due to inaccurate PTV-measurements of water levels and surface velocities and due to an incorrect CFD-model description to obtain the corresponding computed values. The inverse formulation implies further error sources. It performs the discharge estimation by evaluating the best agreement between measurements and computations.

The following table lists possible error sources for the estimation of discharge, which are further classified into systematic and random error. Systematic errors have their origin in an error of the functional model that links an input with an output and cannot be eliminated by increasing the number of measurements/computations, while random errors tend to zero for an increasing number of measurements/computations.

<table>
<thead>
<tr>
<th>Error sources</th>
<th>systematic</th>
<th>random</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Measuring procedure</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>localization of particles (due to camera resolution, particle size)</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>calibration</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>tracking algorithm</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td><strong>CFD-model</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>boundary conditions</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>- river-bed geometry</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>- bed/wall roughness</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>- inflow/outflow velocity distribution</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>simplifications</td>
<td></td>
<td>x x</td>
</tr>
<tr>
<td>- discretization</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>- dimensionality</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>- physical processes</td>
<td>x x</td>
<td></td>
</tr>
<tr>
<td>round off error</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td><strong>Inverse calculation</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>objective function</td>
<td>x x</td>
<td></td>
</tr>
<tr>
<td>minimizing algorithm</td>
<td>x</td>
<td></td>
</tr>
</tbody>
</table>

Most error sources are systematic, thus do not allow a statistical error analysis. These errors should therefore be quantified and, if possible, eliminated a priori. The error sources listed in table 5.1 are described in more details in the following.

Measurement errors can occur through the measurement setup itself. The accuracy of the PTV-measuring technique depends on the resolution of the image by the CCD-sensor, the size and
shape of the particles, the flow conditions (e.g., surface velocity magnitude, spatial variability, turbulent fluctuations, etc.), and the imaging rate. Typical cameras have a resolution of about 1000 x 1000 pixels, which allow to determine the position of a suitable particle with a sub-pixel accuracy of 1/10 pixel. If an area of 2 x 2 m is recorded, for example, the position of particles can be determined to an accuracy of 0.2 mm. When assuming an average surface velocity of 1 ms\(^{-1}\) and an image rate of 1/50 sec., a particle moves 10 pixels within this time, i.e., 20 mm. A surface velocity can then be determined to an accuracy of 2%. This estimation implies optimal laboratory conditions and does not include the effect of irregular particles nor effects due to distortion of the recorded images. A detailed error description in the measuring procedure can be found in Maas (1992), Maas et al. (1993), Virant (1996) and Stuer (1999).

Deviations between the true physics and the CFD-model can emerge due to a lack of observations, producing mainly uncertainties in the boundary conditions, or due to the complex flow field, requiring simplifications in the governing system of equations.

Typical uncertainties in boundary conditions are:

- In natural rivers, the actual river-bed geometry is usually not known or measurements are only available at a limited number of locations. Significant sediment transport during flood events may further lead to an unknown river bed geometry. A sensitivity analysis performed with CFD-simulations, which considers possible bed geometries, can provide information on the influence of a variable river bed geometry on the estimated discharge.
- The bed roughness is usually only known at a limited number of locations or not known at all. The influence of different bed roughness values can be estimated by a sensitivity study.
- The inflow velocity distribution cannot be measured in a continuous way, resulting in sparse measurement data (see also section 1.1.1 for more information on velocity measurements). The sensitivity to different inflow velocity distributions can be analyzed. If the uncertainty interval is not acceptable, the influence of the inflow velocity distribution can be suppressed by having the inflow boundary at a distance of about 25-50 times the hydraulic diameter upstream of the measurement section. This distance allows for an upstream uniform velocity profile to develop into a fully turbulent profile (Schlichting 1965).

The typical simplifications in the description of a complex flow field in a river section are:

- The flow field is usually too complex to be solved analytically, necessitating a numerical discretization and solution. The discretization error can be reduced by refining the grid and choosing regular and not distorted cells. Higher order interpolation schemes can reduce the error, too.
- A turbulence model allows to take into account turbulence without resolving each vortex, allowing for a coarser grid. But such models are based on empirical assumptions, where the degree of empiricism depends on the model. The \(k\)-\(\varepsilon\) turbulence model chosen here has deficits in, e.g., modelling large anisotropy of the turbulence. Furthermore, the flow field was com-
computed by solving the Reynolds averaged Navier-Stokes equations, where turbulent fluctuations are eliminated. The amplitude of the fluctuation can be calculated conservatively by considering the turbulent kinetic energy \( k \) and neglecting the dissipation rate \( \varepsilon \),

\[
v' \equiv 2 \sqrt{k}, \quad h' \equiv \frac{v'^2}{2g} = \frac{2k}{g},
\]

with \( v' \) the fluctuation of the velocity and \( h' \) the fluctuation of the water depth. This approach is very simplistic, but it is sufficient to roughly estimate the maximum expected amplitudes.

- The free surface is estimated on a discretized grid, often leading to a smeared surface due to numerical diffusion. A refined grid and higher order interpolation schemes near the surface lead to a more accurate estimation.
- The steady-state transport equations were solved within inverse calculations, neglecting transient wave patterns.
- The roundoff error depends on the computer precision and the selected precision of the implemented variables in the inverse- and CFD-codes.

These CFD-model errors were indirectly quantified by verifying the forward simulations with laboratory measurements, assuming correct measurements. Sensitivity studies were performed regarding the uncertainties in bed roughness and inflow velocity distribution.

The uncertainties in estimating the discharge resulting from the inverse calculations, have their origin either in the objective function or in the minimizing algorithm.

- An objective function should have steep gradients to the searched minimum, leading to a clear finding of the minimum.
- The success of finding this minimum is not only dependent on the form of the objective function but also on the minimizing algorithm.

The uncertainties originating from the inverse calculations were quantified by considering synthetically generated series of measurements.

### 5.3 Synthetic Measurement Series

The applicability of the inverse method was investigated by using synthetically generated series of measurements from the forward computations for a given discharge \( Q \). Measurement data were obtained by sampling the computational results at a number of locations, yielding in a series of surface velocities and water level data. The concept of synthetically generated data was the preferred approach at this stage as an identical CFD-model was used for both data generation and inverse calculation. Unlike true measurements, these synthetic data are free of measurement errors but include the assumptions made in the CFD-model.
5.4. Feasibility Study

Subsequently, the discharge was estimated based on these synthetic surface velocity and water level data. The implemented inverse method could be verified since the correct discharge was known and its applicability was quantified regarding uniqueness and stability in estimating the discharge. The stability of the inverse method was investigated by perturbing the synthetic series of measurements within a known magnitude allowing for the exact quantification of the deviation in the estimated discharge. In order to obtain a realistic estimation of the magnitudes $m_v$ and $m_h$ for surface velocity and the water level data, the magnitudes were defined according to the amplitudes of the turbulent fluctuations $v'$ and $h'$ (see equation 5-1).

$$m_v = v'(k_m), \quad m_h = h'(k_m).$$

Here, $k_m$ is the mean value of the turbulent kinetic energy $k$ at the water surface of the measurement section, which was obtained from the corresponding CFD-calculations. These magnitudes were used to systematically or randomly perturb the measurements. Subsequently, the term error is used for the perturbation of the synthetic series of measurements, knowing that these errors are a combination of measurement and model error.

5.4 Feasibility Study

The feasibility study outlined here and performed in the following two chapters provides information on the applicability of the proposed inverse numerical model to estimate the discharge, which uses forward CFD-simulations within inverse calculations. The model is applicable, if the discharge can be estimated uniquely within a desired accuracy. Thus, the feasibility study includes the selection of an appropriate CFD-model to reproduce the flow field with a desired accuracy, as well as the validation of the inverse method, which is performed using synthetically generated series of measurements as described in the above section.

First, the CFD-model was validated with laboratory measurements. Then, the inverse method was verified by examining the following criteria:

- The objective function was inspected. Only one global minimum with steep gradients should exist. The contributions of each measured variable on the entire objective function indicate the suitability of each variable, because variables, which are more sensitive to discharge changes are more suitable for optimization.
- Suitable locations for the cameras for recording of particles were evaluated preliminarily by investigating the sensitivity distribution of each measured variable to discharge changes supplied by the Jacobian matrix.
- Information on the needed number of particles was obtained by performing the discharge estimation with a varying number of measurements. This information is of particular interest when considering randomly perturbed measurements to estimate the influence of the number of
measurements on regression.

- The stability of the discharge estimation was quantified by considering measurements with a systematic error at different locations.

The computations presented in the following chapters 6 and 7 applied these tests for the feasibility of the method.
6 2D Computations

The selected test case, which is suitable for 2D computations in a vertical plane, is described in section 6.1. The CFD-simulations and the inverse calculations were validated separately to strictly quantify both influences on the discharge estimation. Section 6.2 presents the validation of the CFD-model, whereas the applicability of the inverse method was determined in section 6.3 using synthetically generated series of measurements. The results of these sections were summarized and discussed in section 6.4.

6.1 Test Case

The Saltina river near Brig in Switzerland, which has a transcritical flow regime during flood events, is chosen as case-study. For this test case, measurements were performed in a Froude-similar laboratory model at a scale of 1:25 by the Laboratory of Hydraulics, Hydrology and Glaciology (VAW 1994A). The configuration was a straight rectangular channel with two sills 0.2 m apart (see figure 6.1, VAW 1994A). Non-uniform flow conditions were observed between the two sills, with a hydraulic jump for smaller flood events ($Q = 10$ to $20 \text{ m}^3\text{s}^{-1}$). The hydraulic jump moved downstream with increasing discharge.

Within this work, flow in a vertical plane along the river axis was computed, whereas secondary flows perpendicular to that plane were neglected. The following computations refer to this test case. The results of which were scaled up to the prototype dimensions.

6.2 Forward Simulation

The 2D computations were performed with the finite element code FEMTOOL (Rutschmann 1993, 1994) and its extended implementation of free surface flows (Bürgisser 1998). This section presents the results from the forward computations with constant discharge $Q$ to verify the CFD-model chosen. A sensitivity analysis was performed for different bed roughness values. Moreover,
the forward computations provided synthetic series of measurements, which were employed in
the following inverse calculations (section 6.3).

6.2.1 Geometry and Generated Grid

The river bed geometry for the computations was defined in analogy to the laboratory experiments
(VAW 1994a). Its physical dimensions are displayed in figure 6.2.

![Physical dimensions of the river bed](image)

For an initial guess of the water surface, a locally refined triangulated grid was generated with the
preprocessing program NEGEFF (Bürgisser 1998). The viscous sublayer at the solid boundary
was not resolved. The grid was only discretized to a distance from the wall, where the law-of-the-
wall is valid (equations 3-40 to 3-43). Figure 6.3 shows a generated triangular grid for a discharge
\( Q = 40 \text{ m}^3\text{s}^{-1} \), with an initial guess of the water surface.

![Generated grid with an initial guess of the water surface for a discharge \( Q=40 \text{ m}^3\text{s}^{-1} \).](image)

The grid was locally refined towards the river bed, where high velocity gradients occur. Such re-
finement was also necessary to calculate the near wall boundary conditions with the method of
Benim (section 3.4.2). This method requires that all nodes of the elements closest to the wall lie
within the validity of the law-of-the-wall. A refined section is enlarged in figure 6.4, where the dis-
tance between the discretized area and the wall is apparent.
6.2.2 Initial and Boundary Condition

The computations were performed with the steady-state transport equations (2-10, 2-16 and 2-17). Although initial conditions were not needed, an initial guess for all variables within a convergence radius was essential, because of the non-linearity in the RANS equations (2-10) as well as in the $k$- and the $\varepsilon$-transport equations (2-16 and 2-17). The initial values for the following 2D computations are listed in the table below.

<table>
<thead>
<tr>
<th>variable</th>
<th>dimensions</th>
<th>values</th>
</tr>
</thead>
<tbody>
<tr>
<td>horizontal velocity component $U_1$</td>
<td>[m s$^{-1}$]</td>
<td>0.5</td>
</tr>
<tr>
<td>vertical velocity component $U_3$</td>
<td>[m s$^{-1}$]</td>
<td>0.0</td>
</tr>
<tr>
<td>relative pressure $P$</td>
<td>[Pa]</td>
<td>hydrostatic</td>
</tr>
<tr>
<td>friction velocity $u_*$</td>
<td>[m s$^{-1}$]</td>
<td>0.0</td>
</tr>
<tr>
<td>eddy viscosity $\nu_t$</td>
<td>[m$^2$s$^{-1}$]</td>
<td>0.00005</td>
</tr>
<tr>
<td>kinetic turbulent energy $k$</td>
<td>[m$^2$s$^{-2}$]</td>
<td>0.0011 - 0.0015</td>
</tr>
<tr>
<td>turbulent dissipation rate $\varepsilon$</td>
<td>[m$^2$s$^{-3}$]</td>
<td>0.5 - 0.9</td>
</tr>
</tbody>
</table>

The initial values for the two turbulence variables $k$ and $\varepsilon$ were estimated for three examined discharge values, $Q = 20, 40, 70$ m$^3$s$^{-1}$, with equations (3-48) - (3-50) stated in section 3.4.4.

The following table provides an overview of the boundary conditions for the 2D simulations. The equation numbers stated in parentheses refer to the corresponding equations in section 3.4 for the recalculation of the boundary conditions during the computations.
Table 6.2  Boundary conditions for the 2D computations.

<table>
<thead>
<tr>
<th></th>
<th>inflow</th>
<th>outflow</th>
<th>free surface</th>
<th>solid</th>
</tr>
</thead>
<tbody>
<tr>
<td>horizontal velocity $U_1$</td>
<td>(3-47)</td>
<td>$\frac{\partial U_1}{\partial n}=0$</td>
<td>$\frac{\partial U_1}{\partial n}=0$</td>
<td>(3-40), (3-44)</td>
</tr>
<tr>
<td>vertical velocity $U_3$</td>
<td>0.0</td>
<td>$\frac{\partial U_3}{\partial n}=0$</td>
<td>$\frac{\partial U_3}{\partial n}=0$</td>
<td>(3-40), (3-44)</td>
</tr>
<tr>
<td>relative pressure $P$</td>
<td>$\frac{\partial P}{\partial n}=0$</td>
<td>$\frac{\partial P}{\partial n}=0$</td>
<td>0.0</td>
<td>$\frac{\partial P}{\partial n}=0$</td>
</tr>
<tr>
<td>kinetic turbulent energy $k$</td>
<td>0.0011 - 0.0015</td>
<td>$\frac{\partial k}{\partial n}=0$</td>
<td>$\frac{\partial k}{\partial n}=0$</td>
<td>(3-45)</td>
</tr>
<tr>
<td>turbulent dissipation rate $\varepsilon$</td>
<td>0.5 - 0.9</td>
<td>$\frac{\partial \varepsilon}{\partial n}=0$</td>
<td>$\frac{\partial \varepsilon}{\partial n}=0$</td>
<td>(3-46)</td>
</tr>
</tbody>
</table>

The free surface was calculated with the velocity-driven grid adaptation in all computations. Therefore, the relative pressure was set to zero and the free surface was calculated with the non-tangential velocity components (see section 3.3.1 for details).

The conditions at the solid boundary were calculated with the law-of-the-wall, which is also a function of the bed roughness expressed by the equivalent roughness height. This roughness was set equal to 50 mm, which corresponds to a fine- to middle-sized gravel bed (Dracos 1990). A sensitivity study was performed by choosing an equivalent roughness height of 5 mm that corresponds to quarystone revet. Figure 6.5 illustrates the influence of the two different roughness values on the water level and the surface velocities.
The sensitivity to the bed roughness is very small for the flood conditions computed here and has not been further examined for that reason. The subsequent computations were performed with an equivalent roughness height of 50 mm, because this roughness corresponded better to the river conditions in the laboratory experiments.

6.2.3 Results and Verification with Measurements

Figure 6.6 presents the velocity field of the horizontal velocity $U_1$ in the computed vertical section for the discharge $Q = 40 \text{ m}^3\text{s}^{-1}$. 

---

Fig. 6.5 Sensitivity of the water level (a) and the surface velocity (b) to bed roughness.

Fig. 6.6 Computed flow field for the discharge $Q = 40 \text{ m}^3\text{s}^{-1}$. 
The separation zones at the forward- and backward-facing steps can be recognized clearly, where the separation zone behind the first sill is displayed in an enlarged view in figure 6.7 with velocity vectors indicating the flow pattern.

![Fig. 6.7 Enlarged section of the separation zone after the first backward facing step.](image)

Figures 6.6 and 6.7 confirm that the CFD-code captures complex flow fields with Froude numbers around 1. A quantitative comparison follows, where computed water levels were compared with corresponding measurements from laboratory experiments (VAW 1994a). The following figure 6.8 shows the section with available measurements for the three computed discharge values $Q = 20, 40, 70 \text{ m}^3\text{s}^{-1}$.

![Fig. 6.8 Comparison between computed water levels and water depths measured in laboratory experiments.](image)

The average relative deviations between the computed and the measured water depths at a given discharge were between 6 and 11% of water depth. The largest relative deviation occurred at the smallest measured discharge ($Q = 20 \text{ m}^3\text{s}^{-1}$). This can be explained by an undular hydraulic jump.
which was observed at this discharge in nature as well as in the laboratory experiments. The Froude number in this case was about 1.1. This unstable flow field could not be reproduced exactly. Generally, an acceptable accuracy was obtained even though secondary cross-stream flow was neglected.

6.3 Inverse Calculations

Numerically generated series of measurements with a given discharge served as synthetic measurement data for all inverse calculations, as explained in section 5.3. For the remainder of this work, the term measurement refers to the synthetically generated measurements. The feasibility study included the investigation of the influence of different variables, number and position of measurements on the estimation of discharge as described in section 5.4. If perturbed data were considered in the calculations, the magnitude \( m_v \) to vary the velocity data was fixed by equation (5-2) using values of \( k_m = 0.01 \) and \( 0.04 \text{ m}^2\text{s}^{-2} \), resulting in relative errors of 10 and 20% with reference to the average velocity. A relative error of 20% was considered for the water level data. Furthermore, the influence of the unknown inflow velocity distribution was evaluated and additionally a form parameter for the velocity distribution was estimated by the inverse method.

6.3.1 Measurement Variables

The contributions of the horizontal and vertical surface velocity components \( (\zeta, \zeta_h) \) and water level \( (\zeta_h) \) data to the entire objective function, \( \zeta(p) \), were quantified to study their influence on the estimated discharge (see equation 4-4 for the definition of the objective functions). Figure 6.9 reveals the objective functions as well as the contributions of the different variables for the three discharge values \( Q = 20, 40, 70 \text{ m}^3\text{s}^{-1} \) considering all 250 correct measurements at the surface.
Fig. 6.9 Objective functions for the discharge values $Q = 20, 40, 70 \text{ m}^3\text{s}^{-1}$.

Each objective function, $\zeta(p)$, for the respective discharge value has only one minimum near the expected discharge. The objective function of the water level data, $\zeta_{h}(p)$, shows only small gradients for discharges of 40 and 70 $\text{m}^3\text{s}^{-1}$. The sensitivity of water level to discharge changes is only relevant for the smallest discharge of 20 $\text{m}^3\text{s}^{-1}$. Overall, the contributions of the water level, $\zeta_{h}(p)$, and the vertical velocity component, $\zeta_{z}(p)$, in the objective function are considerably smaller than that of the horizontal velocity component, $\zeta_{x}(p)$.

The sensitivity of each variable to discharge changes is provided by the Jacobian matrix (section 4.3.2). It was examined along the river axis to study the suitability of each variable for estimating the discharge in relation to its position. Figure 6.10 displays the sensitivities of the vertical and horizontal surface velocity components and of the water level for a discharge of $Q = 40 \text{ m}^3\text{s}^{-1}$.

Fig. 6.10 Sensitivities of the surface velocities in horizontal and vertical direction and for the water level to variations of discharge (around $Q = 40 \text{ m}^3\text{s}^{-1}$).
The horizontal velocity component $U_1$ is the most sensitive variable with respect to discharge changes in the entire measured region. The vertical velocity component $U_3$ and the water level respond to discharge changes only in the region of curved streamlines. The generally small influence of the vertical velocity component and the water level is in agreement with the flat form of the objective functions for these two variables (figure 6.9).

Table 6.3 lists the estimated discharges by considering correct measurement data of the horizontal and vertical surface velocity components as well as the water levels. These results were compared with the estimated discharges by taking into account only velocity-magnitude data, where the measurements of the water level were implicitly considered by generating the grid through these water levels. All 250 nodes at the free surface in the computed domain were taken as measurements for these calculations.

<table>
<thead>
<tr>
<th>expected discharge $[\text{m}^3\text{s}^{-1}]$</th>
<th>estimated discharge $[\text{m}^3\text{s}^{-1}]$</th>
<th>deviation [$%$]</th>
<th>velocity-magnitude deviation [$%$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>19.96</td>
<td>-0.2</td>
<td>19.93</td>
</tr>
<tr>
<td>40</td>
<td>40.02</td>
<td>0.05</td>
<td>40.01</td>
</tr>
<tr>
<td>70</td>
<td>69.73</td>
<td>-0.39</td>
<td>70.09</td>
</tr>
</tbody>
</table>

The discharges could be estimated with a high accuracy of less than 0.4% deviation, where the difference between case 1) and 2) is negligible. The following optimizations were carried out by only considering velocity-magnitudes, while the position of the water surface was implicitly considered by generating the grid through these measurement points. The computations were then performed on a rigid grid with a linearly interpolated water surface between the measurements. Subsequently, the term velocity is used to describe velocity-magnitude.

### 6.3.2 Number of Measurements

The number of measurements was incrementally decreased from 250 down to 5 linearly distributed measurements in the computed section to examine the influence of the number of measurements on the estimated discharge. The measurements were not perturbed for this purpose. Figure 6.11 shows the estimated discharges as a function of the number of measurements for an expected discharge $Q = 40 \text{ m}^3\text{s}^{-1}$. The standard deviations for the estimated discharges (equation 4-23) are also given. They were calculated by assuming constant standard deviations of the measured surface velocities of 0.13 ms$^{-1}$. This corresponds to 10% of the average of measured velocities.
The calculated standard deviations of the estimated discharges increase with a decreasing number of measurements (see equation 4-23). The estimated discharges have a maximum deviation of 2% from the expected discharge for all computations. This is surprising, because the water surface was only linearly interpolated between the measurement locations and therefore could only be imprecisely reproduced with smaller number of measurements. Figure 6.12 illustrates the differences between the water surfaces used, as a function of the number of water level measurements.

With 25 or more measurements, the correct water surface from the forward computation was reproduced well, whereas the water surface was poorly reproduced with 10 and 5 measurements.

The following discharge estimations were performed with perturbed measurements to estimate the influence of an increasing number of perturbed measurements on regression. This was examined for three different cases with 5, 10 and 25 measurements. For each case, ten data sets were
generated adding different white noise components of ±20% of the correct surface velocity, or ±20% of the correct water depth. Figure 6.13 shows the results with perturbed surface velocities, whereas figure 6.14 shows the results including perturbed water levels.

The calculated standard deviations of the estimated discharges, and similarly the intervals between the largest and the smallest estimated discharge for both types of errors are largest for the case with 5 measurements, and decrease when the number of measurements is increased. The reduction of the standard deviation becomes negligible when increasing the number of measurements from 10 to 25.

6.3.3 Position of Measurements

The influence of the position of measurements on the estimated discharge was examined by taking only one data point for the optimization. Two different cases were analyzed using either a data point in the upstream region at [-0.213 m, 0.144 m] or one in the downstream region at [0.582 m,
0.069 m]. The assumed water surface corresponded to the water surface in figure 6.12 for 5 measurements. Tables 6.4 and 6.5 show the estimated discharges with correct measurements as well as with a velocity error to analyze the robustness of the discharge estimation with respect to the position of measurements. The estimated discharges with a velocity error of 10% are listed in table 6.4, whereas table 6.5 refers to an error of 20%.

**Table 6.4** Estimated discharges with a velocity error of 10% for an expected discharge $Q = 40 \text{ m}^3\text{s}^{-1}$.

<table>
<thead>
<tr>
<th>estimated discharge (\text{m}^3\text{s}^{-1})</th>
<th>correct</th>
<th>deviation [%]</th>
<th>+10%</th>
<th>deviation [%]</th>
<th>-10%</th>
<th>deviation [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>upstream point ([-0.213m, 0.144m])</td>
<td>40.65</td>
<td>1.6</td>
<td>45.88</td>
<td>14.7</td>
<td>35.28</td>
<td>-11.8</td>
</tr>
<tr>
<td>downstream point ([0.582m, 0.069m])</td>
<td>39.20</td>
<td>-2.0</td>
<td>56.15</td>
<td>40.4</td>
<td>14.73</td>
<td>-63.2</td>
</tr>
</tbody>
</table>

**Table 6.5** Estimated discharges with a velocity error of 20% for an expected discharge $Q = 40 \text{ m}^3\text{s}^{-1}$.

<table>
<thead>
<tr>
<th>estimated discharge (\text{m}^3\text{s}^{-1})</th>
<th>correct</th>
<th>deviation [%]</th>
<th>+20%</th>
<th>deviation [%]</th>
<th>-20%</th>
<th>deviation [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>upstream point ([-0.213m, 0.144m])</td>
<td>40.65</td>
<td>1.6</td>
<td>50.99</td>
<td>27.5</td>
<td>29.67</td>
<td>-25.8</td>
</tr>
<tr>
<td>downstream point ([0.582m, 0.069m])</td>
<td>39.20</td>
<td>-2.0</td>
<td>71.35</td>
<td>78.4</td>
<td>not converged</td>
<td></td>
</tr>
</tbody>
</table>

A surface velocity error of 10 or 20% at the upstream point led to a discharge error of a similar magnitude. However, a surface velocity error at the downstream measurement had a much larger influence on the estimated discharge. The relative error of the estimated discharge was between 40 and 60% with a 10%-error of the surface velocity and almost 80% with a 20%-error of the velocity. No convergence was achieved, when decreasing the velocity by 20% at the downstream data point. With such a velocity, subcritical flow would dominate in the downstream, which is not realistic. By increasing the velocity error from 10 to 20%, the error in the estimated discharge was also about doubled compared to a velocity error of 10%.

The different behaviour of the two measurement locations is due to the difference in sensitivity of the local surface velocity to discharge changes (see figure 6.10). Figure 6.15 illustrates this relation between stability and sensitivity by displaying the objective functions for the case with a 10%-velocity error.
6.3. Inverse Calculations

The objective functions for the downstream measurement location are flatter than the ones for the upstream measurement location, because of the less sensitive measurements on discharge changes. Furthermore, the discharge estimation was more stable for velocity measurements, which are more sensitive to discharge changes, i.e., a velocity error led to a smaller discharge error by considering more sensitive velocity measurements.

Table 6.6 lists the estimated discharges when considering water level data perturbed by 20% of the correct water depth, but with correct velocity measurements.

<table>
<thead>
<tr>
<th>estimated discharge $[\text{m}^3\text{s}^{-1}]$</th>
<th>correct</th>
<th>deviation [%]</th>
<th>+20%</th>
<th>deviation [%]</th>
<th>-20%</th>
<th>deviation [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>upstream point $[-0.213\text{m}, 0.144\text{m}]$</td>
<td>40.65</td>
<td>1.6</td>
<td>42.03</td>
<td>5.1</td>
<td>37.34</td>
<td>-6.7</td>
</tr>
<tr>
<td>downstream point $[0.582\text{m}, 0.069\text{m}]$</td>
<td>39.20</td>
<td>-2.0</td>
<td>40.39</td>
<td>0.97</td>
<td>40.10</td>
<td>0.25</td>
</tr>
</tbody>
</table>

When a water level error was considered, the results were opposite to the results with a velocity error. An error in the water level had a larger influence on the discharge at an upstream measurement point and was negligible at a downstream point. The negligible influence of a water level error for the downstream measurement is due to the supercritical flow regime.
6.3.4 Inflow Velocity Distribution

In this section, the influence of the velocity distribution at the inflow boundary on the estimated discharge was examined. In the previous inverse calculations, the velocity distribution was assumed to be a logarithmic profile (equation 3-47) as for the forward computations. Because the measurements were generated synthetically by the forward computations, the “correct” velocity profile was assumed for the inverse calculations, although it is usually unknown.

The velocity distribution was varied by assuming either an exponential distribution

\[ U_h = \frac{q(r_{e1} + l)}{H + \delta_w(l - r_{e2})} \left( \frac{Y_h + \delta_w}{H + \delta_w} \right)^{r_{e1}}, \]  

(6-1)

with \( r_{e1} = 0.5 \) and \( r_{e2} = 0.1 \), or a uniform distribution with equal velocities over the entire water depth, and comparing the results with the previous results for the logarithmic distribution. The different velocity distributions at the inflow boundary are shown in figure 6.16.

![Fig. 6.16 Velocity distributions at the inflow boundary.](image)

Four different data sets were examined. Two sets considered only one data point, one upstream \([-0.213 \text{ m}, 0.144 \text{ m}]\) and the other one downstream \([0.582 \text{ m}, 0.069 \text{ m}]\). Another data set considered 5 data points and the last set used 25 data points. All data sets considered correct measurements. Table 6.7 gives an overview of the discharges estimated with different inflow velocity distributions in comparison to the original logarithmic distribution which was taken for the forward computations.
Table 6.7  Estimated discharges for a varying velocity distribution at the inflow boundary for an expected discharge \( Q = 40 \, \text{m}^3\text{s}^{-1} \).

<table>
<thead>
<tr>
<th></th>
<th>estimated discharge ([\text{m}^3\text{s}^{-1}])</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>original deviation</td>
</tr>
<tr>
<td></td>
<td>[%]</td>
</tr>
<tr>
<td>1 upstream point</td>
<td>40.65</td>
</tr>
<tr>
<td>([-0.213 , \text{m}, 0.144 , \text{m}])</td>
<td>1.6</td>
</tr>
<tr>
<td>1 downstream point</td>
<td>39.20</td>
</tr>
<tr>
<td>([0.582 , \text{m}, 0.069 , \text{m}])</td>
<td>-2.0</td>
</tr>
<tr>
<td>5 data points</td>
<td>39.67</td>
</tr>
<tr>
<td></td>
<td>-0.82</td>
</tr>
<tr>
<td>25 data points</td>
<td>40.63</td>
</tr>
<tr>
<td></td>
<td>1.6</td>
</tr>
</tbody>
</table>

The velocity distribution at the inflow boundary had a significant influence on the estimation of discharge. For the exponential distribution, the discharge was estimated to be too small by 12-15\% for any number of exact measurements. This is explained due to larger surface velocities for a given discharge. Correspondingly, the estimated discharge was 3-16\% larger, when assuming a uniform distribution. The closest match was obtained, when only one downstream data point was taken into account, at a distance where the asymptotic velocity profile had already developed downstream of the boundary.

Further investigations were made by fitting the discharge \( Q \) and the parameter \( p_H \) in equation (3-47) which specifies the form of the logarithmic velocity distribution at the inflow. Figure 6.17 shows the objective function as a function of \( Q \) and \( p_H \) for the expected discharge \( Q = 40 \, \text{m}^3\text{s}^{-1} \). All 250 exact measurements in the interval \([-0.35 \, \text{m}, 0.65 \, \text{m}]\) were included.
The objective function shows a minimum in the form of a flat valley. The solution of the inverse problem is therefore non-unique and depends on the starting values.

The results in table 6.7 indicate that the estimation of the discharge is sensitive to the velocity distribution at the inflow boundary. An additional parameter, which describes the inflow velocity distribution cannot be estimated, since the solution is then non-unique. The influence of the inflow velocity distribution can be suppressed by choosing the inflow boundary at a distance of about 25-50 times the hydraulic diameter upstream of the measurement section. This distance allows for a uniform velocity profile to develop into a fully turbulent profile (Schlichting 1965).

6.4 Summary and Discussion of the 2D-Computations

The 2D vertical model used can be applied to complex river bed geometries and transcritical flow regimes, if secondary cross-stream flow can be neglected. The water surface could be computed with an acceptable accuracy. The average relative deviations between the computed and the measured water depths at a given discharge were between 6 and 11% of water depth. The sensitivity of the water levels and the surface velocities due to different bed roughness values is negligible for the studied flood conditions, due to the decreasing influence of bottom friction at larger discharges.

The sensitivity of the water level to discharge changes is very small. This decreasing sensitivity for larger discharges is a general phenomenon in open channel flow and can be observed at probably all stage-discharge curves where no special hydraulic phenomena occur, such as hydraulic jumps and standing waves.
Few measurements are needed for the optimization of the discharge. In principle, one measured surface velocity in the upstream region is sufficient to predict the discharge with a high accuracy (i.e., within 2%), in case no errors in measurements or in the CFD-model are assumed. The water surface between the measurement locations can be reproduced approximately without loss of accuracy for the estimated discharge.

When assuming an error in the surface velocity or water level data, the number of measured data should be at least 10, for the case presented. More reliable discharge estimates were obtained with an increasing number of measurements for small numbers of measurements, but the improvement of the reliability was negligible for more than 10 measurements in the presented case. The larger number of measurements can help to reduce the influence of uncertainties or errors in measurements and model assumptions, such as turbulent fluctuations.

The influence of errors in the surface velocity data on the discharge estimation becomes larger for measurements further downstream, where the sensitivity to discharge changes is smaller. The relative discharge error was around 1.5 times the magnitude of the relative velocity error in the upstream region, and exceeded the magnitude of a surface velocity error by a multiple (4-6 fold) in the downstream region. An error in water level data had a small influence on the discharge. This influence was even smaller for measurements further downstream.

The estimation of the discharge is sensitive to the velocity distribution at the inflow boundary. The optimization of an additional parameter describing the velocity distribution at the inflow boundary resulted in a non-unique solution. Thus, the inflow boundary should be set upstream of the measuring area at a distance of about 25-50 times the hydraulic diameter, to rule out the influence of the inflow velocity distribution.

Generally, only very few inverse iteration cycles were necessary (i.e., 3-4 iterations) in the investigations presented. The CPU-time of one CFD-cycle performed on a Sun SPARC 10 with 512 Mbytes of memory was about 1 hour. Thus, one optimization took about 6-8 hours.
7 3D Computations

The results of the 3D computations are presented in a similar fashion as those of the 2D computations. The selected test case is described first in section 7.1. The CFD-model as well as the inverse formulation were validated separately, with the CFD-model verified in section 7.2, followed by the validation of the inverse formulation in section 7.3. The last section (7.5) discusses the results obtained from the 3D computations.

7.1 Test Case

A 90° bend in a river section with a naturally graded river bed, examined by HERSBERGER (2000) in a laboratory experiment, was chosen as case-study. Measurements were available for the position of the river bed and for the water surface at 1404 points, as well as for the velocity distribution at 10 cross-sections in the bent section for a discharge $Q = 0.15 \text{ m}^3\text{s}^{-1}$, corresponding to an inflow Froude number $Fr = 0.89$. The river bed geometry of the flume is displayed in figure 7.1.

![River bed geometry of the flume.](image)

Fig. 7.1 River bed geometry of the flume.
The characteristic particle diameter for the base sediment mixture, $d_{g0}$, varied between 19.7 mm at the outside of the bend and 5.5 mm at the inside of the bend, with an average characteristic diameter of $d_{g0(\text{avg})} = 14.83$ mm. Thus, the equivalent roughness height $k_s$ is (Jäggi 1995),

$$k_s = 2d_{g0(\text{avg})} = 30 \text{ mm},$$

which corresponds to sandy gravel. Figure 7.2 displays the measured water level and water depth, respectively, for a discharge $Q = 0.15 \text{ m}^3\text{s}^{-1}$.

![Fig. 7.2 Measured water level (left) and water depth (right).](image)

The left figure shows a higher water level at the outside of the bend due to the centrifugal force, whereas the right figure reveals the large differences in water depth between the inside and the outside of the bend. At about a 40°-angle, the water depth is 10 times larger at the outside than at the inside. These measurements already indicate that the corresponding flow-field is non-trivial and that a 3D CFD-model is required to accurately model such a flow-field.

### 7.2 Forward Simulation

The commercial CFD-code FLUENT (2000) was chosen for the 3D computations, where the free surface was calculated with the Volume-of-Fluid (VOF) method (section 3.3.2) and the turbulence was considered with the standard $k$-$\varepsilon$ model (2.3). Sensitivity studies were performed for different bed roughness values and different velocity distributions at the inflow boundary. The computations were verified with measurements introduced in section 7.1 (HERSBERGER 2000) and provided a synthetic set of data for the inverse calculations.
7.2.1 Geometry and Generated Grid

The computational domain was defined according to the geometry of the laboratory flume with the river bed displayed in figure 7.1 and horizontal side walls. A regular hexahedral grid was generated with the preprocessor GAMBIT (2000), which is part of the FLUENT package. Figure 7.3 shows the initial regular grid in a horizontal section, as well as in a cross-section at 40° of the bend.

The initial grid was refined near the side walls and also from the inflow and outflow boundary towards the bend, having the finest grid near 40°. During the computations the grid was locally refined at the near-wall region to fulfill the condition for the cell-centroids of the closest cells to the wall to lie within a distance $Y$ of the wall, where the law-of-the-wall is valid. The region of the free surface was also refined during the computations. The resulting refined grid at the river bed after the computations, which satisfies the criterion at the wall, is displayed in figure 7.4.
The grid is finer at the outer bend, where higher shear stresses exist (see section 3.4.2, equation 3-42, about the relation between shear stress and distance to wall).

7.2.2 Initial and Boundary Condition

The transient transport equations (2-10, 2-16 and 2-17) were solved to approximate the final result, whereas the final solution as well as the computations in an inverse cycle were based on the steady-state transport equations. Since only the final solution is of interest, the initial conditions chosen are irrelevant as long as all variables are initialized within a convergence radius, because of the non-linearity of the RANS equations (2-10), and the $k$- and $\varepsilon$-transport equations (2-16 and 2-17). The discretized domain was initially divided up into a region filled with water and on top of it a layer of air, assuming a horizontal interface. The initial velocity field in the domain was assumed to be uniform with the velocity magnitude equal to the corresponding inflow boundary condition. The turbulence variables $k$ and $\varepsilon$ in the flow field were also initialized to the values chosen for the inflow boundary condition.

The inflow boundary was divided up into two separate boundaries, one for the water phase and one for the air phase, resulting in a fixed water depth at the inflow. A logarithmic velocity profile was defined in the water phase according to equation (3-47) in section 3.4.4. A sensitivity analysis for different velocity distributions at the inflow boundary follows in section 7.2.3. A uniform inflow
velocity profile for the air phase was defined as described in section 3.4.4. The turbulence variables \( k \) and \( \varepsilon \) at the inflow boundary were defined as described in equations (3-49) and (3-50), respectively.

At the solid boundaries, the law-of-the-wall was applied for the calculation of the shear stress, set as Neuman boundary condition, according to equation (3-40). The turbulence variable \( \varepsilon \) was calculated with equation (3-45) and a Neuman boundary condition equal to zero was defined for \( k \). The law-of-the-wall is a function of the bed roughness expressed by the equivalent roughness height. Since the roughness varies at the river bed between \( k_s = 10 \text{ mm} \) and 40 mm, a sensitivity study was performed for different uniform roughness values in section 7.2.3. A uniform roughness value for the entire river bed was applied in the computations, because only the range is known but not its distribution.

At the upper boundary, zero convective and diffusive flux over the boundary was assumed (see section 3.4.3 for details), while Neuman boundary conditions equal to zero were chosen for all variables at the outflow boundary (section 3.4.5).

### 7.2.3 Sensitivity Studies

#### Inflow Velocity Distribution

The inflow velocity distribution was assumed as a logarithmic profile as described by equation (3-47). The velocity distribution was not measured in the laboratory experiments. A sensitivity analysis was performed by defining a uniform velocity distribution at the inflow boundary and comparing the computed water levels and surface velocities with the corresponding results with a logarithmic velocity profile at the inflow boundary. Figure 7.5 shows the difference in water level and surface velocity between computations with the two different inflow velocity distributions.

![Fig. 7.5](image-url)  
**Fig. 7.5** Difference in water level and surface velocity due to different inflow velocity profiles.
The difference in water levels is negligible, whereas the surface velocities differ by about 5% in the upstream region. By assuming a uniform distribution, surface velocities were lower at the upstream region, but higher at the inner bend, compared to the results with a logarithmic profile. The difference in surface velocity decreases with increasing distance from the inflow boundary and is negligible downstream from approximately 45°. Figure 7.6 illustrates the development of the two velocity distributions in the cross-sections at distances of 1 to 7 meters from the inflow boundary for the logarithmic (left) and the uniform (right) inflow velocity profile.

![Figure 7.6](image)

Fig. 7.6 Development of a logarithmic (left) and a uniform (right) inflow velocity profile.

The cross sections reveal that the two velocity profiles still differ at a distance of 7 meters from the inflow boundary, which is at the end of the straight channel section. This agrees with the results shown in figure 7.5, where the differences in surface velocities due to the two inflow velocity distributions are not yet negligible at a distance of 7 m from the inflow boundary.

**Bed Roughness**

A sensitivity study was performed by varying the bed roughness, with one roughness assumed as the average roughness in the river bed $k_s = 30$ mm and the other roughness $k_s = 15$ mm representing the locations with the finest material in the inner bend of the river bed. Figure 7.7 shows the influence of the two different roughness values on the water level and the surface velocity.
The surface velocity is generally higher for the computations with a smaller roughness, leading to negative differences. The smaller velocities for the computations with the smaller roughness around the end of the bent river section might be caused by a stronger separation zone. The water level is lower in the entire displayed river section for the computations with the smaller bed roughness. Despite the significant difference in bed roughness, the computed differences in water level and surface velocities are negligible, i.e., the surface velocity difference is less than 0.1% of the average surface velocity and the difference in water depth is less than 0.5% of the corresponding water depth.

A further sensitivity study was performed by considering a roughness value of $k_s = 3$ mm, which corresponds to a stone wall bed. Such a roughness value was not present in the flume of the case study in section 7.1, but the sensitivity provided general information on the influence of the bed roughness in similar geometries. The differences between the computed surface velocity (left) and water level (right) for the two roughness values $k_s = 30$ mm and $k_s = 3$ mm are displayed in figure 7.8.
The differences in the computed surface velocities and water levels are generally higher than those presented in figure 7.7, because of the larger difference in bed roughness. This allows to draw more distinct conclusions than for the computations presented above. The surface velocities are higher in the entire displayed river section for the computations with the smaller bed roughness, the difference being larger at the outside of the bend than at the inside. The difference in water levels is correspondingly larger at the outside of the bend. Generally, the differences are no longer negligible, with a difference in surface velocity up to 5% of the average surface velocity and a difference in the water level up to 10% on average. The computations performed subsequently considered an equivalent roughness height $k_s = 30 \text{ mm}$ only.

### 7.2.4 Results and Verification with Measurements

This section presents computed details of the separation zone at $90^\circ$, followed by the verification of the computed water surface and velocities with laboratory measurements.

Figure 7.9 illustrates the separation zone at $90^\circ$ with surface velocity vectors and contours of the velocity magnitude at the water surface.
The velocity vectors indicate the vortex in the separation zone, where the velocity is close to zero. The computed water depths were compared with laboratory measurements in figure 7.10 for the given discharge $Q = 0.15 \text{ m}^3\text{s}^{-1}$.

Fig. 7.9 Surface velocity vectors around the separation zone at 90°.

Fig. 7.10 Comparison between computed and measured water depth.
The computed water depths agree well with the measurements both in location and magnitude. The computed minimum in water depth at around $40^\circ$ was less stretched-out compared to the measurements, whereas the computed minimum at around $90^\circ$ has a smaller water depth than the corresponding measured minimum. Between the two minima a higher water depth was computed. A quantitative comparison is given in figure 7.11, where the absolute differences in water depth are displayed, besides the relative differences.

![Differences between computed and measured water depth](image)

**Fig. 7.11** Differences between computed and measured water depth.

The deviations in water depth are largest around the separation zone at $90^\circ$. The amplitude is between minus and plus 3 cm. For more than 90% of the river section, the difference between computed and measured water level is less than 20%. The largest relative differences occur at the inner side of the bend, where the water depth is very small. The absolute differences in water depth are more equally distributed over the entire section. The average relative deviation, calculated from the deviations at all measurement locations, is 6.2%.

Figure 7.12 shows the comparison between the computed and the measured velocity magnitude in a cross-section at $40^\circ$ of the bend, where the difference in water depth between inner and outer side of the bend is largest. The contour of the computed velocity magnitude for the entire cross-section is shown in (a), together with the vectors of the computed velocity magnitude (white arrows) at the measurement locations (black arrows). (b) displays the difference between computed and measured velocity magnitude.
The deviations in velocity magnitude are largest at the inner bend, where the computed velocity magnitude is generally higher than the measured. The near bed region cannot be considered as no measurements were available there. The relative deviations are between 13 and 18% for the measurements at the inner bend and are less than 5% at the outer bend where the main stream is.

7.3 Inverse Calculations

The applicability of the inverse method was investigated by using synthetically generated series of measurements from the forward computations presented in section 7.2. A feasibility study investigated the influence of different number and locations of measurements on the estimation of discharge as described in section 5.4. To study the robustness of the inverse method, perturbed data were applied (see section 5.3). The velocity data were perturbed with the magnitude $m_v$ calculated with equation (5-2), using values of $k_m = 0.005$ and $0.025 \text{ m}^2\text{s}^{-2}$. The resulting relative errors were 7 and 16% of the average surface velocity.
Measurement Variables

Velocity data were considered by their magnitude, thus, the spatial velocity components were not treated as separate measurements. An independent consideration of the three components would not be appropriate, because of the bent river section geometry, where the sensitivity to discharge changes would be dominated by the x-velocity component, before the bend and by the y-velocity component after the bend. All following calculations considered water level and surface velocity measurements as variables, with the term velocity referring to the velocity-magnitude.

The sensitivity of these two variables to discharge changes, given by the Jacobian matrix, was examined for the whole river section to study the suitability of each variable for estimating the discharge in relation to its position. Figure 7.13 displays the sensitivities of the water level (left) and the surface velocities (right) for a discharge $Q = 0.15 \text{ m}^3\text{s}^{-1}$ in the bent section, while figure 7.14 corresponds to a discharge $Q = 0.17 \text{ m}^3\text{s}^{-1}$.
The high sensitivity of the surface velocity to discharge changes at the upstream region for both discharges is misleading, because it originates from the fixed inflow water depth (see section 7.2.2 on page 72). At the inflow boundary, a variation in discharge only leads to a variation in velocity. Thus, the following interpretations are limited to the downstream section, where the influence due to the fixed water depth at the inflow boundary is negligible.

The sensitivity of the water level to discharge changes decreased with increasing discharge. This can be clearly seen on the left of the two figures 7.13 and 7.14. The sensitivity of the surface velocity to discharge changes increased for an increasing discharge at the outside of the bend, whereas it decreased at the inside of the bend. This decreasing sensitivity indicates a stronger developed separation zone at the inside. Generally, a reduced sensitivity was determined in the separation zones on the inside of the bend for both variables.

### 7.3.2 Number of Measurements

The influence of the number of measurements on the discharge estimates was evaluated by considering 5, 10 or 25 measurements. All measurements were selected from a section of the computed flow field where the sensitivities of the measurements to discharge changes are similar. Figure 7.15 illustrates the locations of the selected measurements.

![Fig. 7.15 Locations of the chosen measurements for the investigation of the number of measurements.](image)

The discharge estimations were performed by either using the correct measurements, or by adding/subtracting a systematic error to the velocity data. A 10%-error of the correct surface velocity was applied, in accordance to the calculated error magnitude on page 79. The resulting estimated discharges are listed in table 7.1.
Table 7.1  Optimized discharges either with correct velocities or with a systematic velocity error of 10% for cases with 5, 10 and 25 measurements.

<table>
<thead>
<tr>
<th>Measurements</th>
<th>Correct Discharge [m³s⁻¹]</th>
<th>Deviation [%]</th>
<th>+10% Discharge [m³s⁻¹]</th>
<th>Deviation [%]</th>
<th>-10% Discharge [m³s⁻¹]</th>
<th>Deviation [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>5 measurements</td>
<td>0.1468</td>
<td>-2.1</td>
<td>0.1980</td>
<td>32.0</td>
<td>0.1227</td>
<td>-18.2</td>
</tr>
<tr>
<td>10 measurements</td>
<td>0.1524</td>
<td>1.6</td>
<td>0.1964</td>
<td>30.9</td>
<td>0.1155</td>
<td>-23.0</td>
</tr>
<tr>
<td>25 measurements</td>
<td>0.1492</td>
<td>-0.53</td>
<td>0.1983</td>
<td>32.2</td>
<td>0.1047</td>
<td>-30.2</td>
</tr>
</tbody>
</table>

If correct measurements were considered, the discharge could be estimated with a high accuracy of less than 2.1% deviation from the expected discharge. More accurate results were obtained with more measurements. A systematic error of 10% in velocity measurements leads to a significant error of up to 30% in the estimated discharge, and a larger number of measurements does not decrease the discharge error. Subtracting 10% from the correct velocity measurements, the largest deviation from the expected discharge was obtained with 25 measurements. The larger discharge error, when considering more systematically perturbed measurements, indicates that some of the additional measurement locations lead to a significant error increase. But if no error was considered, the flow field can be represented better with more measurements. This is also illustrated with the objective functions in figure 7.16.

![Figure 7.16](image.png)  
**Fig. 7.16** Objective functions for 5 and 25 measurements with the contribution of surface velocities and water levels.
Both objective functions show only one minimum near the expected discharge. The minimum obtained with 25 measurements agrees better with the expected value. This may be due to better representation of the flow field with more measurements.

The results presented above considered a systematic error, where each velocity measurement was altered by exactly 10% of its correct value. The subsequent investigation reveals the influence of the number of measurements on the estimated discharge by adding different white noise components between ±10% to the correct surface velocity. The three cases were examined with 5, 10 and 25 measurements, where for each case ten data sets were generated adding these different white noise components. Figure 7.17 shows the results for the cases with 5, 10 and 25 measurements.

The calculated standard deviations of the estimated discharges as well as the intervals between the largest and the smallest estimated discharge are largest for the case with 5 measurements, and become smaller with the number of measurements added. The deviations of all estimated discharges from the expected discharge are overall significantly smaller than the deviations obtained for data with a systematic error.

### 7.3.3 Position of Measurements

The influence of the location of perturbed measurements on the estimated discharge was examined using only one measurement point for the optimization. Two different cases were analyzed using either a measurement halfway through the bend at 45°, where the sensitivity of the velocity on discharge changes is high \(\frac{\partial U(Q)}{\partial Q} = 3.7\), or one at the outside of the bend at 90° with a smaller sensitivity \(\frac{\partial U(Q)}{\partial Q} = 2.7\), see figure 7.18.
Table 7.2 lists the optimized discharges for the two examined cases considering either correct surface velocity measurements or adding, respectively subtracting, 10% of the correct surface velocity.

Table 7.2  Optimized discharges with correct velocities and with a 10%-error for two different locations.

<table>
<thead>
<tr>
<th>Location</th>
<th>Correct Discharge</th>
<th>Deviation [%]</th>
<th>+10% Discharge</th>
<th>+10% Deviation [%]</th>
<th>-10% Discharge</th>
<th>-10% Deviation [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 measurement at 45°</td>
<td>0.1473</td>
<td>-1.8</td>
<td>0.1774</td>
<td>18.3</td>
<td>0.1273</td>
<td>-15.1</td>
</tr>
<tr>
<td>1 measurement at 90°</td>
<td>0.1491</td>
<td>-0.6</td>
<td>0.1929</td>
<td>28.6</td>
<td>0.1253</td>
<td>-16.5</td>
</tr>
</tbody>
</table>

A surface velocity error of 10% for the more sensitive measurement (45°) to discharge changes led to a smaller discharge error than for the less sensitive measurement (90°). The difference between the two cases is larger when adding 10% to the correct velocity measurement: The error in the estimated discharge for the more sensitive measurement is +18%, compared to a +28% discharge error when considering the less sensitive measurement. The difference between the two estimated discharges is less when considering velocity measurements which are 10% too small.
7.4 Accuracy of the Discharge

The accuracy of the estimated discharge depends on the accuracy of the measurements, the assumptions in the CFD-model and the inverse formulation. Measurement errors and errors resulting from assumptions in the CFD-modelling lead to water level and surface velocity errors in the objective function (equation 4-3, formulated for the discharge $Q$ as the only optimization parameter),

$$\zeta(Q) = \sum_{i=1}^{N} \frac{|y_i^*-y_i(Q)|^2}{\sigma_i^2}. \quad (7-2)$$

A measurement error leads to deviations in the measured quantities $y_i^*$ and a model error results in deviations of $y_i(Q)$. Both effects may shift the minimum of the objective function on the parameter axis leading to a discharge error. This discharge error is a combination of the two effects, which are discussed separately in the following.

The characteristics of a measurement error was found to be mainly random (see section 5.2). This allows to minimize the influence of a measurement error on the estimated discharge by increasing the number of measurements. The presented 3D case-study showed that a randomly distributed 10%-error in surface velocity resulted in a discharge error of up to 20% when considering 5 measurements but was no larger than 8% when considering 10 measurements. In section 5.2 a velocity error originating from PTV-measurements was estimated to be 2% for optimal laboratory conditions. For river sections, measurement errors may be larger (e.g., 5%, Siedschlag 2001) through less accurate calibration, reflection at the surface, surface waves, irregular particles, etc. A discharge error of 4% is deduced when considering 10 measurements. If the measurement error is not only random, a larger discharge error must be expected.

An error in the computed quantities, $y_i(Q)$, can lead to a significant discharge error, because these errors are mainly systematic (see section 5.2). The results in section 7.2.4 revealed that the velocities could be computed with a high accuracy in the main stream with deviations less than 5%. The deviations were larger at the inside of the river bed, but this region is of minor interest in the discharge estimation procedure as the contribution to total flow is small. Also, the sensitivity of velocity to discharge changes is generally low in this region and therefore it is not suitable for the discharge estimation (see section 7.3.1). A relative velocity error of 5% would lead to a relative discharge error of 7.5% with an error propagation factor of 1.5 as was evaluated for optimal measurement positions (see section 7.3.3).

The inverse formulation can be responsible for a part of the discharge error too, because it may not describe and/or find the exact minimum of the objective function. The results with correct synthetic measurements showed that the estimated discharge was within 2.1% of the exact discharge. The error associated with the inverse procedure is definitely smaller than that originating from the other two sources of error.
The accuracy of the discharge is affected by the 3 error sources discussed above. Assuming a discharge error of 5% from PTV-measurements, 7.5% from CFD-modelling, and 2% from the inverse problem, the expected error is the geometric sum and amounts to 9%.

7.5 Summary and Discussion of the 3D-Computations

The employed 3D CFD-code can be applied to complex river geometries with a naturally eroded river bed and also for flow fields with separation zones. The VOF-algorithm used to calculate the position of the free water surface obtained acceptable results with a deviation of less than 20% from the measured water surface. The largest relative deviations occurred at the inside of the bend, where the water depth was only around 3 cm and the average relative deviation from all measurements is 6.2%. The velocity magnitude in a complex cross section at 40° of the bend could be computed with deviations of less than 5% in the main stream. The deviations were larger at the inside of the bend (13-18%), where the velocity magnitude was generally smaller. The relative inflow velocity distribution at fixed discharge influences the surface velocity up to about 45° into the bend. Downstream of this distance, the influence of the assumed inflow velocity profile is negligible. The influence of the river bed roughness on surface velocities and water levels is small for the roughness values measured in the flume.

The CFD-code chosen is adaptable to the inverse problem formulation without code modifications. A shell-script can be formulated, which is executed automatically after the CFD-code was started from the inverse program routines. This script can include the definition of the inflow boundary with the actual estimation of the discharge Q and also the output of water level and surface velocity at the end of one CFD-cycle. The free surface information may be saved in a file, to allow for the comparison between measurements and corresponding computed quantities within the inverse program routines. The output of the free surface contains a few zero values for the water level. These values were not considered, when searching the closest computed value for a measurement location.

The sensitivity of the water level to discharge changes becomes smaller for increasing discharge due to a decreasing influence of bottom friction. This is in accordance with the results obtained by the 2D computations. The sensitivity of the surface velocity to discharge changes increases at the outside of the bend for increasing discharge and decreases at the inside of the bend, where the separation zone becomes larger.
Few measurements are needed to estimate the discharge. One measured surface velocity is enough to predict the discharge with a high accuracy (i.e., within 2.1%), when no measurement error is assumed and a model error through uncertainties in geometry, bed roughness or empirical assumptions is neglected.

Considering a surface velocity error, an increasing number of measurements can decrease the error in the estimated discharge, if the velocity error is random. More reliable discharge estimates were obtained with an increasing number of measurements for a small number of measurements, but the improvement of the reliability is small for more than 10 measurements in the present case. Consequently, a larger number of measurements can help to minimize the influence of, e.g., outliers and turbulent fluctuations. The number of measurements showed, however, no effect on the estimated discharge, when a systematic error was considered.

The influence of an error in surface velocity measurements on discharge estimates becomes larger for measurements with smaller sensitivities to discharge changes. An a priori estimation of these sensitivities for an expected discharge range, based on computations only, will therefore allow to optimize the selection of locations for velocity measurements.

The error of the estimated discharge was calculated to 9% for the 3D computations under consideration of a 5% measurement error of the surface velocity, and a 5% velocity error resulting from CFD-modelling. A larger deviation must be expected in natural rivers. The PTV-measurement error was assumed under consideration of prototype dimensions, but the error resulting from CFD-modelling may be larger due to uncertainties in river bed geometry and roughness.

Only 3 to 4 inverse iteration steps were needed to find the minimum of the objective function. Nevertheless, the CPU-time was rather high with one CFD-cycle consuming about 5 hours on a HP PA8500 with 2GB of memory. One inverse iteration step included three CFD-cycles: One was needed for calculating the deviations between computations and measurements and two were required to build the central differences for the Jacobian matrix. Thus, 50-65 hours were needed for one optimization of the discharge.
8 Summary and Conclusions

This chapter summarizes and concludes the findings of this work and gives recommendations for future research. Section 8.1 summarizes the motivation, the proposed method and the case-studies performed. The main conclusions that reveal the advantages, limitations and expected accuracy of the proposed method are stated in section 8.2. The last section 8.3 directs the perspective towards future work and points out aspects for further investigations.

8.1 Summary

Flows in rivers are commonly evaluated using gauging station records and the corresponding stage-discharge curve. This curve is obtained with calibration measurements, usually only for moderate flows. For large flood events, the curve has to be extrapolated leading to major uncertainties in the estimation of the corresponding flood discharge and any further hydrologic calculations.

The proposed method to estimate flood discharge in rivers is based on an inverse numerical model, which uses water level and surface velocity measurements. This inverse numerical model consists of an inverse problem formulation around a CFD-model. The CFD-model provides the connection between the flow field in the section where measurements are available and the inflow to the section modelled. Thus, the inverse method adjusts the flow field to the measurements by varying the discharge, defined at the inflow boundary. The inverse method uses the Levenberg-Marquardt optimization algorithm and was combined either with a 2D CFD-model to compute a vertical section, or with a full 3D CFD-model.

The inverse numerical model was applied to two different case-studies. One test case was a straight rectangular channel allowing for computations with the 2D CFD-model, whereas the other case required a full 3D CFD-model because of a 90° bend in its geometry. For both cases, laboratory measurements were available for flood situations with high Froude numbers, \(Fr \geq 0.89\), to verify the respective CFD-model. The results of the forward simulations of both case-studies showed acceptable agreement between the computed free-surface flow and the measurements (i.e., the average relative error in water depth was between 6 and 11% for the 2D-computations, and 6.2% for the 3D-computations, the error in velocity magnitude in a cross-section was between...
3 and 18% for the 3D computations). A sensitivity analysis was performed for different roughness values, where the influence of different realistic roughness values on the water level and surface velocity was found negligible.

The inverse method was tested regarding uniqueness and stability, whereby synthetically generated series of measurements were considered. The discharge could be estimated uniquely, if the inflow velocity distribution and the river bed geometry were assumed to be known. One measurement was enough to predict the discharge with a high accuracy (i.e., within 2.1% for both case-studies), when no error in water level and surface velocity data was assumed. The sensitivity of water level data to discharge changes was small in the entire computed river section, for both case-studies. It was smaller even for higher discharge values.

The influence of random errors on the estimated discharge was minimized by increasing the number of measurement points. However, the improvement of the reliability of the discharge estimate was small for using more than 10 measurements in the presented two cases.

The stability of the proposed method depended considerably on the measurement location in the river section. The discharge estimation was more stable, when measurements were taken at locations where the sensitivity of the measurements to discharge changes was higher. By choosing appropriate measurement locations, the relative discharge error was around 1.5 times the magnitude of the relative velocity error applied in the investigated cases. The relative discharge error surpassed the magnitude of the relative velocity error 4-6 fold in the 2D computations, if the measurement locations were poorly selected.

The influence of different inflow velocity distributions was examined and the estimated discharge was found to be sensitive to the chosen distribution in the 2D computations. In the 3D computations, the sensitivity of water level and surface velocity to discharge changes was negligible downstream from approximately 45° of the bend. The optimization of an additional parameter describing the velocity distribution at the inflow boundary showed that the solution then becomes non-unique, if only surface measurements are available.

The error of the estimated discharge was calculated to be at most 9% for the 3D computations under consideration of a 5% measurement error of the surface velocity, and a 5% velocity error resulting from CFD-modelling.

8.2 Conclusions

The inverse numerical model is a powerful tool for identifying river discharge and the reliability of the prediction from surface measurements. Water level and surface velocity data can be obtained through non-intrusive methods (e.g., Particle Tracking Velocimetry, PTV), which can be used even for extreme floods. Surface velocity data are important for the estimation of flood discharge,
8.2. Conclusions

because the suitability of water level data drops for larger discharges due to the decreasing sensitivity of water levels to discharge changes. For surface velocities the tendency is just the other way round. The CFD-models can be applied to complex river bed geometries with naturally eroded river beds and also to flow fields with separation zones and transcritical flow regimes. This broad applicability adds to the attractiveness of the proposed method.

The applicability to complex river geometries allows to select measurements in a river section with high sensitivity of the measurement variables to discharge changes. The results in sections 6.3.3 and 7.3.3 revealed that the estimation of discharge is more stable for more sensitive measurements to discharge changes. A complex flow field may have sections where the sensitivity of measurement variables is larger than for a uniform flow field with the same discharge. The examined 90°-bend, for example, has small sensitivities at the inside of the bend due to flow separation, but has higher sensitivities at the outside of the bend. These higher sensitivities of the measurement variables to discharge changes may allow for a more stable discharge estimation.

An advantage of taking measurements with the PTV-technique is the possibility of having a sufficient number of measurements, which can help to minimize the influence of outliers and random errors (e.g., due to turbulent fluctuations) on the estimated discharge. However, the influence of systematic errors can not be reduced with more measurements.

The accuracy of the discharge estimated in section 7.4 cannot be expected in natural rivers. While the PTV-measurement error was assumed under consideration of prototype dimensions, the error resulting from CFD-modelling may be larger due to uncertainties in river bed geometry and roughness. An evaluation of the proposed method in comparison to the conventional discharge estimation is not possible for flood events, because no generally valid estimation of accuracy is available for conventionally predicted discharges. However, relating to the examples mentioned in section 1.1.2, the proposed method still seems attractive even if a discharge error of up to 20% may be expected.

The uncertainties of the proposed method to estimate the discharge derive from the following:

• The velocity distribution at the inflow boundary is usually unknown and has to be assumed.
• The river bed geometry and its roughness may change during a flood event due to sediment transport.

The inflow boundary for modelling should be set upstream of the measurement-region at a distance of about 25-50 times the hydraulic diameter. This distance allows for a uniform velocity profile to develop into a fully turbulent profile (Schlichting 1965). Thus, the assumed inflow velocity profile does not affect the discharge estimation. Yet, the longer computational region leads to higher CPU-times and more errors due to poor bed characterization.

The influence of an unknown bed geometry was not examined within this work, because the river bed was known in both presented cases. The following section (8.3) describes possibilities to quantify the influence of different river bed geometries on the estimated discharge, and how an
unstable river bed can be treated within the discharge estimation procedure, if the resulting influence is unacceptable.

The minor influence of different bed roughness values on water levels and surface velocities in the two case-studies can not be generally expected, because both geometries examined had vertical side walls. Natural rivers with inclined river banks have smaller water depths, especially along the edges, for the same discharge. This can lead to a stronger influence of the bed roughness on water levels and surface velocities.

8.3 Outlook

This section gives recommendations for future research, where the research direction may be twofold. On one hand, the inverse numerical model may be further developed, adding different options. On the other hand, experience with prototype dimensions should be gathered by measuring water levels and surface velocities in natural rivers and applying the proposed method to estimate the discharges. This section first suggests possible improvements to the inverse numerical model and then describes a procedure to setup measurements.

Inverse Numerical Model

The previous section indicated that uncertainties about the river bed geometry were not considered in the validation of the proposed method for discharge estimation. But these uncertainties may be a major source of error in estimating the discharge in natural rivers. The stability of the river bed can be estimated roughly with the Shields parameter $\theta$,

$$\theta = \frac{\tau_0}{\rho_w \cdot g \cdot (s - 1) d_m},$$  \hspace{1cm} (8-1)

where $\tau_0$ is the bed shear stress, $g$ is the gravitational acceleration and $s$ is the ratio between the specific weight of sediment $\rho_s$ and the specific weight of water $\rho_w$. $d_m$ is the mean diameter of the bed material. Sediment is transported above a critical Shields parameter of $\theta_{cr} = 0.047$.

The influence of an unstable river bed on the estimated discharge should be evaluated, if instabilities are to be expected. A sensitivity study with different possible river bed geometries yields the expected uncertainty for the estimated discharge. Possible geometries can be obtained by a CFD-model, coupled with a sediment transport module. If the uncertainty in discharge estimates due to possible river bed geometries is not acceptable, either the river bed has to be measured during the PTV-measurements or sediment transport calculations have to be performed within the inverse numerical modelling procedure. The river bed geometry could be measured with, e.g., non-intrusive ground-penetrating radar (GPR). Spicer et al. (1997) have successfully applied this technique for high floods. Additional computation of sediment transport necessitates to solve the
transient transport equations to estimate sediment erosion or deposition, which would lead to a significant expenditure in CPU-time.

Another possible improvement of the inverse numerical model concerns the minimization algorithm. The computations in section 6.3.4 showed that with inclusion of an additional form parameter to describe the inflow velocity profile the problem cannot be optimized. Consequently, the discharge $Q$ is recommended as single optimization parameter if only surface measurements are available. This allows to use a simpler and faster minimization algorithm than in this work (see section 4.3.3). The algorithm used here is generally applicable for any number of optimization parameters and includes the determination of the Jacobian matrix. This matrix allows for the evaluation of suitable measurement locations, which is an important piece of information for reliable discharge estimations. An additional algorithm that does not require the determination of the Jacobian matrix could be implemented, allowing to choose between the two minimizing algorithms. The original algorithm serves then for calculations where a statistical analysis is of interest and the additional, faster algorithm is suitable for the optimization if only the final optimized parameters are of interest.

**Prototype Measurements**

Information from prototype measurements is essential to validate this method of discharge estimation in application, which comprises PTV-measurements and the presented inverse numerical modelling. First measurement setups in rivers should be chosen at locations with conventional gauging-stations to verify the proposed method at moderate flows.

Objects floating on the water surface are needed to carry out PTV-measurements, where naturally existing drifts or air bubbles during flood events are possibly sufficient. If supplemental particles have to be used, they could be naturally available near the river (such as leaves) to avoid additional pollution of the river.

The above section indicated that several preliminary studies can help to optimize the measurement setup. The following list gives suggestions of possible studies.

- A river section should not be chosen where large sediment erosion/deposition occurs. The stability of the river bed can be estimated with equation (8-1). If a river section with an unstable bed is unavoidable, additional conditions (as described above) have to be considered.
- The sensitivity distribution of measurement variables, provided by the Jacobian matrix, can give information on the optimal position for cameras.
- The minimal number of measurements (particles) required in a measurement section can be estimated by using randomly perturbed synthetic measurements, as it was demonstrated in sections 6.3.2 and 7.3.2. This information allows to determine whether additional particles have to be used.

These studies allow to increase the reliability of estimated discharges. But an uncertainty estima-
tion for the discharge is difficult to perform a priori. A time-consuming method to predict the reliability of the discharge is to estimate discharges with different combinations of possible assumptions (e.g., river bed geometry, bed roughness, inflow velocity distribution, etc.). An alternative, less time-consuming method is to estimate the influence of different model assumptions on the computed water levels and surface velocities. This requires only forward computations. Once a realistic interval for water levels and surface velocities is known, the discharge may be calculated with synthetic measurements, which were perturbed by the range of that interval. This results in an uncertainty-interval for the discharge.
9 Bibliography


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11 Curriculum Vitae

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