Numerical Modelling of Shallow Flows
with Horizontal Density Variation

Feifei Zhang Leighton
St. Hugh’s College
Michaelmas Term, 2005

Thesis submitted in partial fulfilment for the degree of
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ABSTRACT

A numerical model is presented of vertically homogeneous shallow flows with variable horizontal density. The governing equations represent mass and momentum conservation of a liquid-species mixture, and mass conservation of the species within a control volume. Here, the term species refers to material transported with the liquid flow. For example, when the species is taken to be suspended sediment, the model provides an idealised simulation of hyper-concentrated sediment-laden flows. The volumetric species concentration acts as an active scalar, allowing the species dynamics to influence the flow structure. The model can simulate flows driven by depth and density differences in the horizontal. The governing equations are written in a deviatoric, hyperbolic form to facilitate their solution by means of a Godunov-type finite volume scheme appropriate for flows containing sharp fronts. The deviatoric governing equations ensure that flux gradient and source terms are balanced (and there is no need for further numerical balancing).

The numerical model is first verified for constant density cases, for which the governing equations reduce to the conventional coupled shallow water and species transport equations. Close agreement between numerical predictions and benchmark test solutions illustrate the model’s ability to capture rapidly-varying flow features over uniform and non-uniform bathymetries.

For variable-density cases, analytical steady-state solutions are derived for two simple cases, one with uniform bathymetry and the other with sinusoidal bathymetry. Detailed parameter studies are then undertaken to examine the effects of varying the initial density and depth in different regions. The shock-capturing scheme resolves all sharp features in the flow such as bore, shear waves, shock diamond like features, contact discontinuities and locally intense vortices. These interesting and novel nonlinear features are unique to variable density flows.

The validated numerical model is applied to an idealised case of a hyperconcentrated sediment-laden debris-type flow along a tributary entering a river. The predicted evolution of the free surface flow field is qualitatively similar to observations of an actual debris flows into a river connected to the Upper Yangtze.
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CHAPTER 1 INTRODUCTION

This chapter provides a general background to shallow flow systems, a literature review on existing shallow flow and species transport modelling techniques and the objectives and synopsis of the thesis.

1.1 Background

Many water systems in the natural environment can be treated as shallow flows in which the flow domain is much larger than the flow depth. Typical examples include rivers, lakes, lagoons, reservoirs and estuaries. Many of these systems are close to populated areas as they provide the water supply needed for the domestic and industrial requirements of nearby inhabitants and form an important part of the local ecosystem (an ecosystem is an ecological community together with its environment, functioning as a unit). Of particular interest is the spatial and temporal variation of the various species that are transported in the shallow flows. The species can be suspended sediment, dissolved oxygen, nitrogen, phosphorus, carbon, mercury, cadmium, salt, fertilisers, pesticides, micro-organisms, etc.

Shallow flow ecosystems are sensitive to the changes in water quantity. Too little water leads to supply shortages, increased sedimentation, reduced capacity, shrinkage of the main course of a water basin, no-flows, and perhaps desertification. Conversely, too much rainfall can cause rivers to become swollen, and eventually overtop the riverbanks or cause dams/dykes to fail.
One of the most common risks for any ecosystem is riverbank overtopping caused by prolonged rainfall. Flooding has become a major issue in most parts of the world due to climate change, population growth and floodplain development. Consequences of flood disasters are loss of life, damage to the economy and society. For instance, the 1998 flood in the Yangtze River in China is reported by the National Climatic Data Centre (2005) to have killed 3,656 people, affected 240 million people, destroyed 5 million houses and caused over $20 billion in estimated damages. Flooding can also be triggered by dam or dyke failures. A dam break is characterised by a sudden bore-like flow along the main course of the downstream river, with water cascading onto the adjacent flood plain. Dyke breaks are laterally directed flows with respect to the main course of the river, which are characterised by water overtopping or penetrating the riverbanks. Dam and dyke breaks are usually accompanied by steep-fronted flows that are highly transient and often supercritical.

In 2005, one of the strongest storms during the last 100 years, Hurricane Katrina generated strong winds, heavy rainfall and storm surges along the central Gulf Coast of the US, causing huge damage to life and property. In New Orleans, the damage was worsened by breaks in the levees separating the city from surrounding lakes. At least 80% of the city became inundated, mainly due to the levee failure from Lake Pontchartrain. The earthen levee also broke, leaving some parts of the city under 20 feet (6 m) of water (according to data provided by the National Climatic Data Centre, 2005).

An important flood related fluvial process is debris flow, which involves the transport of water-charged debris containing sediment and other material. Debris flows are transient and usually are characterised by having a high flow velocity, huge discharge, large transport capacity and short time scale. Consequently, debris flows are much more destructive than
floods and can lead to extensive deposition of material in the middle and lower reaches of a riverbed.

For example, the Jinshan debris reservoir broke on 30th April 1986 in Anhui, China with total debris-water discharge of about 800,000 m$^3$ (Han and Wang, 1996). The debris flow in the downstream only lasted less than 5 minutes but caused the death of all residents in a downstream village. Another example is the July 29, 1998 debris flow and landslide dam at Capricorn Creek within the Mount Meager Volcanic Complex, southern Coast Mountains in British Colombia. This debris flow created a landslide-dammed lake with approximate length of 800 m and a total volume of about 1,200,000 m$^3$, followed by a three-day hyperconcentrated flow surge, causing significant deposition in the local flood plain (Bovis and Jakob, 2000). In 2000, four significant debris flows were observed in the Swiss Alps with total volumes ranging from 5,000 to 35,000 m$^3$, front velocities between 2 and 5 m/s and peak discharges in the range of 20 to 125 m$^3$/s (Hurlimann et al., 2003).

Apart from flooding and dam-break debris flows, some ecosystems can also encounter earthquake and volcano triggered flows that carry a significant amount of material. Although relatively rare, these events can have huge environmental and socio-economic consequences. For instance, the May 1980 eruption of Mount St Helens created a 60-km$^2$ debris avalanche (largest recorded landslide in history), a 15-km$^2$ pyroclastic flow and massive mudflows (Dale and Adams, 2003). These disturbances together with snowmelt caused ash, mud and other materials to scour downstream, fill local watercourses and destroy local river ecosystems. After the eruption, geologists, geophysicists, geochemists and hydrologists have worked as teams to integrate information needed for forecasting and monitoring future events and construct infrastructure such as debris-trap dams.
The June 1991 eruption of Mount Pinatubo in the Philippines is another recent large volcanic eruption. The combination of abundant fine-grained material and intense tropical rainfall led to the development of volcanic debris flows and hyperconcentrated flows, referred to collectively as lahars. River valleys were buried by as much as 200 m of loose pyroclastic debris (Gran and Montgomery, 2005). At volcanoes like Mount Pinatubo and St. Helens, hydrologic hazards including excess sedimentation and downstream flooding are still of concern many years after the major eruptions.

The nature of dam break and debris flows is unsteady and includes steep fronts. The understanding of the material transport process of steep-fronted flows is essential to predict consequent impacts and to design engineering countermeasures. By studying the fundamental flow behaviours and exploring existing data, it is possible to develop numerical models specially targeted for this type of steep-fronted flow with large material transport capacity. Numerical modelling has proved to be a very effective tool for providing quantitative and reliable information on hydrodynamics, species transport and water quality. The information is analysed and used by engineers in designing schemes to minimise the effects of future events.

1.2 Literature Review

1.2.1 Historical Development of the Shallow Water Equations

In 1755, Euler derived the equations of motion for an inviscid fluid by combining the principle of linear momentum with Bernoulli’s concept of internal pressure. In the 19th Century, Navier and Stokes independently obtained the governing momentum equation for
an incompressible fluid including Newtonian viscous effects by considering the force balance over an elemental volume. Reynolds made a further advance by separating the dependent variables of velocity and pressure into mean and fluctuating components, and derived locally time-averaged mass and momentum equations, the Reynolds-averaged Navier-Stokes (RANS) equations. Around the same time, de St Venant and Boussinesq formulated 1-D unsteady, incompressible flow equations based on mass and momentum principles applied over a control volume extending over the depth. Lamb (1879) was among the first to approximate shallow flows by considering analytical solutions of the simplified 2-D depth-averaged equations, the so-called Nonlinear Shallow Water Equations (NSWE). In the derivation of NSWE, it is assumed that water is an incompressible liquid, the horizontal dimensions of the flow domain are much larger than the depth, that any free surface waves have long wavelength and small amplitude, and the pressure variation in the vertical is hydrostatic (a consequence of assuming the vertical component of particle acceleration is negligible compared to the horizontal acceleration components). The nonlinear shallow water equations form the mainstay of many contemporary numerical models of free surface shallow flows considered in water engineering.

1.2.2 Discretization Methods

The nonlinear shallow water equations consist of a set of partial differential equations that can not be solved analytically in all but a few simple cases. As a result, the equations are usually approximated by a system of algebraic equations for the variables at discrete locations in space and time. The discrete locations are known as cells or grid points. There are three main types of discretization methods: finite difference method, finite element method and finite volume method. Comprehensive reviews of these methods are given by Abbott and Basco (1989), Anderson (1995), Baker (1985), Canuto et al. (1988), Ferziger and
Perić (2002), Fletcher (1991), Toro (1997, 2001) and Peyret and Taylor (1983). Other discretization methods such as spectral schemes, boundary element methods, smoothed particle hydrodynamics and cellular automata are less widely utilised but are growing in popularity.

The finite difference method (FDM) is based on Taylor series approximations to the governing equations and boundary conditions in partial differential form (see e.g. Abbott and Basco 1989; Anderson, 1995). In general, the accuracy of the approximations improves if the additional higher-order terms are included (Anderson, 1995). The FDM is straightforward and easy to implement, but does not preserve mass and momentum at jumps where there are discontinuous solutions. Consequently, the FDM is not well suited to flow problems with steep gradients.

The finite element method (FEM) is classified by Fletcher (1991) as weighted residual method, which assumes the existence of analytical representations of the solution. The FEM solves fluid-flow problems by reducing the original partial differential equations to a set of ordinary differential or algebraic equations (Peyret and Taylor, 1983). The FEM involves spatial integration of the governing equations over the problem domain and is therefore capable of resolving steep gradients and discontinuities. Although the FEM is accurate and robust, it can be complicated to code especially with regard to nodal ordering and matrix solution, affecting the efficiency. Another disadvantage of the FEM is the difficulty in dealing with both subcritical and supercritical flows such as dam-breaks (Fennema and Chaudhry, 1990; Zoppou and Roberts, 1999).

The finite volume method (FVM) is based on the integral form of the partial differential equations (see e.g. Vertseeg and Malalasekera, 1995). The computational domain is
discretized into smaller cell volumes within which the integration is carried out so the method inherently obeys conservation laws. Implementation of the method is usually straightforward and the computational cost is relatively low. In addition, the cell discretization procedure enables the FVM to deal with complex geometry without the need of curvilinear co-ordinate transformations. One distinctive advantage of the FVM is its ability to simulate subcritical, supercritical and transcritical flows accurately and efficiently.

Both FVM and FEM are capable of capturing steep fronts and therefore widely used in modern computational fluid dynamics (Anderson 1995; Baker 1985). In general, the FEM approach is more complicated to apply and less efficient than the FVM. This is because the FEM requires the values of conserved variables to be stored at the nodes or the surfaces of each cell and the computation of a large matrix at each time step. Moreover, an investigation by Rabbani and Warner (1994) revealed that in the formulations of subsurface pollution modelling, the transformation of nodal/surface values to element values could violate fundamental principles of both flow and transport processes and cause instability in the matrix solution. The same problem does not occur with FVM since the values of conserved variables are located at the centre of each cell. The FVM has become perhaps the most suitable scheme for simulating subcritical, supercritical and transcritical flows and wet/dry bed problems.

1.2.3 Choice of Grid

The arrangement of the discrete grid points used in the discretization process is called a grid (Anderson, 1995). The choice of grid used with the discretization method depends on the geometries of the flow domain and the dimensions of any obstacles in the geometric domain. The main options are structured grids, block-structured grids or unstructured grids.
A structured grid comprises families of grid lines with the property that members of a single family do not cross each other and cross each member of the other families only once (Ferziger and Perić, 2002). The position of each grid point is defined uniquely and each grid point has four nearest neighbours in 2D and six in 3D. This simple and consecutive grid structure offers perhaps the simplest means to discretize a computational domain. However, structured rectangular grids are only suited to domains with simple geometry. For geometrically complex domains, a much smaller grid size may be required for reasons of accuracy but at high computational expense. Alternatively, an analytical transformation can be applied to stretch a rectangular grid in one or more coordinate directions so that local solution can be increased (Anderson, 1995).

In a blocked-structured grid, the domain is subdivided into two or more smaller sub-mains. The different regions may or may not overlap. The fineness of grids in each region is set depending on the resolution required. The benefit of the block-structured grid over the regular-structured grid is the flexibility to allow finer grids in target areas and also the ability to follow moving bodies in complex domains (Ferziger and Perić, 2002). The disadvantage is the complicated programming and the difficulty in coupling overlapping grids at boundaries (Falconer, 1991; Rodenhuis, 1994).

Unstructured grids are made up of an arbitrary collection of elements of any shape and size, which thus offers maximum flexibility in matching grid points with the boundary surfaces (Anderson, 1995). There is no restriction on the number of neighbouring elements and unlike for a structured grid, the elements may intersect (Ferziger and Perić, 2002). In principle, unstructured grids can be used with any discretization scheme but are best adapted to finite volume and finite element approaches (Ferziger and Perić, 2002). A typical 2D unstructured
grid consists of triangles and quadrilaterals cells whereas for a 3-D grid, tetrahedra and hexahedra are used instead (Ferziger and Perić, 2002). Although highly flexible, the generation of an unstructured grid is extremely complex.

1.2.4 Godunov-Type Riemann Solvers

The Riemann problem for a set of partial differential equations is an initial value problem in which the initial data states consist of two constant states separated by a discontinuity. For the shallow water equations, the Riemann problem is a generalisation of a dam-break problem. The shock tube problem in gas dynamics is also a type of Riemann problem. The solution methodology for the Riemann problem is the fundamental building block for solving flow problem involving discontinuities.

Exact solutions to the Riemann problem require the identification of left and right shock and rarefaction waves (as the middle wave is always a shear/contact wave) and the devising of numerical algorithms for the unknown data states. Stoker (1992) and Toro (2001) give the mathematical derivation. Godunov (1959) was the first to develop a method for solving the Riemann problem of Euler equations exactly. Marshall and Méndez (1981) applied this method for the Euler equations of gas dynamics as well as developing a general procedure for an exact Riemann solver using the case of a wet bed. Toro (2001) describes exact Riemann solvers of the shallow water equations for both wet and dry beds. The analogue of the dry bed problem for gas dynamics is the shock tube problem expanding into a vacuum.

In a landmark paper, Godunov (1959) presented a novel approach for the numerical solution of fluid flows by piecing together exact solutions of a set of local Riemann problems. This is fundamentally different from direct implementation of a numerical solution of the Riemann
problem discretized by the finite difference approach (Anderson, 1995). The Godunov
approach utilises the exact solution to the Riemann problem locally based on an explicit
conservative formula by computing the upwind intercell numerical flux, the so-called
Godunov flux. By using the wave propagation information of hyperbolic PDEs for updating
the conserved variables in time, the Godunov method is conservative with the ability to
capture behaviour of shock waves. Being an upwind scheme, the Godunov method is capable
of accounting for the physically correct propagation of information throughout the flow field
over the entire computational domain.

In most commonly used, Godunov-type methods, the local Riemann problems are usually
solved using either exact or approximate Riemann solvers, which provide sufficiently
accurate results at a competitive computational cost. Exact Riemann solvers are accurate and
can be efficient for simple flows. However, for more complex (e.g. real compressible gases)
equations, the use of exact Riemann solvers becomes prohibitively expensive due to the
complex structure of the states encountered (Toro, 2001). Moreover, the structure of the
exact Riemann solver is lost in the Godunov method in the final cell average operation
(Guinot, 2003). Therefore, approximate Riemann solvers are more often used for complex
flow problems. Toro (2001) provides a detailed description of various types of approximate
Riemann solver.

The approximate Riemann solver of Roe (1981) was first constructed to obtain solutions of
the Euler equations. Roe’s scheme estimates intercell fluxes directly by considering the
linearised Jacobian flux matrix. The entries of the matrix are interpreted as averaged values,
the so-called Roe averages, following the Roe-Pyke approach (1984). The Roe averages are
obtained from the left and right data state values of the primitive variables. The Roe
approach was utilised to solve the shallow water equations by Glaister (1987) who followed
the Roe-Pyke approach to derive the approximate Riemann solver. The Roe scheme is an accurate and efficient method that can be applied to a large variety of physical problems. The matrix formulation ensures the robustness of the scheme which can be particularly beneficial for flows with large gradients in depth, velocity and density.

Harten, Lax and van Leer (1983) suggested the HLL approximate Riemann solver that automatically satisfies the entropy condition and yields solutions for isolated shocks. Given the initial signal velocities, the HLL approach estimates the left and right wave speeds by assuming a two-wave structure of the Riemann problem solution that separates into three constant states. The two-wave assumption neglects the influence of the intermediate wave. As a consequence, the HLL method is only adequate for one-dimensional systems without extra species transport equations (Toro, 2001).

The HLLC approximate Riemann solver is a modification of the HLL scheme to include the effect of the intermediate waves. In the modified HLLC solver of Toro et al. (1994), the missing contact surface is restored so there are two distinct fluxes for the intermediate region compared with only one flux in the HLL solver. Unlike linearised approximate Riemann solvers, the HLLC scheme is positively conservative, which preserves the initially positive pressure and densities. Numerical examples to demonstrate this property are given by Batten et al. (1997). The HLLC solver is inherently capable of modelling wet/dry bed conditions without special treatment. The approach by Fraccarollo and Toro (1995) using the HLLC solver has been successfully applied to the shallow water model for 2-D dam breaks involving dry bed situations.

The Osher-Soloman approximate Riemann solver was devised and used by Engquist and Osher (1981) and Osher and Soloman (1982). The Osher-Soloman scheme is based on the
splitting of the Jacobian matrix and the physical flux according to the sign of the eigenvalues. The intercell flux obtained using the splitting approach is therefore smooth. The scheme has been proven to be entropy satisfying and is suitable for dealing with sonic flows and slow moving shock waves. The evaluation of the intercell flux requires the choice of the ordering of the integration path, namely the O-ordering (original ordering) and the P-ordering (physical ordering). The ordering process requires the correct identification of the flux out of 16 possible cases at each time step and hence is rather expensive to compute. Details of the solver for the Burgers equation, isothermal equations and the time-dependent Euler equations are given by Toro (1999) and its applications to shallow water equations are given in the report by Zhao et al. (1996).

The basic Godunov scheme is first order accurate in space and time. Extension into second and higher order Godunov-type methods can be implemented and used in conjunction with exact and approximate Riemann solvers. The Weighted Average Flux (WAF) and the MUSCL-Hancock schemes are second order extensions of the Godunov-type methods. The WAF scheme computes the flux via an integral average so that the flux is a weighted average across the wave structure of the Riemann problem solution. The MUSCL-Hancock scheme requires a piecewise linear reconstruction of the data states, evolution of the boundary extrapolated values in time and solution of the Riemann problem with data consisting of evolved boundary extrapolated values. Higher order schemes may offer increased accuracy but can also predict spurious oscillations near steep gradients. In discussing Godunov’s (1959) original method, Toro (2001) pointed out that such oscillations were in general unavoidable with higher order schemes. To overcome the unphysical oscillations near discontinuities in higher order schemes, a constraint is enforced in the data reconstruction to limit the slopes by means of a flux limiter. This modification approach is referred to as total variation diminishing (TVD).
The Godunov approach has proven to be a powerful technique in the computation of incompressible shallow flows where the free surface and velocity field can experience steep gradients. In particular, the application to pollutant transport modelling is distinguished for its ability to resolve strong wave interaction and flows with steep discontinuities such as bores, shear waves and contact discontinuities, along with the correct propagation speeds while free from local spurious oscillations (Toro, 2001). In addition, Godunov-type schemes can be particularly useful when dealing with two-phase flows (Guinot, 2001), e.g. in predicting phase boundaries using the shock-capturing approach. Like any other numerical method, Godunov-type Riemann solvers have certain disadvantages. The major disadvantage is the complexity introduced by the Riemann solver and relatively high computational cost.

1.2.5 Numerical Imbalance between Flux Gradient and Source Terms

Most numerical methods for solving shallow flows experience problems in the presence of variable topographies, due to the imbalance between the flux gradient and source terms (Mohamadian et al., 2005). The numerical imbalance is created by the artificial splitting of the flux gradient and source terms in the governing equations. The splitting is necessary for preserving the hyperbolic nature of the equations, expressing the equations in conservative form and treating the advection and diffusion terms in the discretization.

The numerical imbalance is particularly problematic for flows over variable bathymetries in which unphysical fluxes are generated in even initially still water. Great efforts have been made in order to preserve the correct balance at steady states. The quasi-steady wave-propagation algorithm proposed by LeVeque (1998) balances the flux gradient and source terms by introducing an artificial discontinuity within each cell such that the flux differences
exactly cancel the source terms. Vázquez-Cendón (1999) devised an algorithm that achieves equilibrium balancing by upwinding the source terms. This source-term upwind technique was extended to higher order TVD schemes by García-Navarro and Vázquez-Cendón (2000) and Hubbard and García-Navarro (2000). Zhou et al. (2001) developed a surface gradient method that requires a piecewise linear data construction for the treatment of balancing the source terms.

Most of the approaches mentioned above rectify the balancing problem by a posteriori numerical means. Recently, Rogers et al. (2003) developed a priori generalised flux gradient and source term balancing technique that is accurate, simple and efficient. This algebraic approach can be applied widely to systems of hyperbolic conservation laws and merely involves subtracting any equilibrium-state from the governing equations prior to the simulation.

1.2.6 Numerical Modelling of Shallow Flows with Species Transport

During the latter half of the 20th Century, many computational schemes were developed to solve nonlinear shallow water equations in conjunction with the species transport equation. The additional transport equation is used to describe the transport of (solute and insoluble) species such as salinity, suspended sediment and contaminants. In addition to the hydrodynamics, the transport equation can provide extra information on water quality, sediment transport and bed morphology.

To date, species transport processes in shallow flows are modelled using either a single phase or a two (multi)-phase approach depending on whether the mixtures are considered as homogeneous. For non-homogenous mixtures with large vertical gradients of concentrations,
two-phase models are used to treat separately solids and the liquids in order to simulate morphological evolution and stratification flows. For example, see a review by Hutter et al. (1996) and work by Zhang and Dong (2000). Due to the complexity of the interaction between fluid and sediment, a typical two-phase model can consist of six governing equations plus complex boundary and interface conditions at the fluid-sediment interface. Such complicated models are of course costly in terms of computer resources.

In the majority of rivers and streams of naturally buoyant species, fully turbulent conditions achieve rapid vertical mixing and it is therefore appropriate to assume the mixture to be vertically well mixed. It is therefore possible to consider the mixture as homogenous and single phase in situations with no significant morphological changes (Fraccarollo and Papa, 2000). Single phase models are based on solving the combined shallow water and species transport equations using a coupled or a decoupled algorithm. Decoupled algorithms solve the flow pattern first and then deduce the species transport whereas the decoupled algorithms obtain information on flow hydrodynamic and species transport simultaneously. The decoupled approach is easy to implement but requires the physical assumption of low species concentrations so that the species dynamics do not influence the flow structure (Murillo et al., 2005).

Many single-phase shallow water and species transport models are solved using the coupled approach (for example Liang et al., 2001; Murillo et al., 2005; Sommeijer and Van Der Houwen, 2002). The vast majority of these models are based on solving the nonlinear shallow water and species transport equations by considering the species as a passive scalar (i.e. a quantity that is passively advected with the fluid). The passive tracer assumption is a prerequisite for simplifying the mass and momentum equations by treating the density variable as a constant. As the species concentration increases, the role of the species changes
from passive to active and the mechanical properties of a liquid-species mixture becomes very different from those of a pure liquid.

In many practical applications (e.g. dam break debris flows), the properties of the flow change rapidly in time and space and the advection velocity is dependent on both the total depth of the mixture and the species concentration distribution. A literature review on the existing single-phase models revealed that there is a lack of development into the model’s ability to incorporate density effects on the flow hydrodynamics. This is due to the difficulties in the derivations of conservation laws for a liquid-species mixture, the treatment of the flux and source terms and the accurate detection of the stopping of the flow in space and time (Fraccarollo and Papa, 2000).

When the variation in concentration of the species in the mixture is sufficiently significant to influence the flow, the conventional shallow water and species transport models become inappropriate. A new density-dependent hydrodynamic model is necessary to describe the behaviour of the liquid-species mixture. By considering the mixture as homogenous in the vertical direction, conservation laws obtained for the mixture can be expressed as a 2-D depth-averaged model. It is sensible to start with a 2-D depth-averaged model and consider additional spatial density variation in the horizontal direction. The governing equations take similar form as those derived by Abbott (1979) for vertically homogeneous fluids. The new density-dependent hydrodynamic model considers the species concentration as an active scalar that partly determines the subsequent flow behaviours along with the depth profile and velocity distribution.
1.3 Objectives

The overall aim of this thesis is the development of a numerical model for shallow flow and species transport that provides a description of the horizontal free surface flow field for vertically homogenous liquid-species mixtures, where sharp gradients in depth and density may occur locally. The governing equations have to be derived in hyperbolic form in order to retain the desirable conservation properties. It is intended that the numerical scheme be accurate, efficient and robust, with the ability to capture steep-fronts and to preserve steady states over non-uniform bathymetries. The detailed objectives of this thesis are:

- To derive the variable-density shallow flow and species transport equations in Cartesian co-ordinates from physical principles by applying balances of the mixture mass, momentum flux and species mass to an infinitesimal elemental control volume of unit depth, in depth-averaged form.

- To cast the coupled variable-density shallow flow and species equations in equilibrium-corrected hyperbolic matrix form by applying a flux gradient and source term balancing technique.

- To develop an explicit second-order Godunov-type finite volume numerical solver of the equilibrium-corrected shallow flow and species equations and to adapt Roe’s approximate Riemann solver in the finite volume scheme to evaluate the intercell fluxes.
To validate the numerical model under the constant-density condition using benchmark tests for shallow water and species transport equations:

To verify the numerical model under the variable-density condition using analytical steady-state solutions, approximate analytical solutions and parameter tests.

To demonstrate the potential of the model by considering an idealised application case of a debris flow from a tributary of a river.

The variable density model offers physical insight into the behaviour of shallow flows driven by local density differences. It is intended that the model could eventually be applied to the prediction of hyper-concentrated sediment transport and debris flows.

1.4 Synopsis

The next chapter presents a derivation of the coupled variable-density nonlinear shallow flow and species transport equations, starting from the governing equations in primitive form. An equilibrium-corrected hyperbolic form of the deviatoric governing equations is utilised in order to permit shock-like behaviour to be modelled correctly in cases where the bed is non-uniform. Integral expressions for mass, volume and energy are obtained so that validation tests can be established to verify the conservation of these quantities. Chapter 3 describes the second-order Godunov-type numerical scheme used to solve the variable-density nonlinear shallow flow and species transport equations in equilibrium-corrected form. The corresponding flux Jacobian and eigensystem is derived in order to implement Roe’s approximate Riemann solver. Chapter 4 presents numerical model validation for constant
density benchmark cases. The results from the present model are found to be in close agreement with those obtained from alternative numerical models. Chapter 5 presents further results for variable density shallow cases including 1-D cases with analytical steady-state solutions (on flat and sinusoidal beds), 1-D dam break analogues with one or two initial discontinuities in density and 2-D circular dam break analogues. Chapter 6 lists the main conclusions of the thesis and makes recommendations for future research.
CHAPTER 2  MATHEMATICAL MODEL

This chapter presents a mathematical model of variable-density shallow flow processes coupled with species transport in a Cartesian coordinate system. By applying the balance of mass and momentum across an infinitesimal control element of a liquid-species mixture, conservation laws are obtained and expressed in hyperbolic form. However, the hyperbolic form of the governing equations may experience numerical imbalance of the flux gradient and source terms in quiescent conditions over non-uniform bathymetry. To rectify this problem, a novel method of subtracting an equilibrium solution from the governing equations is adopted, following the ideas of Rogers et al. (2003). This algebraic technique eradicates the numerical imbalance without the loss of any physical information because the flux Jacobian of equilibrium-corrected equations is the same as that of the original equations.

2.1 2-D Governing Equations for Vertically Homogeneous Liquid-Species Mixture

Consider an infinitesimal control element of plane dimensions dx and dy, where x, y are the horizontal flow directions. In the vertical direction z, the liquid-species mixture is homogeneous with a depth h. The time interval dt is considered relatively small. In order to establish the primary form of equations of mass conservation, momentum flux balance and species transport for the control volume (shown in Figure 2.1), the following hypotheses are prescribed. It is assumed that the flow is nearly horizontal and incompressible, vertical accelerations may be neglected, pressure is hydrostatic, surface waves are long with respect to the mean flow depth and the wave amplitude and the liquid-species mixture is vertically
homogeneous. The governing equations are written as conservation laws in hyperbolic partial differential form in terms of the depth-averaged variables $\rho, u, v, c$ and the total depth $h$ of the liquid-species mixture. In the foregoing, $\rho$ is the depth-averaged density of the liquid-species mixture, $u$ and $v$ are depth-averaged horizontal velocity components and $c$ is the depth-averaged species concentration by volume. It is inherently assumed that the species and the liquid are mixed uniformly in the vertical throughout the flow and do not react with each other chemically.

The following fundamental conservation laws (see e.g. Abbott, 1979) are obtained by balancing the net inflow of mass, $x$- and $y$- momentum and species through the sides of the control volume with the corresponding accumulation of mass, resultant forces and species within the control volume.

Mass conservation of the mixture:

$$\frac{\partial(p h)}{\partial t} + \frac{\partial(p u h)}{\partial x} + \frac{\partial(p v h)}{\partial y} = 0$$  \hspace{1cm} (2.1)

Momentum flux balance in the $x$-direction:

$$\frac{\partial(p u h)}{\partial t} + \frac{\partial(p u^2 h + \frac{1}{2} \rho gh^2)}{\partial x} + \frac{\partial(p u v h)}{\partial y} = \tau_{xx} - \tau_{yx} - \rho g h S_{ax} + \rho v h f + \frac{\partial(h T_{x})}{\partial x} + \frac{\partial(h T_{y})}{\partial y}$$  \hspace{1cm} (2.2)

Momentum flux balance in the $y$-direction:
\[
\frac{\partial (\rho v h)}{\partial t} + \frac{\partial (\rho u v h)}{\partial x} + \frac{\partial (\rho v^2 h + \frac{1}{2} \rho g h^2)}{\partial y} = \tau_{wx} - \tau_{wy} - \rho g h S_{ox} - \rho uh f + \frac{\partial (h T_{xx})}{\partial x} + \frac{\partial (h T_{yy})}{\partial y} \tag{2.3}
\]

where \( \tau_{wx} \) and \( \tau_{wy} \) are the tangential surface stress components, \( \tau_{hsx} \) and \( \tau_{hsy} \) are the bed shear stress components, \( S_{ox} \) and \( S_{oy} \) are the bed slopes in the Cartesian directions, \( f \) is the Coriolis parameter, and \( T_{xx}, T_{xy} \) and \( T_{yy} \) are effective stresses due to viscous effects.

Species mass conservation:

\[
\frac{\partial (\rho_s c h)}{\partial t} + \frac{\partial (\rho u c h)}{\partial x} + \frac{\partial (\rho v c h)}{\partial y} = \frac{\partial}{\partial x} \left( K_x h \frac{\partial (\rho_s c)}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y h \frac{\partial (\rho_s c)}{\partial y} \right) \tag{2.4}
\]

where \( c \) is the depth-averaged species concentration of the liquid-species mixture by volume \((0 \leq c \leq 1)\), \( K_x \) and \( K_y \) are the longitudinal mixing coefficients and \( \rho_s \) is the density of the species (e.g. suspended sediment). The above equation is used to model the dispersion process of the species, which consists of differential convection and longitudinal mixing. Detailed description of the modelling of transport of pollutants is available in Cunge, Holly and Verwey (1980).

The density of the liquid-species mixture, \( \rho \) is defined as

\[
\rho = \rho_w + c(\rho_s - \rho_w) \tag{2.5}
\]

where \( \rho_w \) is the density of the liquid and \( \rho_s \) is the density of the species. The species can be a solid or another liquid so the mixture is either a solid-liquid mixture (e.g. suspended
sediment in water) or a binary liquid mixture. For clarity, the liquid with density \( \rho_w \) will be referred to as the (ambient) liquid and the liquid or solid with density \( \rho_s \) will be denoted as the species.

Alternatively, the volumetric concentration \( c \) can be expressed in terms of \( \rho_w \), \( \rho \), and \( \rho_s \) as

\[
c = \frac{\rho - \rho_w}{\rho_s - \rho_w} \quad \text{if} \quad \rho \neq \rho_w
\]

Therefore the variables \( \rho \) and \( c \) are coupled, and if one of the variables is known then the value of the other can be determined using Equations (2.5) or (2.6). For the sake of simplicity and clarity in displaying results of the species transport process, the density is expressed as a function of the volumetric concentration in this thesis. Another advantage of choosing concentration over density to represent the transport process is that the role of variable \( c \) switches from an active scalar to a passive scalar when \( \rho = \text{constant} \) and \( c \neq 0 \). Under such conditions, the governing equations reduce to the coupled shallow water and species transport equations.

The conservation laws and momentum equations (2.1)-(2.4) can be expressed as a hyperbolic system of partial differential equations in following vector form.

\[
\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{f}}{\partial x} + \frac{\partial \mathbf{g}}{\partial y} = \mathbf{h}
\]

where the vector of the conserved variables \( \mathbf{q} \), the flux vectors \( \mathbf{f}(\mathbf{q}) \), \( \mathbf{g}(\mathbf{q}) \) and the source terms vector \( \mathbf{h}(\mathbf{q}) \) are
The bed shear stress \( \tau_b \) is a measure of the retarding effect on the flow due to the bed roughness and can be approximated by a quadratic form:

\[
\tau_{bx} = \rho C_f u \sqrt{u^2 + v^2}, \quad \tau_{by} = \rho C_f v \sqrt{u^2 + v^2}
\]  

(2.9)

where \( C_f \) is an empirical friction coefficient related to bed roughness. In the present work, \( C_f \) is evaluated using the Chézy friction law

\[
C_f = \frac{g}{C_{ch}^2}
\]  

(2.10)

where \( g \) is the gravitational acceleration and \( C_{ch} \) is the Chézy coefficient.
The bed slope components \( S_{ox} \) and \( S_{oy} \) are the gradients of the bed profile \( z_b(x, y) \) (shown in Figure 2.2, above an arbitrary datum) in the x- and y-direction respectively, i.e.

\[
S_{ox} = \frac{\partial z_b}{\partial x}, \quad S_{oy} = \frac{\partial z_b}{\partial y}
\]  

(2.11)

The Coriolis parameter is given by \( f = 2 \omega \sin \phi \), with \( \omega \) as the angular velocity of the earth and \( \phi \) the north latitude (Abbott, 1979).

The mean depth-averaged effective stresses \( T_{xx} \), \( T_{xy} \) and \( T_{yy} \) may be derived as (McGuirk & Rodi, 1978)

\[
T_{xx} = \frac{1}{h} \int \left[ \frac{2}{h} \frac{\partial \bar{u}}{\partial x} - \rho \bar{u}'u' - \rho (\bar{u} - u)^2 \right] dz
\]

\[
T_{xy} = \frac{1}{h} \int \left[ \mu \left( \frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} \right) - \rho \bar{u}'v' - \rho (\bar{u} - u)(\bar{v} - v) \right] dz
\]

\[
T_{yy} = \frac{1}{h} \int \left[ \frac{2}{h} \frac{\partial \bar{v}}{\partial x} - \rho \bar{v}'v' - \rho (\bar{v} - v)^2 \right] dz
\]

(2.12)

where \( \bar{u}(x, y, z) \) and \( \bar{v}(x, y, z) \) are the time-averaged velocity components, \( u'(x, y, z, t) \) and \( v'(x, y, z, t) \) are the turbulent fluctuating velocity components, \( u(x, y, t) \) and \( v(x, y, t) \) are the mean depth-averaged velocities over the total depth \( h \), and \( \mu \) and \( \rho \) are the density and coefficient of fluid dynamic viscosity of the fluid respectively. Each equation has three terms on the right hand side: the first one is for viscous stresses; the second term represents turbulent Reynolds stresses arising from time-averaging the instantaneous Navier-Stokes equations; and the last term expresses the dispersive effect of the non-uniform velocity.
profile in the vertical direction. McGuirk and Rodi (1978) noted that the turbulent Reynolds stress terms dominated, such that

\[ T_{xx} = -\frac{1}{h} \int_0^h \rho \overline{u' u'} dz, \quad T_{xy} = -\frac{1}{h} \int_0^h \rho \overline{u' v'} dz, \quad T_{yy} = -\frac{1}{h} \int_0^h \rho \overline{v' v'} dz \] (2.13)

The effective stresses can be approximated using Boussinesq’s (1877) eddy viscosity concept with a kinematic eddy viscosity coefficient \( \varepsilon \) as follows.

\[ T_{xx} = 2 \rho \varepsilon \frac{\partial u}{\partial x}, \quad T_{xy} = \rho \varepsilon \left[ \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right], \quad T_{yy} = 2 \rho \varepsilon \frac{\partial v}{\partial y} \] (2.14)

For a flow in a domain \( \Omega \) with boundary \( S \), the hyperbolic system of conservation equations in vector form (2.7) can be written in integral form as (Chan, 1997):

\[ \frac{\partial}{\partial t} \int_\Omega q \, d\Omega + \int_\Omega \left( \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} \right) \, d\Omega = \int_\Omega h \, d\Omega \] (2.15)

Applying Gauss’ theorem to the second term gives

\[ \frac{\partial}{\partial t} \int_\Omega q \, d\Omega + \oint_S (fn_x + gn_y) \, dS = \int_\Omega h \, d\Omega \] (2.16)

where \( n_x \) and \( n_y \) are the Cartesian components of the unit vector \( n \) normal to \( S \).
The above integral equation can easily be discretized and solved on a collocated grid using a finite volume method. Before proceeding to the development of an algorithm for solving the equations numerically, it is important to realise that many numerical models for shallow flows experience difficulty in preserving the balance between flux gradient and source terms. The result of this numerical imbalance is an unphysical, non-zero flux generated in a system which is initially in equilibrium. When integrated in time this imbalance will accumulate to produce further unphysical fluxes and eventually the numerical scheme will break down. To overcome this problem, a novel method is selected for the balancing of the flux gradient and source terms to the governing hyperbolic equations. Details of the method are explained in the following section.

2.2 Generalised Flux Gradient and Source Term Balancing

The generalised flux gradient and source term balancing technique derived by Rogers et al. (2003) is adopted here to obtain the equilibrium-corrected variable-density shallow flow and species transport equations. The solution methodology involves subtracting a primarily known equilibrium solution from the governing equations. The reformulated hyperbolic conservation equations are balanced a priori, and so there is no need to carry out numerical upwinding of source terms at each time step during the simulation.

To apply this technique, first consider the integral form of the hyperbolic system of the conservation laws given in (2.15). Let \( \mathbf{q}^{eq} \) denote the vector of the equilibrium values of the conserved variables which is defined as \( \frac{\partial \mathbf{q}^{eq}}{\partial t} = \mathbf{0} \). Subtracting the integrated equilibrium values of the flux gradients from each side of the equation to gives
\[
\frac{\partial}{\partial t} \int_{\Omega} \mathbf{q} \, d\Omega + \int_{\Omega} \left( \frac{\partial f(q)}{\partial x} - \frac{\partial f(q^e)}{\partial x} + \frac{\partial g(q)}{\partial y} - \frac{\partial g(q^e)}{\partial y} \right) d\Omega = \int_{\Omega} h^* \, d\Omega \quad (2.17)
\]

where the equilibrium-corrected source term \( h^* \) is given by

\[
h^* = h - \frac{\partial f(q^e)}{\partial x} - \frac{\partial g(q^e)}{\partial y} \quad (2.18)
\]

The vector of the conserved variables, \( \mathbf{q} \) can also be expressed as deviations \( \bar{q} \) from the equilibrium values \( q^e \) as

\[
\mathbf{q} = q^e + \bar{q} \quad (2.19)
\]

If an equilibrium state is assumed preceding the simulation, then Equation (2.17) reduces to

\[
\frac{\partial}{\partial t} \int_{\Omega} \bar{q} \, d\Omega + \int_{\Omega} \left( \frac{\partial f(q^e)}{\partial x} + \frac{\partial g(q^e)}{\partial y} \right) d\Omega = \int_{\Omega} h^* \, d\Omega \quad (2.20)
\]

The equilibrium state also satisfies the integral form of the conservation laws in (2.15), which is

\[
\frac{\partial}{\partial t} \int_{\Omega} q^e \, d\Omega + \int_{\Omega} \left( \frac{\partial f(q^e)}{\partial x} + \frac{\partial g(q^e)}{\partial y} \right) d\Omega = \int_{\Omega} h(q^e) \, d\Omega \quad (2.21)
\]

This implies, for an arbitrary domain \( \Omega \),
\[
\frac{\partial f(q^{*y})}{\partial x} + \frac{\partial g(q^{*y})}{\partial y} = h(q^{*y})
\]  

Hence from the above equation, Equation (2.18) implies

\[h^* = h - h(q^{*y})\]  

(2.23)

Let

\[
\tilde{q} = q - q^{*y}, \\
\tilde{f} = f(q) - f(q^{*y}), \\
\tilde{g} = g(q) - g(q^{*y}), \\
\tilde{h} = h(q) - h(q^{*y}).
\]  

(2.24)

Thus Equation (2.20) becomes

\[
\frac{\partial}{\partial t} \int_{\Omega} \tilde{q} \, d\Omega + \int_{\Omega} \left( \frac{\partial \tilde{f}}{\partial x} + \frac{\partial \tilde{g}}{\partial y} \right) \, d\Omega = \int_{\Omega} \tilde{h} \, d\Omega
\]  

(2.25)

Application of Gauss’ theorem to the above equation gives

\[
\frac{\partial}{\partial t} \int_{\tilde{\Omega}} \tilde{q} \, d\Omega + \int_{\tilde{\Omega}} \left( \tilde{f}_{n_x} + \tilde{g}_{n_y} \right) \, dS = \int_{\tilde{\Omega}} \tilde{h} \, d\Omega
\]  

(2.26)

By inspection, the equilibrium-corrected equations (2.26) can be solved in the same manner as the original governing equations (2.16). The advantage of this particular flux gradient and source terms balancing approach over other posteriori balancing methods is that it overcomes...
the problems associated with unbalanced flux gradient and source terms. Furthermore, this approach preserves the hyperbolicity of the original equations and is independent of the order of the numerical approximation (Rogers et al., 2003).

2.3 Invariance of the Flux Jacobian

For a complex system of equations, the equilibrium-corrected flux Jacobian may be very difficult to derive algebraically. However, an important property of the flux gradient and source terms balancing approach is that the equilibrium-corrected flux Jacobian is the same as the flux Jacobian of the original hyperbolic system of conservation laws. This invariance property of the flux Jacobian permits the substitution of the simpler original Jacobian matrix for the more complicated equilibrium-corrected Jacobian matrix. The following restates the proof of the invariance property of the flux Jacobian (originally given in 1-D by Rogers et al., 2003).

By applying the generalised flux gradient and source term balancing technique, the hyperbolic system of conservation laws in (2.7) is transformed to

\[
\frac{\partial \tilde{q}}{\partial t} + \frac{\partial \tilde{f}}{\partial x} + \frac{\partial \tilde{g}}{\partial y} = \tilde{h}
\]

(2.27)

where \( \tilde{q} \) is the equilibrium-corrected vector of conserved variables, \( \tilde{f} \) and \( \tilde{g} \) are the equilibrium-corrected flux vectors, and \( \tilde{h} \) is the equilibrium-corrected source term vector given in Equation (2.24).
Applying linearization to the system (2.27), so that

\[ \frac{\partial \mathbf{q}}{\partial t} + \mathbf{A}_x \frac{\partial \mathbf{q}}{\partial x} + \mathbf{A}_y \frac{\partial \mathbf{q}}{\partial y} = \mathbf{h} \]  

(2.28)

where \( \mathbf{A}_x \) and \( \mathbf{A}_y \) are the equilibrium-corrected flux Jacobian in the \( x \)- and \( y \)-direction respectively, which can be expressed in the following form.

\[
\mathbf{A}_x = \frac{\partial \mathbf{f}}{\partial \mathbf{q}} = \frac{\partial \mathbf{f}}{\partial \mathbf{q}} \cdot \frac{\partial \mathbf{q}}{\partial \mathbf{q}}
\]

\[
\mathbf{A}_y = \frac{\partial \mathbf{g}}{\partial \mathbf{q}} = \frac{\partial \mathbf{g}}{\partial \mathbf{q}} \cdot \frac{\partial \mathbf{q}}{\partial \mathbf{q}}
\]

(2.29)

Differentiating \( \mathbf{q} = \mathbf{q}^{eq} + \bar{\mathbf{q}} \) with respect to \( \bar{\mathbf{q}} \) gives \( \frac{\partial \mathbf{q}}{\partial \bar{\mathbf{q}}} = \mathbf{I} \) since \( \frac{\partial \mathbf{q}^{eq}}{\partial \bar{\mathbf{q}}} = \mathbf{0} \). In addition,

\[ \frac{\partial \mathbf{f}(\mathbf{q}^{eq})}{\partial \mathbf{q}} = \mathbf{0} \quad \text{and} \quad \frac{\partial \mathbf{g}(\mathbf{q}^{eq})}{\partial \mathbf{q}} = \mathbf{0} \].

Hence the above flux Jacobian matrices (2.29) can be simplified as

\[
\mathbf{A}_x = \frac{\partial \mathbf{f}}{\partial \mathbf{q}} = \frac{\partial [\mathbf{f}(\mathbf{q}) - \mathbf{f}(\mathbf{q}^{eq})]}{\partial \mathbf{q}} = \frac{\partial \mathbf{f}(\mathbf{q})}{\partial \mathbf{q}} = \mathbf{A}_x
\]

\[
\mathbf{A}_y = \frac{\partial \mathbf{g}}{\partial \mathbf{q}} = \frac{\partial [\mathbf{g}(\mathbf{q}) - \mathbf{g}(\mathbf{q}^{eq})]}{\partial \mathbf{q}} = \frac{\partial \mathbf{g}(\mathbf{q})}{\partial \mathbf{q}} = \mathbf{A}_y
\]

(2.30)

This completes the proof of the invariance property of the flux Jacobian matrix.
2.4 Governing Equations in Equilibrium-Corrected Form

The equilibrium-corrected variable-density shallow flow and species transport equations can be expressed in vector form as that given in Equation (2.27) with the equilibrium-corrected vectors of the conserved variables, fluxes and source terms given by

\[
\begin{align*}
\mathbf{\hat{q}} &= \begin{bmatrix}
\rho h - \rho^{eq} h^{eq} \\
\rho u h \\
\rho v h \\
\rho, ch - \rho, c^{eq} h^{eq}
\end{bmatrix}, \\
\mathbf{\hat{f}} &= \begin{bmatrix}
\rho u h \\
\rho u^2 h + \frac{1}{2} \rho g h^2 - \frac{1}{2} \rho^{eq} g (h^{eq})^2 \\
\rho u v h \\
\rho, u c h
\end{bmatrix}, \\
\mathbf{\hat{g}} &= \begin{bmatrix}
\rho v h \\
\rho v^2 h + \frac{1}{2} \rho g h^2 - \frac{1}{2} \rho^{eq} g (h^{eq})^2 \\
\rho u v h \\
\rho, v c h
\end{bmatrix}
\end{align*}
\]

\begin{align*}
\mathbf{\hat{h}} &= \begin{bmatrix}
\tau_{wx} - \tau_{hx} - \rho g h S_{sx} + \rho^{eq} g h^{eq} S_{sx} + \rho v h f + \frac{\partial (h T_{sx})}{\partial x} + \frac{\partial (h T_{sy})}{\partial y} \\
\tau_{wy} - \tau_{hy} - \rho g h S_{sy} + \rho^{eq} g h^{eq} S_{sy} - \rho u h f + \frac{\partial (h T_{sy})}{\partial x} + \frac{\partial (h T_{sx})}{\partial y} \\
\frac{\partial}{\partial x} \left( K_x h \frac{\partial \rho c}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y h \frac{\partial \rho c}{\partial y} \right)
\end{bmatrix}
\end{align*}

(2.31)
When defining the equilibrium for the system prior to the simulation, it is usually the most convenient to choose the quiescent state equilibrium which is defined as: $u^{eq} = v^{eq} = 0$, $\rho^{eq} = \rho_\infty$, $c^{eq} = 0$ and $h^{eq} = h_s$, where $h_s$ is the still liquid depth given by (volume average)

$$h_s(x, y) = \frac{1}{ab} \int_{(0,0)}^{(a,b)} \left[ h(x, y) + z_b(x, y) \right] \, dx \, dy - z_b(x, y) \tag{2.32}$$

in which $z_b(x, y)$ is the bed profile and $h(x, y)$ is the total depth of the liquid-species mixture given in the domain $0 \leq x \leq a$, $0 \leq y \leq b$. Figure 2.2 gives a sketch of a typical flow domain illustrating the free surface, bed profile and the still liquid depth.

Another equilibrium state is the steady state equilibrium which is defined by $u^{eq} = v^{eq} =$ constant and $\partial q / \partial t = 0$. The steady state equilibrium may be difficult to compute because the calculation requires solving a system of partial or ordinary differential equations and is therefore less often used.

### 2.5 Comparison with Conventional Formulation

The coupled equilibrium-corrected variable-density shallow flow and species transport equations have advantages over the conventional uncoupled formulations for their ability to model shallow flows with variable horizontal density. Conventional formulations assume a low concentration of species so that the transport process does not affect flow properties. This assumption becomes unrealistic for large concentration of the species which, being a part of the liquid-species mixture, does have an impact on flow velocities. Even at low concentration, a discontinuity in the concentration can have an effect on the flow whereby
the higher density region will try to balance the lower density region. This is an analogue to the dam break problems (with a discontinuity in water depth) that may lead to contact discontinuity, rarefaction and shock wave.

In the variable-density shallow flow and species transport equations, the variables $h, u, v, c$ and $\rho$ are solved in a fully coupled manner. The role of the volumetric concentration $c$ is an active scalar so any effect due to the variation of species concentration is embodied in the solution of other variables which include the depth, density and the flow velocities.

The conventional shallow water and species transport equations are simplifications of the variable-density shallow flow and species transport equations for constant density cases with non-zero species concentration. In this case the variable $c$ has changed its role from active to passive. This can be shown by taking $\rho = \rho^{eq}$ and $c^{eq} = 0$ in Equation (2.31) and dividing each equation by the common density constant. By expressing the deviated depth $h - h^{eq}$ as the free surface elevation $\eta$, the following equations are obtained.
\[
\begin{align*}
\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{f}}{\partial x} + \frac{\partial \mathbf{g}}{\partial y} &= \mathbf{h} \\
\begin{bmatrix}
\eta \\
\mathbf{u} \\
\mathbf{v} \\
\mathbf{c}
\end{bmatrix} &= \\
\begin{bmatrix}
u h \\
\frac{u^2 h}{2} + \frac{1}{2} g(\eta^2 + 2 \eta h_y) \\
v \mathbf{u} h \\
v \mathbf{u} \mathbf{c} \\
v \mathbf{v} \\
v \mathbf{v} \mathbf{c}
\end{bmatrix}, \\
\begin{bmatrix}
v h \\
u \mathbf{v} h \\
v \mathbf{u} \mathbf{c} \\
v \mathbf{v} \mathbf{c}
\end{bmatrix} &= \\
\begin{bmatrix}
u^2 h + \frac{1}{2} g(\eta^2 + 2 \eta h_y) \\
v \mathbf{u} \mathbf{v} h \\
v \mathbf{u} \mathbf{v} \mathbf{c} \\
v \mathbf{v} \mathbf{v} \mathbf{c}
\end{bmatrix}, \\
\begin{bmatrix}
u^2 h + \frac{1}{2} g(\eta^2 + 2 \eta h_y) \\
v \mathbf{u} \mathbf{v} h \\
v \mathbf{u} \mathbf{v} \mathbf{c} \\
v \mathbf{v} \mathbf{v} \mathbf{c}
\end{bmatrix}
\end{align*}
\]

The above equations are essentially the coupled shallow water and species transport equations (see e.g. Liang et al., 2004 and Huang, 2005). This indicates that the model has a wide range of applicability in that the new variable-density shallow flow and species transport equations transform to the conventional shallow water equations plus the advection equation for species transport when \( \rho = \text{constant} \) and \( c \neq 0 \).

### 2.6 Conservation of Mass, Volume and Energy

The governing equations of the variable-density shallow flow and species transport model are derived from physical laws stating the conservation of mixture mass, momentum flux and species mass. In the absence of any source or sink, volume conservation is the consequence of the mass conservation of both the mixture and the species. If the bed friction, wind stress, Coriolis parameter, viscosity and diffusivity are all set to zero so that there is no loss or gain
of energy to or from the system’s surroundings, then the flow is driven purely by the interchange of kinetic energy \((KE)\) and potential energy \((PE)\). Moreover, the sum of \(KE\) and \(PE\) is a constant wherever the flow is varying continuously with \(KE\) and \(PE\) being out of phase at all time. At flow discontinuities such as finite hydraulic jumps, energy is lost according to the first law of thermodynamics.

For the variable-density shallow flow and species transport model, the volume \((V)\), mass \((M)\), kinetic energy \((KE)\) and potential energy \((PE)\) of the liquid-species mixture can be interpreted at any given time as

\[
V = \int_{a(0,0)}^{(a,b)} h \, dx \, dy \quad (2.34)
\]

\[
M = \int_{a(0,0)}^{(a,b)} \rho h \, dx \, dy \quad (2.35)
\]

\[
KE = \int_{a(0,0)}^{(a,b)} \frac{1}{2} \rho h(u^2 + v^2) \, dx \, dy \quad (2.36)
\]

\[
PE = \int_{a(0,0)}^{(a,b)} \rho h g \left( \frac{h}{2} + z_h \right) \, dx \, dy \quad (2.37)
\]

where \(h = h(x, y)\), \(\rho = \rho(x, y)\), \(u\) and \(v\) are the total depth, mixture density and horizontal velocity components defined in the domain \(0 \leq x \leq a, \ 0 \leq y \leq b\) and \(z_h = z_h(x, y)\) is the bed level above the initial reference datum.
Tests are carried out on cases performed in this thesis in order to check the conservation of volume, mass, and energy. The volume and mass of the system are expected to be conserved at all time if there is no mass leaving or entering the system and the boundaries are perfectly reflective. The total energy of the system is also expected to be conserved whenever the flow variables are continuous (i.e. without hydraulic jumps or bores).

2.7 Concluding Remarks

This chapter presents the governing equations of the coupled variable-density nonlinear shallow flow and species transport equations for vertically homogeneous liquid-species mixture. These equations are also presented in equilibrium-corrected form in order to rectify the numerical imbalance between the flux gradient and source terms. It is shown that the flux Jacobian matrix for the equilibrium-corrected system is the same as that of the original system. Integral expressions for mass, volume and energy are also established for validating conservations of these quantities.
Figure 2.1 Sketch of the control volume for vertically homogenous liquid-species mixtures

Figure 2.2 Sketch illustrating the free surface, bed profile and still liquid depth
CHAPTER 3  NUMERICAL SOLUTION

This chapter presents the numerical solution of the variable-density shallow flow and species transport model utilising a Godunov-type finite volume scheme in conjunction with an approximate Riemann solver. The finite volume scheme transforms the integral form of the governing partial differential equations to a system of algebraic equations which can be solved on a collocated grid. At each time step, the values of the conserved variables are stored at the centre of each cell and the corresponding interface values are computed using a second order linear interpolation. The interface fluxes through adjacent cells are calculated using either Roe's or the HLL approximate Riemann solver. The source terms are discretized using a second-order central difference method. The conserved variables are updated in time using an explicit second-order Adams-Bashforth scheme.

3.1  The Godunov-type Scheme

For a vertically homogeneous liquid-species mixture, the equilibrium-corrected shallow flow and species transport equations derived in Chapter 2 can be expressed in the following integral form (omitting tildes in Equation (2.26) for convenience).

\[
\frac{\partial}{\partial t} \int_{\Omega} q \, d\Omega + \int_{\partial \Omega} (fn_x + gn_y) \, dS = \int_{\Omega} h \, d\Omega \quad (3.1)
\]
in which \( \Omega \) is the flow domain with boundary \( S \), \( n_x \) and \( n_y \) are the Cartesian components of the unit vector \( \mathbf{n} \) in the \( x \)- and \( y \)-directions respectively, and \( \mathbf{q}, \mathbf{f}, \mathbf{g} \) and \( \mathbf{h} \) are the corresponding vectors of the conserved variables, inviscid fluxes and source terms given by

\[
\mathbf{q} = \begin{bmatrix}
\rho h - \rho \rho_{eq} \rho_{eq} \\
\rho u h \\
\rho v h \\
\rho, c u h - \rho, c \rho_{eq} \rho_{eq}
\end{bmatrix}
\]

\[
\mathbf{f} = \begin{bmatrix}
\rho u h \\
\rho u^2 + \rho \gamma h - \frac{1}{2} \rho \rho_{eq} \rho_{eq} (h_{eq})^2 \\
\rho u v h \\
\rho c u h
\end{bmatrix}
\]

\[
\mathbf{g} = \begin{bmatrix}
\rho v h \\
\rho v^2 + \frac{1}{2} \rho g h^2 - \frac{1}{2} \rho \rho_{eq} \rho_{eq} (h_{eq})^2 \\
\rho v u h \\
\rho v c h
\end{bmatrix}
\]

\[
h = \begin{bmatrix}
0 \\
\tau_{wx} - \tau_{ex} - \rho g h S_{sx} + \rho v h f + \frac{\partial (h T_{sx})}{\partial x} + \frac{\partial (h T_{sy})}{\partial y} \\
\tau_{wy} - \tau_{ey} - \rho g h S_{sy} - \rho u h f + \frac{\partial (h T_{sy})}{\partial x} + \frac{\partial (h T_{yy})}{\partial y} \\
\frac{\partial}{\partial x} \left( K_h \frac{\partial (\rho, c)}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_h \frac{\partial (\rho, c)}{\partial y} \right)
\end{bmatrix}
\]

where \( \rho, u, v, c \) and \( h \) are the depth-averaged mixture density, velocity components in the \( x \)- and \( y \)-directions, volumetric species concentration, and the total depth of the liquid-species mixture respectively; \( \tau_{wx}, \tau_{wy} \) are surface stress components and \( \tau_{ex}, \tau_{ey} \) are bed stress components; \( S_{sx}, S_{sy} \) are the bed slope components and \( T_{sx}, T_{sy}, T_{yy} \) are the viscous stress components.
components; \( f \) is the Coriolis parameter and \( K_x, K_y \) are the horizontal mixing coefficients.

The superscript \( eq \) refers to the equilibrium state values of the conserved variables, which can be taken at quiescent state or steady state of the system. The liquid-species mixture density and the volumetric species concentration are related by Equation (2.5).

To solve for the conserved variables, the integral equation is discretized on a collocated grid with \( \rho h - \rho^{eq} h^{eq} \), \( \rho u_h \), \( \rho v_h \) and \( \rho_c h - \rho_c^{eq} h^{eq} \) stored at the centre of each cell. For an arbitrary cell \( (i) \) on the grid, Equation (3.1) can be conveniently rewritten as

\[
\frac{\partial \Lambda^q}{\partial t} = - \oint_{\partial C_{(i)}} \left( f_{(i)} n_x + g_{(i)} n_y \right) dS + A_{(i)} h_{(i)}
\]

where \( A_{(i)} \) denotes the area of cell \( (i) \) which has the path of integration \( \partial C_{(i)} \) along the four cell edges.

It is convenient to define and denote the vector of flux functions as

\[
F = fn_x + gn_y
\]

The surface integral in Equation (3.3) can be evaluated in discrete form as a summation by using the following expression

\[
\oint_{\partial C_{(i)}} F dS = - \left( F_{W(i)} - F_{E(i)} \right) \Delta y_{(i)} - \left( F_{S(i)} - F_{N(i)} \right) \Delta x_{(i)}
\]
where $F_W(i), F_E(i), F_S(i)$ and $F_N(i)$ are the corresponding inviscid flux vectors through the west, east, south and north face of cell $(i)$, and $\Delta x_{(i)}$ and $\Delta y_{(i)}$ denote the cell dimensions in the $x$- and $y$-directions respectively. Note that $F_W = f_w n_x$, $F_E = f_e n_x$, $F_S = g_s n_y$ and $F_N = g_N n_y$.

The area of any rectangular cell is simply the product of the cell dimensions, i.e. $A_i = \Delta x \Delta y$.

Hence substitution of (3.5) into (3.3) gives

$$
\frac{\partial \mathbf{q}}{\partial t} \bigg|_{(i)} = \frac{F_{W(i)} - F_{E(i)}}{\Delta x} + \frac{F_{S(i)} - F_{N(i)}}{\Delta y} + \mathbf{h}_{(i)} \tag{3.6}
$$

Now the values of the conserved variables $\mathbf{q}$ and its time derivative $\partial \mathbf{q} / \partial t$ at any given time $t$ are known. The values of the conserved variables at time $t + \Delta t$ can be obtained using a second-order Adams-Bashforth time-stepping method:

$$
\mathbf{q}_{(i)}^{t+\Delta t} = \mathbf{q}_{(i)}^t + \frac{\Delta t}{A_i} \left( \frac{3}{2} \frac{\partial \mathbf{Aq}}{\partial t} \bigg|_{(i)} - \frac{1}{2} \frac{\partial \mathbf{Aq}}{\partial t} \bigg|_{(i)}^{\Delta t} \right) \tag{3.7}
$$

For a uniform rectangular grid, the above equation simplifies to

$$
\mathbf{q}_{(i)}^{t+\Delta t} = \mathbf{q}_{(i)}^t + \Delta t \left( \frac{3}{2} \frac{\partial \mathbf{q}}{\partial t} \bigg|_{(i)} - \frac{1}{2} \frac{\partial \mathbf{q}}{\partial t} \bigg|_{(i)}^{\Delta t} \right) \tag{3.8}
$$
The time step required for a stable solution is determined by the Courant Friedrichs Lewy criterion (CFL), which can be expressed in terms of the Courant number $C_o$. For an arbitrary cell $i$ on a 2-D Cartesian grid, the CFL criterion implies

$$\Delta t \leq \min \left[ \left( \frac{C_o \min(\Delta x, \Delta y)}{\sqrt{gh + \sqrt{u^2 + v^2}}} \right) \right], \quad (0 < C_o \leq 1) \quad (3.9)$$

where $\Delta x$ and $\Delta y$ are the cell dimensions, and $u$ and $v$ are the flow velocities in the $x$- and $y$- directions respectively.

It is evident the system of algebraic equations (3.8) can be readily solved once the interface flux vectors are available. For Godunov-type methods, approximate Riemann solvers can provide an accurate and efficient computational tool to evaluate interface fluxes. Two types of approximate Riemann solvers are considered in this thesis. Details on the methodology used to determine the interface fluxes are presented in the following sections.

### 3.2 Roe’s Approximate Riemann Solver

The flux Jacobian matrix $A$ can be approximated as a constant coefficient Roe matrix with entries written in terms of the Roe averages defined in terms of the left and right data states $u_L$ and $u_R$. If $u = [h, u, \psi]^T$, where $\psi$ is a passive scalar, then the Roe averages can be obtained using Roe-Pike approach (Roe & Pike, 1984) which are given by:

$$u = \frac{u^+ \sqrt{h^+} + u^- \sqrt{h^-}}{\sqrt{h^+} + \sqrt{h^-}}, \quad \psi = \frac{\psi^+ \sqrt{h^+} + \psi^- \sqrt{h^-}}{\sqrt{h^+} + \sqrt{h^-}}, \quad h = \sqrt{h^+ h^-}, \quad a = \sqrt{\frac{g(h^+ + h^-)}{2}} \quad (3.10)$$
where $a$ is the wave celerity given by $a = \sqrt{gh}$ and the superscripts $-$ and $+$ are used to represent the left and right Riemann states respectively.

The interface fluxes can be evaluated by adopting Roe’s approximate Riemann solver at each cell edge as follows

$$
\mathbf{f}_{(i,j)} = \frac{1}{2} [\mathbf{f}(\mathbf{q}_{(i,j)}^+) + \mathbf{f}(\mathbf{q}_{(i,j)}^-) - |\mathbf{A}|(\mathbf{q}_{(i,j)}^+ - \mathbf{q}_{(i,j)}^-)]
$$

in which

$$
|\mathbf{A}| = \mathbf{R}|\Lambda|\mathbf{L}
$$

where $\mathbf{q}_{(i,j)}^+$ and $\mathbf{q}_{(i,j)}^-$ are the reconstructed right and left Riemann states of the conserved variables at the cell interface and $\mathbf{A}$ is the flux Jacobian matrix evaluated using the right and left eigenvector matrices $\mathbf{R}$ and $\mathbf{L}$ and the diagonal matrix of the absolute values of the eigenvalues $|\Lambda|$.

The interface flux through the west, east, south and north edge of the cell can be evaluated using (3.11). For example, the flux through the west face of cell $(i, j)$ can be expressed as

$$
\mathbf{f}_{W(i,j)} = \frac{1}{2} [\mathbf{f}(\mathbf{q}_{W(i,j)}^+) + \mathbf{f}(\mathbf{q}_{W(i,j)}^-) - |\mathbf{A}|(\mathbf{q}_{W(i,j)}^+ - \mathbf{q}_{W(i,j)}^-)]
$$

The flux Jacobian matrix is obtained upon linearization of the original hyperbolic system of conservative equations. Recall from Section 2.3 that the flux Jacobian matrix of the equilibrium-corrected system is the same as the flux Jacobian matrix of the original system.
The latter is less complex and therefore much easier to compute. Taking $f$ and $q$ from (2.8), simple differentiation of $f$ with respect to $q$ leads to

$$A = \begin{bmatrix}
0 & n_x & n_y & 0 \\
(a^2 - u^2 + \frac{(\rho_s - \rho_w)\alpha^2 c}{2 \rho_w})n_x - un_y & 2un_x + vn_y & un_y & -\frac{(\rho_s - \rho_w)\alpha^2}{2 \rho_s \rho_w} n_x \\
-avn_x + \left(a^2 - v^2 + \frac{(\rho_s - \rho_w)\alpha^2 c}{2 \rho_w}\right)n_y & vn_x & un_x + 2vn_y & -\frac{(\rho_s - \rho_w)\alpha^2}{2 \rho_s \rho_w} n_y \\
-\frac{\rho_s \alpha c}{\rho} n_x - \frac{\rho_s \alpha c}{\rho} n_y & \frac{\rho_s \alpha c}{\rho} n_x & \frac{\rho_s \alpha c}{\rho} n_y & un_x + vn_y
\end{bmatrix}$$

in which $a = \sqrt{gh}$ is the wave celerity.

The eigenvalues of the flux Jacobian matrix of the hyperbolic system of equations are determined by solving $\det(A - \lambda I) = 0$, where $I$ is the $4 \times 4$ identity matrix. The eigenvalues of the flux Jacobian matrix are found to be $\lambda_1 = un_x + vn_y - a$, $\lambda_2 = un_x + vn_y$, $\lambda_3 = un_x + vn_y$, and $\lambda_4 = un_x + vn_y + a$. These four real eigenvalues confirm the hyperbolicity of the system (not strictly hyperbolic because two of the four eigenvalues are identical). Furthermore, $\lambda_1$ and $\lambda_4$ define genuinely non-linear fields associated with a shock or rarefaction wave whereas $\lambda_{2,3}$ (with multiplicity two) defines a linearly degenerate field associated with an intermediate contact wave. The characteristic wave speeds are given by the eigenvalues, and the corresponding eigenvectors indicate the directions of wave propagation. In matrix form, the absolute values of the eigenvalues are given by
In order to find a right and a left eigenvector of matrix $A$ corresponding to the eigenvalue $\lambda$, one needs to solve the equation $AR = \lambda R$ and $LA = \lambda L$. For a hyperbolic system of conservation laws, an important property which links the left and right eigenvectors of the Jacobian matrix is the bi-orthonormality condition (Toro, 2001). The left and right eigenvectors $L$ and $R$ are said to be bi-orthonormal if they satisfy the relations

$$L^{(i)} \cdot R^{(j)} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{otherwise}. \end{cases}$$

(3.16)

For the bi-orthonormality condition to be satisfied, appropriate scaling factors must be chosen for each pair of $L^{(i)}$ and $R^{(i)}$. The coefficients are not unique due to the degree of freedom in the system of equations. As a result, there may be many different combinations for each pair of left and right eigenvectors. The left and right eigenvectors of the matrix (3.14) are derived in a form similar to those for the flux matrix of the conventional shallow water and species transport models, which are presented in the following.
Note that when $\rho = \text{constant}$ and $c \neq 0$, the above matrix reduces to the Jacobian matrix for the conventional shallow water and species equations such as that obtained by Liang et al. (2004). This justifies the feasibility of model under constant density conditions.

At each time step, the matrix $|A|$ is evaluated using averaged values by adopting the Roe-Pike approach (Roe & Pike, 1984). The Roe averages of the variables $u, v, c$ and $a$ are given by
\[ u = \frac{u^+ \sqrt{(\rho h)^+} + u^- \sqrt{(\rho h)^-}}{\sqrt{(\rho h)^+} + \sqrt{(\rho h)^-}}, \quad v = \frac{v^+ \sqrt{(\rho h)^+} + v^- \sqrt{(\rho h)^-}}{\sqrt{(\rho h)^+} + \sqrt{(\rho h)^-}}, \quad \frac{c}{a} = \frac{c^+ \sqrt{(\rho h)^+} + c^- \sqrt{(\rho h)^-}}{\sqrt{(\rho h)^+} + \sqrt{(\rho h)^-}}, \quad \text{and} \quad a = \sqrt{\frac{g(h^+ + h^-)}{2}} \]  

(3.19)

where the superscripts + and – denote the right and left Riemann states on either side of a cell interface respectively.

Note that the left and right Riemann states of the variable \( \rho \) can be obtained from \( c \) using Equation (2.5) and the left and right Riemann states of the variable \( h \) are obtained using the following.

\[

h^+ = \frac{(\rho h)^+}{\rho^+} = \frac{(\rho h)^+}{\rho_w + c^+ (\rho_s - \rho_w)} \quad \text{and} \quad h^- = \frac{(\rho h)^-}{\rho^-} = \frac{(\rho h)^-}{\rho_w + c^- (\rho_s - \rho_w)}

(3.20)

Based on the assumption of non-zero depth, Roe’s approximate Riemann solver can not strictly handle situations involving dry bed states. The Roe’s solver deals with dry bed problems by means of artificial bed wetting. This is equivalent to setting the depth over the dry bed to some very small positive tolerance known as the artificial-wetting parameter. The magnitude of the wetting parameter determines the error in the speed of the dry front. Even a tolerance of as small as 0.001 m can give rise to a 25% error in propagation speed (Toro, 2001). It is likely that any error in the propagation speed will grow with time which can then significantly affect the flow features for long evolution times. For problems with dry bed conditions, another approximate Riemann solver that deals with the wet-dry fronts systematically is developed so that comparisons can be made with results obtained using the Roe solver with artificial bed-wetting.
3.3 The HLL Approximate Riemann Solver

The HLL (Harten, Lax and van Leer, 1983) approximate Riemann solver computes the interface flux $f_{i+1/2}$ by direct approximation which is derived using the integral form of the conservation laws. The HLL numerical flux is given by (Toro, 2001)

$$f_{i+1/2} = \begin{cases} 
  f_L & \text{if } S_L \geq 0 \\
  \frac{S_R f_L - S_L f_R + S_R S_L (q_R - q_L)}{S_R - S_L} & \text{if } S_L \leq 0 \leq S_R \\
  f_R & \text{if } S_R \leq 0 
\end{cases}$$

(3.21)

where $f_L$ and $f_R$ are left and right fluxes that correspond to the left and right data states $q_L = q_i^n$ and $q_R = q_{i+1}^n$ respectively; $S_L$ and $S_R$ are left and right wave speed estimates in the two-wave structure of the Riemann problem solution assumed in the HLL approach (see e.g. Toro, 2001).

The two-wave assumption of the HLL solver becomes inadequate for 2-D problems and 1-D problems with extra species-like equations as it ignores the middle wave. The results are excess unphysical smearing of vortices and contact discontinuities (Toro, 2001). However, the HLL approach does offer a simple method of dealing with wet/dry fronts in dry bed situations by estimating the front speed directly.
The left and right wave speed estimates adopted as part of the HLL solver defined in Equation (3.21) are suggested by Davis (1988) and Toro (2001) for wet and dry bed regions respectively. The two cases are combined according to the depth positivity condition (Toro, 2001) to give the following expressions of the left and right wave speeds.

\[
S_L = \begin{cases} 
    u_R - 2a_R & \text{if } h_L = 0 \\
    \min(u_L - a_L, u_R - a_R) & \text{if } h_L > 0 
\end{cases}
\]

\[
S_R = \begin{cases} 
    u_L + 2a_L & \text{if } h_R = 0 \\
    \max(u_L + a_L, u_R + a_R) & \text{if } h_R > 0 
\end{cases}
\] (3.22)

where \( u_L, a_L, u_R \) and \( a_R \) are values of the velocity and wave celerity of the left and right data states \( q_L = q_L^i \) and \( q_R = q_{i+1}^r \) respectively.

### 3.4 Slope Limiter

Evaluation of the intercell fluxes requires values of the left and right Riemann states either side of the cell interfaces. Using cell-centred values of the conserved variables as estimates of cell-face values would give first-order approximations of the intercell fluxes. In order to achieve second-order accuracy, a piecewise linear interpolation of the left and right Riemann states of each conserved variable is required. Within an arbitrary cell \( i \), the second-order spatial information can be obtained from linear interpolation across the cell given by

\[
q = q_i + \nabla q_i \cdot r_i 
\] (3.23)
where \( \mathbf{r}_i \) is the vector from the cell centre to the midpoint of the corresponding cell interface.

Numerical oscillations are common with second and higher-order numerical schemes. In the Godunov-type schemes, unphysical oscillations are generated from linear interpolations across an arbitrary cell. At flow discontinuities these oscillations can lead to physically meaningless results. Unwanted oscillations can be controlled by either employing non-linear limiters or by introducing artificial viscosity in the numerical scheme.

Von Neumann and Richtmyer (1950) proposed an artificial viscosity approach to damp the amplitude of spurious oscillations near discontinuities when solving the Euler equations. A purely artificial dissipative term is added to the solver to adjust the gradients so that discontinuous solutions are represented more accurately. This method is straightforward to implement and computationally efficient. However, it is difficult to achieve the adequate amount of dissipation, which leads to problems such as excess smearing at discontinuities.

Non linear limiters are utilised as scaling factors to the gradient terms during the estimation of conserved quantities at each cell interface. The extreme values are controlled by the limiters in order to avoid grossly unphysical results. The modified cell interface values of the conserved variables are then used in the Riemann solver to estimate the flux across the cell. There are various choices for the limiter function \( \Phi \). A version proposed by Hirsch (1990) is defined as:

\[
\Phi(r) = \max[0, \min(\beta r, 1), \min(r, \beta)] \quad \text{for } 1 \leq \beta \leq 2 \tag{3.24}
\]

where \( \beta \) is the limiter parameter and \( r \) is the gradient ratio given by
In particular, $\beta = 1$ gives the MINMOD limiter and $\beta = 2$ gives the SUPERBEE limiter.

The choice of the limiter greatly depends on the problem that is being dealt with. Among others, Anastasiou and Chan (1997), Suratanakavikul and Marquis (1999) and LeVeque (2002) present comparative studies of flux limiters. It is found that as the limiter increases in strength, the results become less diffusive but admit greater numerical oscillations.

Equation (3.23) can now be modified to include the limiter function in the gradient term. Hence for consecutive east-west cells $(i - 1, j), (i, j), (i + 1, j)$ and south-north cells $(i, j - 1), (i, j), (i, j + 1)$ on a locally uniform gird, the Riemann states for the vector of the conserved variables at each cell interface are given by

\[
\begin{align*}
q_{E(i,j)}^- &= q_{i,j} + \frac{\Phi(r)}{2} (q_{i,j} - q_{i-1,j}) = q_{w(i+1,j)}^+ \\
q_{W(i,j)}^- &= q_{i,j} - \frac{\Phi(r)}{2} (q_{i,j} - q_{i-1,j}) = q_{e(i-1,j)}^- \\
q_{N(i,j)}^+ &= q_{i,j} + \frac{\Phi(r)}{2} (q_{i,j} - q_{i,j-1}) = q_{s(i,j+1)}^+ \\
q_{S(i,j)}^- &= q_{i,j} - \frac{\Phi(r)}{2} (q_{i,j} - q_{i,j-1}) = q_{n(i,j-1)}^- 
\end{align*}
\]

(3.26)

where $E$, $W$, $N$ and $S$ denote the east, west, north and south cell interface, and superscripts + and − denote the right and left Riemann states either side of the cell interface respectively.
3.5 Boundary Conditions

Two types of simple boundary conditions are considered herein, namely transmissive open boundary and reflective closed boundary conditions (Toro, 2001). The boundary conditions for each type are imposed as follows.

At open transmissive boundaries in the $x$-direction:

$$\rho_0 = \rho_1, \quad h_0 = h_1, \quad u_0 = u_1, \quad v_0 = v_1,$$

$$\rho_m = \rho_m, \quad h_{m+1} = h_m, \quad u_{m+1} = u_m, \quad v_{m+1} = v_m. \quad (3.27)$$

At closed reflective boundaries in the $x$-direction:

$$\rho_0 = \rho_1, \quad h_0 = h_1, \quad u_0 = u_1, \quad v_0 = v_1,$$

$$\rho_{m+1} = \rho_m, \quad h_{m+1} = h_m, \quad u_{m+1} = -u_m, \quad v_{m+1} = v_m. \quad (3.28)$$

In the above, $\rho$ is the density, $h$ is the depth, and $u$ and $v$ are the velocity components normal and tangential to the wall respectively. The subscripts 1 and $m$ refer to the cells immediately inside the computational domain and the subscripts 0 and $m+1$ are used to represent fictitious cells outside the domain.
CHAPTER 4  TESTS FOR CONSTANT-DENSITY CASES

For validation purposes, the variable-density shallow flow and species transport model is first verified under constant density conditions. When the fluid density is constant, the governing equations are essentially the coupled shallow water and species transport equations. Benchmark tests with analytical or nearly exact numerical solutions of the shallow water and species transport equations are used to examine the accuracy, adaptability and stability of the numerical model, each focusing on a particular aspect.

For all the cases presented in this chapter (unless otherwise stated): the liquid is taken to be water of density 1,000 kg/m$^3$; the species also has density 1,000 kg/m$^3$; the acceleration due to gravity is $g = 9.8$ m/s$^2$; Turbulence, viscous, wind and Coriolis effects are neglected. The numerical results displayed in this chapter are obtained using the Roe's approximate Riemann solver unless otherwise stated. The Courant-Friedrichs-Lewy condition given in (3.9) and grid convergence are verified for all the computations so that the solutions of the Godunov scheme are linearly stable. In order to give quantitative measures between the numerical and analytical solutions for cases with analytical solutions, the percentage normalised root mean squared (RMS) differences are calculated using the following formula

$$E_{\text{RMS}} = \frac{\sqrt{\frac{1}{n} \sum (f_i - F_i)^2}}{\sqrt{\frac{1}{n} \sum F_i^2}} \times 100\% \quad (4.0)$$

where $f_i$ and $F_i$ are the corresponding numerical and analytical values at point $i$ from a set of $n$ data points.
4.1 Uniform Flow in a Sloping Channel

This test involves flow down a rectangular open channel with a constant non-zero bed slope, which is used to examine the ability of the model to simulate steady inviscid flow conditions. At steady state, the flow speed is uniform everywhere because pressure force component down the channel is balanced with the friction opposing the motion.

The channel used in this test is 1000 m long by 250 m wide with a slope of 1 in 1000. The channel contains water at a constant depth of 5 m which is initially at rest. By taking the Chézy coefficient as 41.42 m$^{1/2}$/s, the depth-averaged velocity $u$ along the channel at steady state is calculated from the Chézy equation as,

$$u = C_{ch} \sqrt{RS_{ox}} = 41.42 \sqrt{5.0 \times 0.001} = 2.92883628767 \text{ m/s} \quad (4.1)$$

where $C_{ch}$ is the Chézy coefficient, $S_{ox}$ is the bed slope and $R$ is the hydraulic radius which approximates to the total water depth for infinitely wide channels.

The model was run on a uniform grid consisting of 40 x 10 cells with a time step of 1.0 s until reaching steady state at $t = 4000$ s. Both the inflow and outflow boundaries were set to be transmissive. The steady state flow speed predicted by the model is 2.92883628767 m/s to 12 significant figures at all grid points. Figure 4.1 shows the velocity field over the domain at $t = 4000$ s.

The numerical prediction is in agreement with the analytical solution to 12 significant figures. The results demonstrate that the model is capable of simulating inviscid flows in a
rectangular sloping channel. This test case validates the ability of the numerical scheme to model advective, gravity, surface gradient and bed stress terms in the steady state.

4.2 Seiching in a Rectangular Basin

If the free surface of a flow in steady state is displaced from its equilibrium position, the subsequent motion will be such as to restore it towards the steady state of the system. The driving force of such free surface motions is gravity, accompanied by frictional and viscous effects that diminish amplitude and dissipate energy. Free surface motions of liquid under gravity exhibit very different behaviour depending on the initial disturbance. For disturbances of very small amplitude, the free surface motions are almost linear and analytical solutions can be sought by application of first-order small perturbation theory. The wave non-linearity increases with wave steepness, which can be observed as a shape change of the wave and a phase-shift that grows with time with respect to the corresponding linear solution.

Provided the amplitude of the initial wave is small compared to the still water depth, the subsequent sloshing motions can be approximated by applying first order small perturbation theory. The solution procedure involves writing the original system of partial differential equations in terms of equilibrium values and perturbation variables and then linearising the resulting equations by neglecting double and higher order product type terms. This transformation gives a completely linear system of partial differential equations which can be solved analytically. The procedure for obtaining the 1-D analytical solution is given briefly in the following.
For a flat-bottomed rectangular basin of constant cross-section, the flow dynamics is determined by the solution of the 1-D shallow water equations (neglecting frictional, diffusive and Coriolis effects):

\[
\begin{align*}
\frac{\partial h}{\partial t} + \frac{\partial uh}{\partial x} &= 0 \\
\frac{\partial uh}{\partial t} + \frac{\partial}{\partial x} \left( u^2 h + \frac{1}{2} gh^2 \right) &= 0
\end{align*}
\] (4.2)

where \( h \) is the total water depth and \( u \) is the depth-averaged flow velocity.

Let the equilibrium state be the quiescent state with zero flow velocity and constant still water depth \( h_s \). Consider the system when it is slightly perturbed from its equilibrium state such that \( h(x,t) = h_s + h'(x,t) \) and \( u(x,t) = 0 + u'(x,t) \), where \( h' \) and \( u' \) are the perturbation variables measured from their equilibrium values. The depth perturbation variable \( h'(x,t) \) is usually denoted by the free surface elevation \( \eta(x,t) \).

Linearising Equation (4.2) by neglecting quadratic and higher order terms in the perturbation variables leads to a linear system of partial differential equations:

\[
\begin{align*}
\frac{\partial \eta}{\partial t} + h_s \frac{\partial u'}{\partial x} &= 0 \\
\frac{\partial u'}{\partial t} + g \frac{\partial \eta}{\partial x} &= 0
\end{align*}
\] (4.3)

This system of equations can be solved analytically by seeking solutions in the form below:
The constants $H_n, U_n, \alpha_n$ and $\beta_n$ which are independent of $x$ and $t$ can be determined from the given initial conditions. The general solutions to Equation (4.4) are given as follows (See e.g. Cunge, Holly and Verwey, 1980).

$$
\eta_n = e^{i\alpha_n x} (A_n e^{i\beta_n t} + B_n e^{-i\beta_n t})
$$

$$
u_n = \frac{g}{\sqrt{gh_s}} e^{i\alpha_n x} (-A_n e^{i\beta_n t} + B_n e^{-i\beta_n t})$$

where $A_n$ and $B_n$ are arbitrary constants.

Suppose the initial free surface disturbance satisfies:

$$
\eta_n \big|_{t=0} = \eta_n(x, 0) = A \cos(k_n x), \quad 0 \leq x \leq L
$$

$$
k_n = \frac{n\pi}{L}, \quad n = 0, 1, 2, 3... (n^{th} \text{ sloshing mode})
$$

where $A$ is the amplitude of the initial wave profile, $x$ is the horizontal distance along the length of the basin and $k_n$ is the wave number.

The solution $\eta_n$ to the partial differential equations (4.3) can be obtained by substituting (4.6) into (4.5). With the initial free surface profile as in (4.6) and zero initial flow velocities everywhere, the first-order free surface elevation for the $n^{th}$ sloshing mode along the length of the tank is
\[ \eta_n(x,t) = A \cos(k_n x) \cos(\omega_n t) = A \cos\left(\frac{n\pi x}{L}\right) \cos\left(\frac{n\pi \sqrt{gh_s} t}{L}\right), \quad 0 \leq x \leq L, \quad t \geq 0 \quad (4.7) \]

where \( \omega_n = k_n \sqrt{gh_s} = \frac{n\pi}{L} \sqrt{gh_s} \) is the sloshing frequency.

The seiching test considered herein is used to investigate sloshing motions due to small amplitude waves. This test has been chosen for verifying the mass and energy conservation in perfectly reflective environments in the absence of any source and sink terms. This is an important check because the linear solution (4.4) is strictly energy conserving.

The test consists of a basin of length \( L = 100 \) m with an initial still water depth of \( h_s = 1 \) m. The aspect ratio is therefore \( h_s / L = 0.01 \). The bed of the enclosed basin is assumed to be horizontal, the walls are assumed to be perfectly reflective and the liquid is assumed to be incompressible, irrotational and inviscid.

The second harmonic (\( n = 2 \) secondary) sloshing mode was selected for demonstration purposes. The effect of non-linearity on free surface motions was investigated by varying the initial wave steepness \( A \) and comparing numerical predictions with first-order analytical solutions derived from small perturbation theory. For the second harmonic mode, the first-order linear free surface profile along the tank is given by Equation (4.7) as

\[ \eta(x,t) = A \cos\left(\frac{2\pi x}{L}\right) \cos\left(\frac{2\pi t \sqrt{g}}{L}\right), \quad 0 \leq x \leq L, \quad t \geq 0 \quad (4.8) \]
In order to compare numerical predictions with first-order linear solutions systematically, the results are presented in non-dimensional form. The non-dimensionalised variables are:

\[ z^* = \frac{\eta}{A}, \quad x^* = \frac{x}{L}, \quad t^* = \frac{2\pi t \sqrt{g}}{L} \]  

The period of the non-dimensionalised solutions is therefore \( 2\pi \) radians. Figures 4.2-4.5 display the predicted wave profiles and time histories of the free surface elevation at the basin centre and time histories of the kinetic, potential and total energy. A uniform grid consisting of 201 cells is used and the time step is \( \Delta t = 0.05 \) s. The limiter is Minmod.

Figure 4.2 illustrates the free surface profiles along the tank at five different times during the second cycle. For amplitude ratio \( A/h_s = 0.0001 \), two sharply defined nodes occur one-quarter and three-quarters the distance along the tank and the profiles have spatial symmetry about the node. For \( A/h_s = 0.01 \), the two nodes are less distinct due to the steeper initial wave profile leading to more apparent nonlinear effects. The crests are narrower and the troughs are shallower (in accordance with the findings of other researchers who use potential flow models, e.g. Chern et al., 1999). Similar effects have been found by many authors, e.g. Greaves et al. (1997), Chern et al. (1999) and Frandsen and Borthwick (2003), for sloshing in a rectangular tank, solved using fully nonlinear potential flow models. It should however be noted that the present model assumes hydrostatic pressure and long wave representation, unlike the aforementioned potential flow models. For amplitude ratio \( A/h_s = 0.1 \), the nonlinear effects are so significant that the initial sinusoidal wave is converted into a bore-like profile. A pair of opposing bores, travelling in the opposite direction to the other, reflecting at the lateral walls and interacting with each other at the centre of the tank is apparent, each of which propagates across the basin reflecting at the lateral walls.
Figure 4.3 shows the evolution of the bores for amplitude ratio $A/h_s = 0.1$, as a series of snapshots in time. The left and right bores have identical amplitudes (at any given time). After reflecting at the walls, the two bores approach each other, their amplitude remaining nearly constant, though appearing to sit lower in the water as the depth behind each bore has to drop (to maintain mass conservation). At the point of collision, the water depth is constant everywhere, and has a value close to that of still water. There is a spike at the point of collision. Afterwards, the two bores re-emerge and continue towards the walls, each retaining approximately the same amplitude as before the collision, but riding progressively lower as the water surface ahead of both bores drops (to compensate for the increasing amount of water at higher elevation between the bore fronts).

Figure 4.4 displays the time histories of the free surface elevation at the centre of the basin according to numerical predictions and first-order analytical solutions. For low amplitude ratio $A/h_s = 0.0001$, the predicted and analytical time histories almost exactly coincide, as would be expected from first-order linear perturbation theory. For $A/h_s = 0.01$, the agreement is close at the beginning, but the phase shift becomes more apparent as time increases due to the more dominant nonlinear effects. The numerically predicted free surface profile becomes less and less sinusoidal over time, showing a steeper front but a more gradual back face compared to the first-order linear approximation of the free surface. For the largest amplitude ratio considered i.e. $A/h_s = 0.1$, the free surface elevation reduces rapidly in amplitude, unlike the first-order linear approximation. This is because the nonlinear effects are so significant that a pair of shock-like bores are generated leading to energy loss at the wave front. The normalised RMS differences for the three different amplitude ratios used here are 0.84%, 9.0% and 49% respectively. The difference is under
1% for the case with the smallest amplitude and grows as the amplitude increases which is expected due to the influence of nonlinearity.

Figure 4.5 shows the time histories of the variations in kinetic energy (KE), potential energy (PE) and the sum of the kinetic and potential energy (KE+PE). For small initial amplitude ratio $A/h_s = 0.0001$, KE and PE are exactly out of phase by half of the period and their sum is approximately constant in time. The numerical prediction of KE+PE is in agreement with the constant total energy principle for small amplitude waves apart from a small loss of 1.27 % (equivalent to 0.1 % per cycle) due to numerical limitations and weak nonlinear effects. As the initial amplitude ratio increases to $A/h_s = 0.01$, the crest of the PE profile has decreased and the trough of the KE profile has decreased in amplitudes although the total energy is still approximately constant (with a loss of 1.42 % over about 12 cycles). For $A/h_s = 0.1$, the nonlinear effects are so great that bores are formed and energy is lost at the flow discontinuities, which has caused a decrease of 63.8 % in the total energy.

4.3 Flow over a Frictionless Hump

The following two cases are benchmark tests that are widely used to validate Godunov-type numerical solvers of shallow water equations. These tests are employed here to validate the model's ability to simulate flows over a non-uniform bathymetry.

4.3.1 Steady Transcritical Flow over a 1-D Hump

This test was used by Vázquez-Cendón (1999) to verify a numerical scheme with an upwind discretization for the bed slope and source terms. This test was also used by Zhou et al.
(2001) who considered both subcritical and transcritical flows with and without shocks by prescribing different boundary conditions. The 1-D hump is defined within a 25-m long domain by

\[
z_h(x) = \begin{cases} 
0.2 - 0.05(x - 10)^2 & \text{if } 8 < x < 12 \\
0 & \text{otherwise}
\end{cases}
\] (4.10)

The boundary conditions have been chosen to provide the most demanding test, i.e. transcritical flow with a shock, over the other flow conditions which are subcritical, supercritical and transcritical without a shock. The initial free surface is 0.33 m above the chosen datum everywhere in the domain, the inflow discharge is specified as 0.18 m²/s and the downstream water depth is 0.33 m. The bed friction is neglected and the flow is assumed to be inviscid with no eddy viscosity. Both inlet and outlet boundaries are treated as transmissive and the no-slip condition is applied at the lateral boundaries.

The global relative error for assessing the convergence is given by Zhou et al. (2001) as

\[
E = \sqrt{\sum \left( \frac{h^n_i - h^{n-1}_i}{h^n_i} \right)^2}
\] (4.11)

Using a grid of 256 cells and a time step of \( \Delta t = 0.0175 \) s, the computed water depth is found to converge in 66 s of flow simulation time with a relative error of less than \( 5 \times 10^{-6} \). The profiles of the free surface elevation, Froude number and flux discharge are displayed in Figure 4.6, along with the corresponding reference solutions.
Analytical solutions are provided by Goutal and Maurel (1997). The computed results are in close agreement with the reference solutions showing the expected discrepancy in the Froude number and flow rate plots at the location of the shock. The corresponding normalised RMS differences in the free surface elevation, Froude number and flow rate are 0.24%, 2.2% and 0.83%, which are all very small. The density distribution predicted by the model is uniform everywhere with no discontinuity at the shock. The discrepancy at the flow discontinuity can be observed in the results reported by Vázquez-Cendón (1999), Hubbard and García-Navarro (2000), Zhou et al. (2001) and Rogers et al. (2003). Rogers et al. (2003) suggest that this discrepancy could be due to the fact the energy conservation is not satisfied in this type of discontinuous shallow flow is when solved using Godunov-type methods.

4.3.2 Wave Propagation over a 2-D Hump

This case was proposed by LeVeque (1998) and later considered by Hubbard and García-Navarro (2000), Rogers et al. (2003). The bed topography is defined within a 1 x 1 m² domain as:

\[
z_b = 0.5 \exp \left[ -50 \left( (x - 0.5)^2 + (y - 0.5)^2 \right) \right], \quad \text{for } 0 < x, y < 1
\]  

(4.12)

The water is initially at rest and the initial free surface profile above the datum is given by:

\[
\eta = \begin{cases} 
1.01 \text{ m} & \text{if } x \in (0.05, 0.15) \\
1 \text{ m} & \text{otherwise}
\end{cases}
\]

(4.13)
Transmissive boundaries are located at \( x = 0, 1 \) m and lateral slip boundaries at \( y = 0, 1 \) m. The bed friction and eddy viscosity coefficients are set to zero, and the acceleration due to gravity is \( g = 1 \) m/s\(^2\). A uniform grid of 100 \( \times \) 100 cells and a time increment of \( \Delta t = 0.002 \) s were used in the numerical computation. The slope limiter used is Minmod.

The predicted results at \( t = 0.1 \) s are shown in Figure 4.7. The initial water surface splits into two waves travelling in opposite directions each with characteristic speed \( \sqrt{gh} \). The leftward wave travels towards the boundary and eventually leaves the domain without any disturbance to the flow. It can be seen from the graph that the rightward wave has propagated over the hump producing a trough just in front of the hump and a crest further ahead of the hump. Wave energy is concentrated near the location of the crest where the amplitude is the greatest. There are no unphysical oscillations present in the numerical solution. The positions of the trough and the crest shown in the numerically predicted contours are at \( x = 0.6 \) m and \( x = 0.75 \) m respectively, both located between \( y = 0.4 \) and \( y = 0.6 \) m approximately (with the crest having a more elongated shape than the trough). These results agree with those obtained by LeVeque (1998), Hubbard and Garcia-Navarro (2000) and Rogers et al. (2003).

### 4.4 Idealised 2-D Circular Dam Break

Circular dam break tests are commonly used to validate shallow water Godunov-type solvers against radial symmetry. The solver is required to simulate accurately the subsequent motions after the sudden collapse of a circular column of water. The wave propagation is characterised by an outward propagating circular bores and a circular rarefaction wave that initially propagates inwards but later develops into a secondary bore. Many researchers (e.g. Alcrudo and Garcia-Navarro (1993), Anastasiou and Chan (1997), Fujihara and Borthwick
(2000), Rogers (2001) and Toro (2001)) have simulated wave propagation due to a circular dam break. The case considered here is proposed by Toro (2001) who has also provided the reference solutions for the problem. This is a very severe test in the way that the water depth at the centre of the initial column almost reaches zero at one stage of the simulation.

The circular column is initially enclosed by an infinitesimally thin cylindrical wall of radius \( R = 2.5 \) m, located at the centre of a square \( 40 \times 40 \) m\(^2\) basin. The initial water depths of the circular column and the surrounding are 2.5 m and 1.5 m respectively. Numerical results are based on computations on a uniform grid of \( 400 \times 400 \) cells, with a time step of \( \Delta t = 0.005 \) s. The domain boundaries are considered to be transmissive. The limiter \( \beta = 1.5 \) is used in order to achieve high resolutions at the flow discontinuities without creating excessive unphysical oscillations.

Numerical results are presented at times \( t = 0.4, 0.7, 1.4, 3.5 \) and \( 4.7 \) s respectively in Figure 4.8, showing the evolution of rarefaction and shock waves. Results are presented as 2-D contours, 3-D visualisations and depth and velocity profiles along the centreline. The contour and surface plots show the computed free surface elevation while the depth and velocity profiles give more information on the wave propagation, especially near the centre.

Figure 4.8 (a) shows the results at \( t = 0.4 \) s. A circular shock wave and a circular rarefaction wave have formed after the sudden collapse of the dam. In the radial direction, the circular shock front travels outwards from the initial interface while the rarefaction wave front travels inwards until almost reaching the centre.
Figure 4.8 (b) shows the results at $t = 0.1$ s. The rarefaction wave has focused at the centre and starts to propagate outward in the radial direction. The free surface elevation has fallen to about two-thirds of the initial value, leaving a concave indentation near the centre.

Figure 4.8 (c) shows the results at $t = 1.4$ s. The reflected inner rarefaction wave continues to propagate outward, expanding the flow near the centre while the free surface drops (in order to conserve mass). This overexpansion of the flow causes a secondary circular shock to form at the circumference of the free surface of the central column.

Figure 4.8 (d) shows the results at $t = 3.5$ s. The front of the primary shock has propagated towards the boundary of the domain, further away from the centre. The secondary circular shock has continued to travel towards the centre and the free surface elevation near the centre rises up again after dropping to almost bed level.

Figure 4.8 (e) shows the results at $t = 4.7$ s. The primary shock has travelled further towards the boundary of the domain. The secondary circular shock reflects immediately after focusing at the centre and propagates outward in the radial direction.

Figure 4.9 (a) shows the time history of the free surface elevation at location (20, 20) over the first 20 s. The graph indicates the propagation of the strong rarefaction wave towards the centre and the ‘implosion’ of the secondary shock at about $t = 4.25$ s. In accordance with Toro’s high resolution results, no further wave activity occurs at the centre after $t = 4.25$ s, with the free surface elevation remaining almost constant at $h = 0.5$ m. The small crest at $t = 14$ s arises because of the simple transmissive boundary conditions, which for shocks generate weak artificial reflections.
Figure 4.9 (b) shows the time history of the free surface elevation at location (24,20) over the first 20 s of the simulation. This location is outside the initial circular dam and thus acts as a passage of the primary and secondary shock after the ‘implosion’. The primary bore reaches this location at about $t = 1.5$ s and the secondary bore propagates through the same location at $t = 6.5$ s approximately.

The above results obtained are almost identical to those obtained by Toro (2001) who used a very fine mesh of 1000 cells in the radial direction in order to achieve high resolution reference solutions. The values of depth and velocity have been checked to agree at all discontinuities along the radial distance of the domain including the primary and secondary bores and the rarefaction waves. The present numerical solver has captured shocks to a high degree of accuracy including the ‘dip’ in the free surface elevation at $t = 0.7$ s, which is very difficult to resolve numerically according to Toro. Slight discrepancies between the present model predictions and Toro’s results are due to machine round off and truncation errors, boundary reflections and Cartesian grid effects. The uniform Cartesian grid used for this test may also give rise to numerical errors because the grid lines are not aligned with the flow. As a result, circular dam break tests with radially symmetric solutions are best solved in polar coordinates. In this context, it should be noted that Alcrudo and Garcia-Navarro (1993) made comparative calculations of a circular dam break test on rectangular and polar meshes. One calculation was computed on a rectangular mesh and the other on a circular mesh. They found that negative square-like features occurred on the rectangular grid, but were not present in the circular grid results. This indicates that there is some dependence on grid alignment to the predominant flow directions.
4.5 Diffusion Modelling

In practice, the density of a liquid-species mixture can vary both in the horizontal and in the vertical direction. The depth-averaged model assumes that the density is constant in any vertical, which is typical of a ‘well-mixed estuary’, where the river depth is small compared with the length. The transport of species is usually referred to as dispersion, which is a combination of convection and diffusion. Convection is dependent on the flow velocity field and is incorporated in the flux gradient term of the species transport equation (2.4).

Molecular diffusion can be described by Fick’s law in such a way that the flux is proportional to the concentration gradient. Molecular diffusion on its own is a very slow process. For example, a point source of dye in still water takes approximately 24 hours to gain a diameter of 1 m. In turbulent flow conditions such that the Reynolds number is higher that about 2000, the phenomenon of turbulent diffusion becomes apparent. For the present model, the molecular diffusion is incorporated in the source term of the species transport equation (2.4) and is evaluated using a central difference method.

4.5.1 Pure Diffusion of a Gaussian Concentration Distribution

This test considers diffusion process of species in still water. Suppose the species has an initial Gaussian distribution and is diffusing into still water. The concentration distribution of pure diffusion of a Gaussian concentration has an analytical solution (Crank, 1957) given by
where \( c \) is the volumetric species concentration, \( M_0 \) is the total amount of species, \( \varepsilon \) is the species diffusion coefficient given by \( \varepsilon = \sqrt{K_x^2 + K_y^2} \) and \((x_c, y_c)\) is the centre of the Gaussian concentration distribution in Cartesian coordinates.

In the test case performed herein \( M_0 \) is chosen such that the initial concentration \( c_0 = 1.0 \), i.e. \( \rho_0 = \rho_s \). The maximum of the initial Gaussian concentration distribution is located at the centre of a \( 1.5 \times 1.5 \) m\(^2\) square basin containing water of 1 m deep. The initial time is set to be \( t = t_0 = 2.5 \) s and the diffusion coefficient is \( \varepsilon = 0.001 \) m\(^2\)/s. The total amount of species is \( M_0 = 0.01\pi \). The boundary conditions imposed are reflective and frictional forces are ignored. For the numerical simulation, a uniform grid of \( 100 \times 100 \) cells is used, with a time step of \( \Delta t = 0.004 \) s. The choice of the slope limiter has no effect on the computation because there is no advection present.

Figures 4.10 (a)-(c) show the mesh (left column) and contour (right column) plots of the concentration distribution at time \( t = 2.5 \), 5 and 10 s. Figure 4.11 displays the numerical predictions of the concentration distribution across the diagonal of the domain at different times, plotted against the corresponding analytical solution. The normalised RMS differences are 0.24\%, 0.15\% and 0.07\% for results at \( t = 2.5 \), 5 and 10 s respectively, confirming close agreement between numerical predictions and analytical solutions given by Equation (4.14). The mixture and species mass satisfy conservation checks, which is consistent with the reflective boundary conditions used.

\[
c(x, y, t) = \frac{M_0}{4\pi \varepsilon t} \exp\left(\frac{-(x-x_c)^2-(y-y_c)^2}{4\varepsilon t}\right)
\]  

(4.14)
4.5.2 Advection Diffusion in a Rotating Flow Field

Another widely used standard diffusion test is the rotating cone problem (Abbott and Basco, 1989). The initial Gaussian concentration distribution is subject to a steady velocity field of a rotational flow corresponding to a solid body rotation. After an integral number of periods, the centre of the initial concentration distribution will return to its original position according to the analytical solution given by Equation (4.14).

The initial conditions are the same as those of the pure diffusion test in the previous section except that the peak concentration is now located at \((x_c, y_c) = (0.55, 0.55)\). The flow field has a constant angular velocity of \(10\pi/3\) rads/s with a period of 0.6 s around the centre of the basin located at \((0.75, 0.75)\). For the simulation, a uniform grid consisting of 100 \(\times\) 100 cells is used, with a time step of \(\Delta t = 0.0005\) s.

Figure 4.12 (a) and (b) show the mesh and contour plots of the concentration distribution at \(t = 2.8\) and 3.1 s, which correspond respectively to 0.5 and 1 revolution after the initial position. Figure 4.13 displays numerical predictions against analytical solutions of the concentration distribution, which are in good agreement (the normalised RMS differences are 2.6\% and 4.2\% for results at \(t = 2.8\) and 3.1 s respectively). Note that the effects of diffusion are not apparent due to the diffusion coefficient (0.001 m\(^2\)/s) and the change in time (from 2.8 to 3.1 s) both being small. Again checks for conservation laws are made to ensure that there is no gain or loss of material through the boundaries. Due to the advection, the results are very sensitive to the choice of limiters. The results presented here are based on the use of the Superbee limiter in order to reduce artificial diffusion and to deal with sharp concentration gradients.
4.6 Toro’s (2001) Wet-bed Tests

In wet-bed regions, the water depth is strictly positive and the depth-positivity condition $2(a_L + a_R) > u_R - u_L$ is satisfied everywhere in the domain (Toro, 2001). Toro (2001) proposed two tests based on this condition, for which high resolution numerical solutions are obtainable using Toro’s exact Riemann solver. These tests are used to investigate the ability of the present model to capture shocks and discontinuities in a channel where the bed is invariably wet. Table 4.1 summarises the initial data for the two test cases of steep-fronted flows in a channel of length 50 m, originally proposed by Toro (2001).

Table 4.1 Initial data for two wet-bed tests with analytical solutions

<table>
<thead>
<tr>
<th>Test</th>
<th>$h_L$ (m)</th>
<th>$u_L$ (m/s)</th>
<th>$c_L$</th>
<th>$h_R$ (m)</th>
<th>$u_R$ (m/s)</th>
<th>$c_R$</th>
<th>$x_0$ (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>W1</td>
<td>1.0</td>
<td>2.5</td>
<td>1.0</td>
<td>0.1</td>
<td>0.0</td>
<td>0.0</td>
<td>10.0</td>
</tr>
<tr>
<td>W2</td>
<td>1.0</td>
<td>5.0</td>
<td>1.0</td>
<td>1.0</td>
<td>-5.0</td>
<td>0.0</td>
<td>25.0</td>
</tr>
</tbody>
</table>

In the above table, $x_0$ denotes the position of the initial discontinuity; $h$, $u$ and $c$ are the total water depth, mean flow velocity and volumetric concentration; subscripts $L$ and $R$ are used to represent values of depth or velocity on the left and the right side of the discontinuity.

In order to assess the performance of the numerical solver, the tests are computed using both Roe and HLL approximate Riemann solvers. For the numerical computations, a uniform grid of 500 cells is used for both tests. Other computational parameters are stated in Table 4.2.

Table 4.2 Computational parameters for Test W1 and W2

<table>
<thead>
<tr>
<th>Test</th>
<th>Output time (s)</th>
<th>Time step (s)</th>
<th>Limiter</th>
</tr>
</thead>
<tbody>
<tr>
<td>W1</td>
<td>7.0</td>
<td>0.005</td>
<td>1.0</td>
</tr>
<tr>
<td>W2</td>
<td>2.5</td>
<td>0.002</td>
<td>1.5</td>
</tr>
</tbody>
</table>
Test W1 involves a right shock wave and a left critical rarefaction. An infinitesimally thin dam at position $x_0$ divides the channel into an upstream and a downstream section. At $t = 0$ s, the dam is suddenly removed. The left-hand plots in Figure 4.14 and Figure 4.15 contain predictions of the water depth and particle velocity profiles by the present model and Toro’s high resolution scheme at time $t = 0.7$ s. A bore travelling downstream and a rarefaction wave moving upstream can be observed from the depth and velocity distributions. The ability of the scheme to resolve shocks is reflected in the accuracy of speed of propagation, strength of the jump, width of the shock layer and the lack of spurious oscillations in the vicinity of the shock. Results based on the Roe and HLL approximate Riemann solvers agree very well with Toro’s result, although results from the Roe scheme are more resolved than those from the HLL scheme at sonic points. This is because the HLL solver can not capture the middle wave i.e. the contact discontinuity as accurately as the Roe scheme.

Test W2 involves two rarefaction waves and a contact discontinuity. This is a case in which the initial depth is constant throughout the channel, but the flow velocity is directed upstream along the left-hand half of the channel and downstream along the right-hand half of the channel. The right-hand plots in Figure 4.14 and Figure 4.15 give profiles of water depth, mean flow velocity and concentration distribution at $t = 2.5$ s. The initial discontinuity at the centre of the channel produces two strong rarefaction waves travelling in opposite direction at the same speed. If a negative water depth were computed in the vicinity of very shallow water, then the solution would blow up and the numerical scheme would be unsatisfactory. Hence this test assesses the accuracy and stability of the numerical scheme. The limiter used for this test is $\beta = 1.5$, which gives less diffusive results than the Minmod limiter without creating additional spurious numerical oscillations. The HLL scheme produces more spurious oscillations in the vicinity of the sonic points due to the misinterpretation of the
contact wave in the numerical solver. The unphysical oscillation in the HLL solver causes the numerical result in concentration to fall outside its domain $0 \leq c \leq 1$.

The numerical predictions by the present model agree very well with those of Toro except at the contact discontinuity. When using the HLL solver, the normalised RMS differences in the depth and velocity are 2.2% and 4.2% for Test W1 while Test W2 results have smaller normalised RMS differences with values of 0.30% and 0.89% respectively. The normalised RMS differences in the depth and velocity results from the Roe solver are 2.0% and 3.8% for Test W1 and 0.84% and 0.82% for Test W2.

It should be noted that most second-order schemes experience problems at the contact discontinuity and the sonic points. Although this is a highly demanding test, the numerical results produced are very satisfactory in comparison with the analytical solution, and hence demonstrate the ability of the solver to model very shallow water induced by strong rarefactions travelling in opposite directions.

### 4.7 Toro’s (2001) Dry-Bed Tests

The test cases considered in the previous sections are all wet-bed problems in which the water depth is strictly positive everywhere. For dry beds, the water depth becomes zero and it is not possible to evaluate the Roe-averages as the denominator becomes zero. Hence, the dry-bed problem is solved using a modified approximate HLL Riemann Solver. The modified HLL solver computes the wet/dry front speeds by imposing appropriate left and right wave speeds according to the water depth.
The three dry-bed tests considered here are proposed by Toro (2001) who obtained high-resolution solutions using exact Riemann solvers. For all test cases in this section, the domain is set to be 50 m. The initial left and right data states for the depth and velocity and the position of the initial discontinuity are displayed in the table below.

Table 4.2 Initial data for three test cases with analytical solutions

<table>
<thead>
<tr>
<th>Test</th>
<th>$h_L$ (m)</th>
<th>$u_L$ (m/s)</th>
<th>$h_R$ (m)</th>
<th>$u_R$ (m/s)</th>
<th>$x_0$ (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>D1</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>20.0</td>
</tr>
<tr>
<td>D2</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
<td>30.0</td>
</tr>
<tr>
<td>D3</td>
<td>0.1</td>
<td>-3.0</td>
<td>0.1</td>
<td>3.0</td>
<td>25.0</td>
</tr>
</tbody>
</table>

Test D1 consists of a right dry-bed state in the initial data, which develops to a single left rarefaction wave. The tail of this rarefaction wave corresponds to the dry/wet wave front whose speed is difficult to capture by many numerical methods (Toro, 2001). Test D2 is the mirror image of test D1 and in consequence the solution of test D2 comprises a single right rarefaction. Test D3 has initial data that do not satisfy the depth-positivity condition $2(a_L + a_R) > u_R - u_L$. Even with non-zero depth everywhere as the initial condition, a dry bed state is generated in-between the two outward rarefaction waves. As a result, there are two wet/dry wave fronts in the solution that are travelling in opposite directions. The two opposite wet/dry wave fronts are more difficult to capture compared with the single wet/dry front in Test D1 and D2. Numerical methods inevitably experience difficulties in resolving the flow especially at the discontinuities.

All three tests were performed using the modified HLL approximate Riemann solver on a uniform grid of 1000 cells with Minmod limiter. The output time, time step and tolerance for dry-bed conditions used in the solver are displayed in the table below.
Table 4.3 Computational parameters for test D1, D2 and D3

<table>
<thead>
<tr>
<th>Test</th>
<th>Output time (s)</th>
<th>Time step (s)</th>
<th>Tolerance (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>D1</td>
<td>4.0</td>
<td>0.001</td>
<td>$1.0 \times 10^{-9}$</td>
</tr>
<tr>
<td>D2</td>
<td>4.0</td>
<td>0.001</td>
<td>$1.0 \times 10^{-9}$</td>
</tr>
<tr>
<td>D3</td>
<td>5.0</td>
<td>0.005</td>
<td>$1.0 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

Figure 4.16 presents the numerical predictions using the HLL approximate Riemann solvers and Toro’s high-resolution solutions of the depth, velocity and concentration profiles for Test D1, D2 and D3 respectively.

The results show that the numerical predictions of the water depth in tests D1 and D2 are in very close agreement with the analytical solutions. The normalised RMS differences in the depth are found to be 0.23% for Test D1 and 0.19% for Test D2, which are both very small. In the velocity results, small discrepancies can be seen near the wet/dry wave front in both tests. This is due to the difficulty in capturing the jump in velocity at the wave front. As pointed out by Toro, even some high-resolution TVD methods produce spurious oscillations near the front. It should also be pointed out that the HLL solver has problems in resolving contact discontinuities, as it does not account for intermediate waves. The results obtained are therefore sufficiently accurate. In addition, the expected symmetries produced from the two tests further verify the accuracy of the numerical solver and the codes.

For the more demanding test D3 that has two opposite travelling wave fronts, the predicted depth and velocity profiles are also very close to Toro’s high-resolution solutions except at the wet/dry fronts (with a normalised RMS difference of 1.8% in the depth). Again this is due to the limitation of the numerical method in computing the wave propagation speed. It is also found that Test D3 is very sensitive to the tolerance parameter that determines whether the depth is treated as being zero (allowing for computer precision).
4.8 Concluding Remarks

The Godunov-type numerical model based on a new set of hyperbolic depth-averaged conservation equations has been validated for a range of benchmark tests. The model correctly balances flux gradient and source terms, and accurately resolves shock and rarefaction waves. It has been demonstrated that the model correctly simulates conventional shallow flows for liquids with constant density. The predicted results are in very close agreement with analytical and alternative numerical solutions for uniform flow in an open channel, steep-fronted flows including dam breaks, transcritical flow over humps and small-amplitude sloshing in a tank. In the latter case, the influence of non-linearity becomes evident as the wave steepness increases, with the model exhibiting a tendency for the waves to shock up into bores.
Figure 4.1 Uniform flow in an open channel: Depth-averaged velocity vector field
Figure 4.2 Seiching in a rectangular basin: Free surface profiles at 5 distinct times for different initial wave steepness
Figure 4.3 Seiching in a rectangular basin: Free surface profiles at 6 distinct times for initial wave amplitude ratio $A/h_s = 0.1$
Figure 4.4 Seiching in a rectangular basin: Time histories of the free surface elevation at the basin centre for different initial wave steepness
Figure 4.5 Seiching in a rectangular basin: Time histories of kinetic and potential energy for different initial wave steepness
Figure 4.6 Steady Transcritical flow over a 1-D hump: Results of the free surface elevation, Froude number and flow discharge at steady state
Figure 4.7 Wave propagation over a 2-D hump: Free surface at $t = 0.7$ s
Figure 4.8 (a) Toro dam break: Results at $t = 0.4$ s
Figure 4.8 (b) Toro dam break: Results at $t = 0.7$ s
Figure 4.8 (c) Toro dam break: Results at $t = 1.4$ s
Figure 4.8 (d) Toro dam break: Results at $t = 3.5$ s
Figure 4.8 (e) Toro dam break: Results at $t = 4.7$ s
Figure 4.9 Toro dam break: Time histories of the free surface elevation
Figure 4.10 2-D Pure diffusion: Mesh and contour plots at $t = 2.5$, 5 and 10 s
Figure 4.11 2-D Pure diffusion: Comparisons with analytical solutions
Figure 4.12 Advection-diffusion: Concentration contour at $t = 2.8$ and $3.1$ s

Figure 4.13 Advection-diffusion: Comparisons with analytical solutions
Figure 4.14 Wet-bed cases W1 ($t = 0.7$ s) and W2 ($t = 2.5$ s): Results obtained using Roe solver
Figure 4.15 Wet-bed cases W1 \((t = 0.7 \text{ s})\) and W2 \((t = 2.5 \text{ s})\):
Results obtained using HLL Solver
Figure 4.16 Dry-bed cases: Results obtained using HLL solver for Tests D1 (at $t = 4.0$ s), D2 (at $t = 4.0$ s) and D3 (at $t = 5.0$ s)
CHAPTER 5 TESTS FOR VARIABLE-DENSITY CASES

In the previous chapter, the variable-density shallow flow and species transport model has been validated for a series of benchmark tests, when the mixture density is uniform throughout the domain and constant in time. This chapter discusses the results of further validation tests designed to examine spatial and temporal variations in mixture density. Analytical solutions are derived for certain idealised cases.

5.1 1-D Analytical Solutions for Idealised Cases

For certain idealised cases where the mixture density distribution varies spatially, analytical solutions can be derived and used to validate the variable-density shallow flow and species transport model. Under appropriate initial and boundary conditions together with a smoothly varying topography, steady state solutions can be obtained analytically for a prescribed spatial distribution of either density or else the total depth of the mixture.

The 1-D variable-density shallow flow and species transport equations (without source term) are:

\[ \frac{\partial (\rho h)}{\partial t} + \frac{\partial (\rho uh)}{\partial x} = 0 \]  
\[ \frac{\partial (\rho u h)}{\partial t} + \frac{\partial (\rho u^2 h + \frac{1}{2} \rho gh^2)}{\partial x} = -\rho gh S_{ex} - \tau_{bx} \]  
\[ \frac{\partial (\rho c h)}{\partial t} + \frac{\partial (\rho u c h)}{\partial x} = 0 \]
where \( h \) is the local total depth of the mixture from the bed to the free surface, \( u \) is the depth-averaged velocity, \( \rho \) is the depth-averaged density and \( c \) is the depth-averaged concentration of the liquid-species mixture, \( S_{ox} \) is the bed slope, \( \tau_{bx} \) is the bed frictional stress, \( \rho_s \) is the density of the species for which \( c = 1 \), and \( g \) is the acceleration due to gravity.

The steady state no-flow solutions are such that \( \frac{\partial (\rho h)}{\partial t} = \frac{\partial (\rho u h)}{\partial t} = \frac{\partial (\rho_s c h)}{\partial t} = u = 0 \). Under this condition, both sides of Equations (5.1) and (5.3) reduce to zero, and Equation (5.2) becomes

\[
\frac{\partial (\rho h^2)}{\partial x} = -2 \rho h S_{ox} \quad (5.4)
\]

As steady state solutions are independent of time, distributions of the mixture density and mixture depth can be expressed as functions of spatial distance alone i.e. \( \rho = \rho(x) \) and \( h = h(x) \). Thus the above partial differential equation is essentially an ordinary differential equation. If the bed is flat \( (S_{ox} = 0) \) then Equation (5.4) simplifies to

\[
\rho h^2 = \text{constant} \quad (5.5)
\]

If the bed is not flat \( (S_{ox} \neq 0) \) then simple differentiation of Equation (5.4) leads to

\[
\frac{h}{\rho} \frac{\partial \rho}{\partial x} + 2 \frac{\partial h}{\partial x} = -2 S_{ox} \quad (5.6)
\]
5.2 1-D Test Cases with Analytical Solutions

Cases HB (horizontal bed) and SB (sinusoidal bed) have continuous analytical steady state solutions involving horizontal bed and sinusoidal bed profile respectively. The analytical steady-state solutions are computed and inputted as initial conditions. Time histories of the variables at the first, middle and last cell in the domain are computed and displayed in non-dimensional form. This verifies whether the quiescent constant-density equilibrium is both calculated and subtracted correctly and whether the steady-state equilibrium solutions remain in equilibrium. The sinusoidal bed case also tests the correct balance of the bed gradient term but is expected to incur additional numerical error due to grid effects.

5.2.1 Case HB: Horizontal Bed Topography

This case comprises a rectangular channel of length $L$, with a flat horizontal bed. The channel contains a liquid-species mixture with initial depth and density distributions prescribed such that Equation (5.5) is satisfied. The initial depth profile of the mixture is the same as that of the sloshing test in the previous chapter, which has a quiescent constant density equilibrium that equals the still water depth. Another equilibrium is the steady-state equilibrium that satisfies the condition $\rho h^2 = \rho_w h_s^2$, where $\rho_w$ is the density of the liquid without the absence of species and $h_s$ is the still liquid depth (see definitions in Chapter 2).

The initial free surface profile of the mixture is designed to take a similar form as Equation (4.8) which has a symmetric sinusoidal profile with zero gradients at the boundaries in order to avoid unphysical oscillations at the boundaries. The initial design depth and the corresponding steady-state density distribution in terms of the distance $x$ along the channel as
In the case considered herein, the parameters are $L = 100$ m, $h_0 = 1$ m, $A = 0.1$ m and $\rho_0 = 1000$ kg/m$^3$. The gravitational acceleration is $g = 9.81$ m/s$^2$.

In examining the difference between the numerical and analytical solutions, the variations in depth, velocity and density are presented in non-dimensional form. Here the non-dimensionalised variables are defined as follows:

$$h^*(x) = h_0 + A \cos\left(\frac{2\pi x}{L}\right), \quad \rho^*(x) = \rho_0 h_0^2 \left[ h_0 + A \cos\left(\frac{2\pi x}{L}\right) \right]^{-2} \quad (5.7)$$

The non-dimensional groups $h^*$ and $\rho^*$ represent errors in depth and density (i.e. deviations from the analytical steady-state equilibrium values), and $M^*$ is the ratio between the flow velocity and the celerity of a first-order solitary wave in the liquid mixture at equilibrium depth.

The numerical domain is discretised spatially using a uniform grid of 1001 cells with $\Delta x = 0.099$ m. Grid convergence has been checked so that the numerical solutions are grid independent. The time step is $\Delta t = 0.01$ s and the total simulation time is $t = 100$ s. The end boundary conditions are reflective. Frictional effects are ignored. The limiter used is Minmod. The numerical solver commences the simulation using the analytical steady-state equilibrium solution as initial values. By integrating the depths along the channel and dividing by the length of the channel at the beginning of the simulation, a static equilibrium value for $h$, $100$
namely $h_s$, is computed using Equation (2.20). The quiescent equilibrium value for $\rho$ is defined to be $\rho_w$ for which $c = 0$. At each iteration thereafter, the equilibrium-corrected flux gradient and source terms are evaluated by subtracting the static equilibrium flux gradient and source terms which are written in terms of $h_s$ and $\rho_w$.

The solid line plots in Figure 5.1 show the initial free surface profile above the horizontal bed and the initial density distribution. These initial conditions are also the steady state equilibrium solutions of the system. The constant density equilibrium states $h = h_s$ and $\rho = \rho_w$ are also plotted as dashed lines.

Figure 5.2 displays the time histories of the depth error, non-dimensional velocity and density error at the first, middle and last cell in the domain, namely at positions $x = \Delta x / 2$, $L / 2$ and $L - \Delta x / 2$ m respectively. The variations in depth, velocity and density at the first and the last cells of the domain are identical, and confirm the expected symmetry of the results. The error in depth appears to repeat itself at approximately 15-second intervals. The non-dimensional velocity error appears to be slowly converging towards zero. The density error is very slightly divergent with an average increase in density of less than $10^{-13}$/s. The discrepancies between the numerical predictions and the analytical solutions are mainly due to discretisation errors in the numerical scheme. Less significant sources include computer round-off errors. The numerical predictions remain very close to the analytical equilibrium solutions, indicating that the scheme is stable and not affected by any initial transient (due to the difference between the discretised and analytical solutions). By $t = 100$ s, the initial transient wave has travelled approximately three times across the channel and hence any small perturbation away from equilibrium would have grown significantly during this time interval. Conservation of the volume, the mixtures mass and the species mass has been checked for $t \leq 100$ s.
5.2.2 Case SB: Sinusoidal Bed Topography

The domain of this case consists of a channel of length $L$, with smoothly varying sinusoidal bed topography. Initial depth and density distributions are imposed such that Equation (5.6) is satisfied and the system is initially at steady-state equilibrium (with zero flow everywhere). The flow system should of course remain stationary throughout the simulation because of the initial equilibrium condition. The design bed topography is defined in terms of horizontal distance $x$ across the channel as

$$z_b(x) = A \left[ 1 - \cos \left( \frac{2\pi x}{L} \right) \right]$$

(5.9)

For this particular bed topography, one set of steady-state equilibrium solutions for the mixture depth and density is

$$h^{eq}(x) = h_0, \quad \rho^{eq}(x) = \rho_0 \exp \left[ \frac{2A}{h_0} \cos \left( \frac{2\pi x}{L} \right) \right]$$

(5.10)

Here the parameters are chosen as $L = 100$ m, $A = 0.1$ m, $h_0 = 1$ m and $\rho_0 = 1000$ kg/m$^3$.

The initial conditions are taken as the equilibrium solutions in (5.10). The depth, velocity and density errors are non-dimensionalised as in Equation (5.8), and give a qualitative measure of the magnitude of the variation of numerical results from the analytical solutions. The numerical domain is uniformly discretised in space using 1001 cells. In time, the variables are updated after every time step of $\Delta t = 0.01$ s. The other parameters and assumptions are the
same as those in the previous case. Like the previous case, the static equilibrium value of $h$ is calculated by integrating the initial depth and bed profiles along the channel and dividing by the length of channel using Equation (2.20).

Figure 5.3 shows the initial free surface (solid line) with the bed profile (dotted line) and the density distribution (solid line), which are also the steady state equilibrium solutions. The constant density equilibrium $h = h_s$ and $\rho = \rho_w$ are plotted for comparison purposes.

Figure 5.4 displays the time histories of the depth error, non-dimensional velocity and density error computed at the first, middle and last cell along the channel; namely at positions $x = \Delta x/2$, $L/2$ and $L - \Delta x/2$. The plots show that the errors in the depth and the non-dimensional velocity are convergent with time, while the error in the density diverges. The magnitudes of the discrepancies between numerical predictions and analytical solutions for this sinusoidal bed case are greater than the magnitudes for the horizontal-bed case. This is due to extra discretisation errors resulting from the effect of the sloping bed. Further errors are due to the order of accuracy of the numerical scheme, truncation errors, and computer round-off errors.

### 5.3 1-D Density Dam Break Tests with One Initial Discontinuity

The two cases considered in this section, namely cases A and B, are parameter tests designed to investigate the perturbation effect to the system caused by having two adjacent liquids of different densities but equal volumes. The results are studied by comparison with the gravity-driven wave motions of a step-like dam break and also with gas dynamics in a shock tube.
The physical domain consists of a horizontal channel of length $L$. An infinitesimally thin wall separates the channel into two equal sections. The liquid to the left of the wall has density $\rho_L$, whereas the liquid to the right has density $\rho_R$. The two liquid regions are at rest initially and both have uniform depth of $h_0$. After the sudden collapse of the wall at time $t = 0$ s, waves are generated due to the hydrostatic pressure difference either side of the liquid interface at the channel centre.

In Case A, densities of the two liquids are $\rho_L = 10$ kg/m$^3$ and $\rho_R = 1$ kg/m$^3$. In Case B, densities of the two liquids are $\rho_L = 1$ kg/m$^3$ and $\rho_R = 10$ kg/m$^3$. In both cases: $L = 100$ m, $h_0 = 1$ m, $g = 1$ m/s$^2$, frictional effects are neglected, the limiter is Minmod, the grid is uniform with 5000 cells, and the time step is $\Delta t = 0.02$ s. The output time is $t = 100$ s.

Figure 5.5 illustrates the stacked $x$-$t$ plots showing time evolution of the depth, velocity and concentration for Case A. Initially the hydrostatic pressure difference at the interface of the two liquids drives a flow of higher density liquid towards the right, pushing the lower density liquid ahead. To conserve mass, the free surface of the lower density liquid rises and a rightward propagating shock-like bore forms (Figure 5.5 a). This is evident also as a step change in velocity (Figure 5.5 b). The bore occurs entirely in the less dense liquid, and so there is no trace of it in the concentration plot (Figure 5.5 c). As can be seen in the free surface elevation $x$-$t$ plot, there is a moving contact surface behind the bore, where the liquid depth drops suddenly as the contact wave passes. This contact surface marks the boundary between the two liquids that were either side of the interface initially, and is where the concentration jumps discontinuously. As diffusion is neglected, the two liquids are permanently separated by the contact surface. The contact shear wave propagates to the right in the depth and concentration $x$-$t$ plots, but is not visible on the depth-averaged velocity either side of the shear.
wave. A leftward propagating expansion-type wave is evident in Figure 5.5 a, and travels leftward, located entirely in the denser liquid. The expansion-type wave fans out with time, smoothing out the change of depth between the region of the denser liquid that has reduced depth near the interface, and the as yet undisturbed region of denser liquid. The expansion-type wave does not appear in the concentration plot of Figure 5.5 (c). From Figure 5.5 (a) it can be discerned that the bore travels to the right at 1.43 m/s, the contact wave to the right at 0.578 m/s and the expansion wave to the left at 1 m/s. The bore speed is in approximate agreement with the wave celerity \( u_b = \sqrt{gh_n} = \sqrt{1.63} = 1.28 \) m/s obtained using the predicted mixture depth. Data of the velocities indicate that the flow velocities before and after the bore passes are zero and 0.567 m/s, respectively.

The mechanisms of the density dam break are similar to that of a dam break induced by change in free surface depth. The resulting effects are analogous in that a leftward rarefaction, a rightward shock and a contact wave are formed. Toro (2001) gives details of the different types of waves, and the related solutions of the Riemann problem. Similar wave structures occur in shock tube gas dynamics (see e.g. Liepmann and Roshko 1957).

Figure 5.6 shows the time evolution of the depth, velocity and concentration for Case B. As would be expected, the results of this case and the previous case are exactly symmetric about the initial interface at \( x = L/2 \).

### 5.4 1-D Density Dam Break Tests with Two Initial Discontinuities

Cases DB1 to DB4 in this section are undertaken as a parameter study in order to investigate the effect of different density ratios either side of a pair of liquid interfaces in a channel with a
horizontal bed. The channel has length $L$, and initially contains liquid of depth $h$. As illustrated in Figure 5.7, the liquid is divided into three regions. At the left-hand side and right-hand side of the channel, the liquid is of density $\rho_1$. At the centre of the channel there is a liquid column of density $\rho_2$ and width $w$. In these parameter tests: $h = 1$ m; $w = 1$ m; $\rho_1 = 1$ kg/m$^3$; $\rho_2 = 0.1, 1, 10, 100$ and 1000 kg/m$^3$; and $g = 1$ m/s$^2$. Frictional effects are ignored.

A simple physical interpretation of the liquid behaviour is as follows. The central liquid column falls or rises to an equilibrium level depending on whether the density ratio $\rho_2/\rho_1$ is respectively greater than or less than unity. At equilibrium there is a balance between the hydrostatic pressure produced by the different liquids either side of the density interface. After being released, the system tries to restore the region of density $\rho_2$ to an equilibrium depth $h_2$ with an equilibrium width $w_2$. Once equilibrium is established, the region of density $\rho_1$ has a new equilibrium depth $h_1$.

The initial and equilibrium states of the system are sketched in Figure 5.7. The hydrostatic balance implies

$$\rho_1 g h_1^2 = \rho_2 g h_2^2$$

Thus, by rearrangement,

$$h_2 = h_1 \sqrt{\frac{\rho_1}{\rho_2}}$$
Provided that the domain length $L$ is sufficiently large, $h_1 = h$. Hence an approximation for $h_2$ can be obtained from Equation (5.12).

The equilibrium width $w_2$, of the central liquid column of density $\rho_2$ can then be estimated from volume (area in 1-D) conservation to be

$$w_2 = w \frac{h}{h_2}$$

(5.13)

The equilibrium depth $h_2$ and the equilibrium width $w_2$ are independent of the domain length $L$. For each of the cases listed below, the computational domain is uniformly discretised in space with $\Delta x = 0.05$ m and the time step is $\Delta t = 0.01$ s so that the CFL condition (see Equation (3.9)) and grid convergence criterion are satisfied. The length $L$ is chosen sufficiently large compared to $w_2$ so that volume conservation approximately holds. The domain also needs to be large enough for the equilibrium width to be achieved before reflected waves disturb the solution. The limiter is Minmod.

5.4.1 Case DB1: $\rho_2 = 1$ kg/m³

In this special case the liquid density is the same throughout the channel. Figure 5.8 displays stacked time plots showing evolution of the depth, velocity and concentration profiles along the channel for time $t \leq 50$ s. All the physical variables remain constant in time. The liquid remains entirely stationary with regard to density throughout the simulation. This is to be expected because there is no driving force to perturb the system from its equilibrium state.
5.4.2 Case DB2: $\rho_2 = 10$ kg/m$^3$

In this case, the liquid in the central region is a factor of ten denser than the liquid either side of the interfaces. The density differences cause liquid motions to occur. The equilibrium depth and width of the central region are estimated from Equations (5.12) and (5.13) to be

$$h_2 = \frac{1}{\sqrt{10}} \approx 0.316 \text{ m} \text{ and } w_2 = \sqrt{10} \approx 3.162 \text{ m}.$$  

Figure 5.9 displays depth and velocity profiles at times $t = 1, 4, 12, 18, 30,$ and $50$ s, respectively. The plots are interpreted as follows.

(a) The initial drop of the central column of higher density liquid under gravity drives left and right shock-type bores into the adjacent lower density liquid regions. The bores commence at the two density interfaces, and are accompanied by rarefaction waves travelling in opposite directions to the bores. By time $t = 1$ s, the initial inward propagating rarefaction waves have already reflected at the centre of the channel where the liquid free surface is at its lowest level. The reflected rarefaction also causes the rapid fall in the free surface of the central column to about half of the initial depth.

(b) The leading shock-type bores continue to travel outwards with almost vertical front faces. The fronts of the bores travel fastest, with liquid behind travelling more and more slowly as the free surface level reduces. Meanwhile the central column of denser liquid continues to fall and spread out under gravity. By $t = 4$ s, a zone of still liquid begins to grow as the denser liquid spreads out. At this stage, the denser liquid has spread out too far, in a similar manner to an over-expanded compressible flow.
(c) At $t = 12$ s, the denser liquid at the centre of the domain has started to readjust for the over-spreading. The depth profile at the centre has risen by a small amount since $t = 4$ s and has become more rectangular in shape and contracts slightly.

(d) By $t = 18$ s, the central rectangular depth profile has almost become established. The adjustment for over-spreading has ceased, releasing a further pair of small bores into a depression region behind the main bores.

(e) At $t = 30$ s, the height of the shock-type bore front has reduced, as the liquid making up the bore has to cover an increasing distance along the channel. The decrease in height is accompanied with a reduction in bore speed. This second pair of bores follows behind, propagating in the outwards directions.

(f) At $t = 50$ s, both pairs of shock-type bores continue to travel outwards from the centre, losing height and speed as liquid is distributed along the channel. The primary bores have almost reached the outer boundary walls of the domain. There is a growing region in the middle of the channel, which is no longer moving and includes the higher density column at the centre. The depth and the width of the central column have now reached steady state. The numerically computed equilibrium depth and width of the liquid at the centre are 0.315 m and 3.1 m respectively.

Figure 5.10 shows time history of the free surface position at the centre of the channel plotted at one-second intervals. The free surface undergoes decaying oscillations until the equilibrium depth, $h_2 = 0.316$ m, is reached after approximately 50 seconds.
Figure 5.11 gives the stacked $x$-$t$ plots showing evolution of the depth, velocity and concentration profiles along the channel from $t=0$ s to $t=50$ s plotted at 1-second intervals. The plots show the wave-like processes as they occur in space and time. The sudden collapse of the denser liquid in the central column causes primary shock waves to be created and propagate as bores in the direction from high to low density. The two outward propagating bores are clearly visible in Figure 5.11 (a) and (b), travelling in opposite directions. Each primary bore decreases in strength with time, which can be seen from the curved shock path. At the same time as the primary bores are created, a pair of rarefaction waves travels inward from the interfaces. The rarefaction waves are almost immediately reflected at the centre, and then move outward weakening rapidly. Two contact waves are also clearly evident at the interfaces between the higher and lower density liquids. These show that over-expansion occurs during the first two seconds. The width of the denser region then contracts, until a minimum width occurs at about $t=10$ s at which time two secondary bores (travelling in opposite direction, away from the centre) are released. After this the contact waves at the interface between the regions of different density become stationary (Figure 5.11 (a) and (c)), and the primary and secondary bores continue to travel outward. The primary bore travels in a curved path on the $x$-$t$ plane as it loses height and speed.

5.4.3 Case DB3: $\rho_2 = 100$ kg/m$^3$

In this case, the liquid in the central region is a factor of a hundred times denser than the liquid either side. Density differences at the interfaces between the regions cause liquid motions to occur, as discussed in detail below. The analytical equilibrium depth and width of the central region calculated using Equations (5.12) and (5.13) are $h_2 = 0.1$ m and $w_2 = 10$ m.
respectively. The time taken for the system to reach equilibrium is much greater than that of the previous case because of the bigger density difference of the two fluids.

Figure 5.12 displays the depth and velocity profiles at times $t = 6, 18, 84, 108, 144$, and $180$ s, respectively. The plots are interpreted as follows.

(a) At first, the hydrostatic pressure differences at the interfaces between the two liquids drive two shock-type bores outwards into the adjacent lower density liquid regions. Rarefaction waves travelling inwards are reflected at the centre, causing the central column to fall rapidly. By time $t = 6$ s, the free surface of the central region has dropped to less than one tenth of the original depth, and the shock-like bore fronts have become fully established.

(b) The leading shock-type bores continue to travel away from the centre, while the free surface of the central region falls almost to bed level at $t = 18$ s. Meanwhile, the width of the central column increases as the depth decreases in order to conserve mass. The fronts of the bores travel fastest, with liquid behind travelling more and more slowly as the free surface level reduces. At this stage, the denser liquid has spread far outwards as a result of the over-expanded flow.

(c) At $t = 84$ s, the denser liquid at the centre of the domain has started to readjust for the over-spreading. The depth profile at the centre has risen by a small amount and the width of the denser liquid has reduced.

(d) By $t = 108$ s, a zone of still liquid begins to grow near the centre. The denser liquid region has become more rectangular in shape and contracted slightly. The adjustment for over-
spreading releases a further pair of small bores into a depression region behind the main bores.

(e) At $t = 144$ s, both the primary and secondary shock wave fronts are continuing to propagate outwards. The depth and width of the denser liquid region are also adjusting in order to approach equilibrium.

(f) At $t = 180$ s, the central denser liquid has a nearly rectangular (and unchanging) depth profile, corresponding to the equilibrium condition. The primary and secondary bores continue to travel outwards from the centre, losing height and speed as liquid is redistributed along the channel. The primary bores have almost reached the outer boundary walls of the domain.

Figure 5.13 shows a time history of the free surface position at the centre of the channel plotted at 6-second intervals. The convergence rate is much slower than that of the previous case and the numerically predicted depth oscillates about the analytical equilibrium position several times. In the first 6 seconds, the free surface drops to about 5 percent of the initial value. The depth continues to fall until $t \approx 84$ s when it reaches its lowest value of 0.01 m, after which the system starts to readjust for the over-spreading of the central denser liquid region. The width and depth of the denser liquid region undergoes damped oscillations as it tends to its equilibrium state. A steady converged depth of $h = 0.1$ m is reached at about $t = 300$ s.

Figure 5.14 gives the stacked $x$-$t$ plots showing evolution of the depth, velocity and concentration profiles along the channel from $t = 0$ s to $t = 300$ s plotted at 6-second intervals. Three pairs of outward propagating shock-type bores can be observed in the depth and velocity plots. As noted before, the primary pair of bores is caused by liquid density
The secondary and tertiary pairs of shock waves are released from the edges of the denser liquid region each time it starts to readjust for over-expansion of its width.

5.4.4 Case DB4: $\rho_2 = 0.1 \text{ kg/m}^3$

In this case, the liquid in the central region is a factor of a ten times less dense than the liquid in the regions either side. As a result, the denser liquid moved inwards towards the centre of the domain, squeezing the less dense region upwards. The analytical equilibrium depth and width of the central region calculated using Equations (5.12) and (5.13) are \( h_2 = \sqrt{10} = 3.16 \text{ m} \) and \( w_2 = 1/\sqrt{10} = 0.316 \text{ m} \) respectively.

Figure 5.15 displays the depth and velocity profiles at times \( t = 1, 2, 4, 8, 30, \) and \( 50 \text{ s} \), respectively. The initial density difference at the liquid interface produces a pair of rarefaction waves propagating outwards and a pair of shock-like bores propagating inwards. The bores collide at the centre, creating a clapotis-type sudden rise in the free surface elevation. By \( t = 1 \text{ s} \), the free surface has already risen close to its highest elevation, corresponding to the analytical equilibrium solution, as can be seen in Figure 5.15 (a). The central column of less dense liquid remains almost unchanged in profile after this for the remainder of the simulation. The rarefaction waves progressively move outwards with time, but with decreasing velocity. Elsewhere the liquid is almost stationary.

Figure 5.16 shows time history of the free surface position at the centre of the channel plotted at 1-second intervals. The free surface asymptotically converges towards the steady state analytical solution of 3.16 m. In this case, convergence is fairly rapid, and non-oscillatory. Steady state appears to be reached by \( t = 10 \text{ s} \).
Figure 5.17 presents stacked $x$-$t$ plots showing evolution of the depth, velocity and concentration profiles along the channel from $t = 0$ s to $t = 50$ s plotted at 1-second intervals. Outward propagating rarefaction waves are initially released from the density interfaces, propagating outwards. Meanwhile, two shock-type bores travel inwards and are reflected at the centre causing the lower density liquid region to contract and almost immediately establish its equilibrium shape (i.e. at about $t = 1$ s). The contact surfaces between the low- and high-density liquid regions remain more or less steady thereafter. With time, the rarefaction waves continue to travel outwards decreasing in strength and speed.

### 5.5 Circular Dam Breaks Driven by Both Depth and Density Differences

The aim of these tests is to interpret physically the numerical predictions of a dam break induced by both depth and density differences. An additional parameter that influences this type of dam break, but not a conventional constant density dam break, is the ratio of the density inside the circular column to that outside. By analogy to the 1-D parameter tests in earlier sections, three different outcomes are expected depending on the hydrostatic pressure ratio either side of the interface i.e. $(\rho_h^2)_\text{in} : (\rho_h^2)_\text{out}$, which can be greater, less than, or equal to unity.

The dam is initially enclosed by an infinitely thin circular wall of radius $R = 2.5$ m located at the centre of a flat-bottomed square basin of $40 \times 40$ m$^2$. The liquid inside the circular wall has initial depth $h_\text{in} = 2$ m and density $\rho_\text{in}$ whose values are listed in the table below. Outside the circular wall, liquid of density $\rho_\text{out} = 1000$ kg/m$^3$ is initially at rest at a constant depth of
\( h_{\text{out}} = 1 \text{ m} \), so that \((\rho h^2)_{\text{out}} = 1000 \text{ kg/m}\). All the initial velocities are set to zero throughout the domain. Table 5.1 lists the values of \( \rho_m \) for each test considered and the other dependent quantities that determine the outcome of the dam break.

<table>
<thead>
<tr>
<th>Test</th>
<th>( \rho_m ) (kg/m(^3))</th>
<th>((\rho h^2)_{\text{in}}) (kg/m)</th>
<th>((\rho h^2)<em>{\text{in}} : (\rho h^2)</em>{\text{out}})</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD1</td>
<td>1000</td>
<td>4000</td>
<td>4:1</td>
</tr>
<tr>
<td>CD2</td>
<td>250</td>
<td>1000</td>
<td>1:1</td>
</tr>
<tr>
<td>CD3</td>
<td>200</td>
<td>800</td>
<td>4:5</td>
</tr>
<tr>
<td>CD4</td>
<td>100</td>
<td>400</td>
<td>2:5</td>
</tr>
</tbody>
</table>

The subsequent motion of the system acts to restore the system's equilibrium state by adjusting the depth and radius of the circular liquid column. This response is similar to that of the 1-D problems discussed in the previous section. The hydrostatic pressure thrust balance implies that the equilibrium depth of the circular liquid column must satisfy

\[
\text{heq} = \sqrt{\frac{(\rho h^2)_{\text{out}}}{\rho_m}} \quad (5.14)
\]

By considering the mass conservation of the circular liquid column at initial time and at equilibrium, the equilibrium radius of the circular liquid column satisfies

\[
R_{\text{eq}} = \sqrt{\frac{R^2 h_{\text{in}}}{\text{heq}}} \quad (5.15)
\]

For cases CD1-CD4, the equilibrium depth and the equilibrium radius of the central circular column are calculated from Equations (5.14)-(5.15) and are listed below in Table 5.2.
Table 5.2 Equilibrium depth and radius of the liquid circular liquid column of density $\rho_m$

<table>
<thead>
<tr>
<th>Case</th>
<th>Equilibrium depth (m)</th>
<th>Equilibrium radius (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CD1</td>
<td>1</td>
<td>3.536 (3 d.p.)</td>
</tr>
<tr>
<td>CD2</td>
<td>2</td>
<td>2.5</td>
</tr>
<tr>
<td>CD3</td>
<td>$\sqrt{5} = 2.236$ (3 d.p.)</td>
<td>2.364 (3 d.p.)</td>
</tr>
<tr>
<td>CD4</td>
<td>$\sqrt{10} = 3.162$ (3 d.p.)</td>
<td>1.988 (3 d.p.)</td>
</tr>
</tbody>
</table>

The numerical domain is discretised spatially on a uniform grid of $401 \times 401$ cells that is sufficiently fine for grid convergence to be achieved. Temporally, the variables are updated with a time step of $\Delta t = 0.0025$ s in the numerical calculations. The gravitational acceleration is $g = 9.8$ m/s$^2$. The limiter is Minmod. Frictional effects and diffusion are neglected. Boundaries are considered to be transmissive unless otherwise stated.

5.5.1 Case CD1

In this case, the initial hydrostatic pressure thrust inside the initial circular column is higher than that outside, with a ratio of 4:1 (which is entirely due to the depth difference, like a conventional dam break). The main features of this type of dam break are similar to those of a conventional dam break such as ones simulated by Toro (2001) and Alcrudo and Garcia-Navarro (1993). Results presented herein are obtained so as to be comparable to those displayed by Toro (2001). Similarities and differences can be observed by comparisons with Figures 13.2 to 13.17 displayed by Toro (2001).

Figures 5.18 and 5.19 present 3-D free surface visualisations and profiles of depth and velocity along the basin centreline, at times $t = 0.35, 0.65, 1, 1.25$ and $1.7$ s respectively. Once the system is released, the hydrostatic pressure thrust difference at the circular interface drives a
circular shock bore radially outward. Accompanied by the outward shock bore is a circular
rarefaction wave, which propagates radially inward. By $t = 0.35$ s, an outward propagating
circular bore and an inward rarefaction wave have formed; the rarefaction wave is about to
focus at the centre. At $t = 0.65$ s, the circular rarefaction has focused causing the liquid depth
to drop rapidly near the centre. By $t = 1$ s, the primary bore continues to propagate outwards
and a secondary bore emerges from the inner circular contact boundary due to the over-
expansion of the flow near the centre. This circular secondary bore propagates radially
inwards forcing the depth to drop (in order to conserve mass) which is evident at $t = 1.25$ s.
As soon as the secondary bore comes to a halt, it begins to propagate in the outward direction
that causes the free surface near the centre to rise. At $t = 1.7$ s, the secondary shock front has
started to propagate outward again after focusing at the centre and the free surface at the centre
has risen to almost equilibrium depth which is 1 m.

Figure 5.20 presents the stacked $x$-$t$ plots showing evolution of the depth, depth-averaged
speed and concentration profiles along the centreline of the domain at $y = y_L/2$ from $t = 0$ s
to $t = 5$ s plotted at 0.05 second intervals. From the plots of the depth and depth-averaged
speed, it can be observed that the primary bore is initially released from the liquid interface,
propagating outwards. Meanwhile, the rarefaction wave travels inward and implodes (i.e.
reflects with itself) at the centre causing the inner liquid region to drop in depth in the early
stages of the simulation. The reflected rarefaction wave then propagates outwards until it
reaches the liquid interface where it is partly reflected by the boundary and partly transmitted
through the interface. The over-expansion of the flow causes the release of the secondary bore
just after the depth has dropped to its first minimum and before rising up again to compensate
the overshoot. The secondary bore reflects at the centre and travels outwards.
Figure 5.21 contains 3-D $r$-$t$-$h$ representations of the wave diagram. The plots show views from above and beneath of the evolving wave pattern. The primary bore can be observed propagating outward with decreasing strength (seen as the curved path in the previous $x$-$t$ diagram). The rarefaction wave initially travels inward and is reflected at the centre. Immediately after the reflection of the rarefaction wave, the free surface drops rapidly. When the free surface rises up again after the first over-shoot, the secondary bore emerges from the centre and propagates outward with less strength compared to the primary bore but at a steadier rate. The bottom view shows clearly the free surface dropping, reaching a minimum and then rising up again with a very sharp gradient.

Figure 5.22 shows the time history of the free surface at the centre of the domain. The convergence rate is relatively quick and there is no over-adjustment from the equilibrium depth after the first rapid fall of the central region compared to the Toro (2001) case. This is because the hydrostatic pressure thrust difference at the interface in the present case is not as big as in Toro’s case (ratio of 4:1 and 25:1 respectively) so the system reaches equilibrium without such a large overshoot.

5.5.2 Case CD2

This is a special case in which the initial hydrostatic pressure thrust inside the circular column is the same as that outside the column. There is no input driving force and therefore the system is expected to remain in equilibrium. This case is particularly sensitive to grid resolution and a grid convergence study indicates that a uniform grid of $421 \times 421$ with a time step of $\Delta t = 0.002$ s is required in order to achieve sufficient accuracy. Because of the Cartesian grid
effects introduced when simulating a circular dam break on a uniform rectangular grid, the numerical scheme is bound to experience difficulties. As a result, the predicted equilibrium contact surface is not perfectly circular but has a slightly circular shape with fringed edges.

Figures 5.23 and 5.24 present 3-D free surface visualisations and profiles of depth and velocity along the centreline of the domain, at times $t = 0.55$ s and $t = 0.7$ s respectively. The interface remains almost unchanged but with fringed edges and step-like features due to the Cartesian grid effects. After the system is released, a very weak circular rarefaction wave emerges from the density interface, propagating radially outwards. Meanwhile, an inward propagating bore reaches at the centre at $t = 0.55$ s causing a small dip in the free surface near the centre. The reflected bore then travels radially outward, forcing the free surface at the centre to rise slightly, which is evident at $t = 0.7$ s. It should be noted that the vertical velocity scales in Figure 5.24 are ten times smaller than those in Figure 5.18.

Figure 5.25 depicts the stacked $x$-$t$ plots showing evolution of the depth, depth-averaged speed and concentration distribution along the centreline of the domain from $t = 0$ s to $t = 5$ s plotted at 0.05 second intervals. This particular cross section shows the Cartesian grid effects on the circular interface. The very slight perturbation from the analytical equilibrium due to the grid effects grows with time but at a very slow rate. The discrepancies can be regarded as a numerical error.

Figure 5.26 shows the 3-D $r$-$t$-$h$ representations of the wave diagram. Along the diagonal of section, the contact surface remains relatively smooth compared to the centreline section. The drop in the free surface at the centre can be clearly observed. After the primary bore focuses and reflects at the centre, it propagates radially outwards until reaching the interface. At the interface, the bore is partly reflected and partly transmitted through the interface, following the
rarefaction wave. From the time when the first reflection takes place at the interface, there is diminishing wave activity, indicating that equilibrium is being approached.

Figure 5.27 displays the time history of the free surface at the centre of the domain. It is almost constant, except for a small undulation from $t = 0.4$ s to $t = 0.8$ s when the small bore implodes and then reflects. From $t = 2$ s onwards, there is no evidence of any change in the free surface, confirming the approach of equilibrium.

5.5.3 Case CD3

In this case, the liquid inside the circular column has smaller density than the liquid outside. The initial hydrostatic pressure thrust on the inside of the circular column is lower than that outside with a ratio of 4:5. After the system is released, the higher hydrostatic pressure thrust outside the circular column drives a radial shock-type bore from the density interface inwards toward the centre, as well as a rarefaction wave that propagates radially outwards.

Figures 5.28 and 5.29 present 3-D free surface visualisations and profiles of depth and velocity along the centreline of the domain, at times $t = 0.3$, 0.6, 1.05, 1.5, and 1.7 s respectively. By $t = 0.3$ s, the higher initial hydrostatic pressure thrust outside the circular region causes low density liquid close to the contact interface to be squeezed upwards. This generates a circular bore that travels radially inward towards the centre and a circular rarefaction wave that propagates radially toward the outer walls of the domain. At $t = 0.6$ s, the circular bore focuses at the centre and forms a spike. The reflected bore propagates radially outward towards the interface. By $t = 1.05$ s, the outward flow has caused a concavity in the free surface. When the reflected bore reaches the interface, it partly reflects towards the centre and partly propagates
though the interface. At $t = 1.5$ s, the part of the reflected bore focuses at the centre and forms another spike; the part that passes through the interface develops into a secondary bore that travels radially outward, following the rarefaction wave. At $t = 1.7$ s, the circular density interface remains delineated by a sharp step depth change; the rarefaction wave and the secondary bore continue to propagate outwards while the reflected bore inside the column travels outwards after the second peak.

Figure 5.30 presents the stacked $x$-$t$ plots showing evolution of the depth, depth-averaged speed and concentration profiles along the centreline from $t = 0$ s to $t = 5$ s plotted at 0.05 second intervals. Immediately after the system is released, a radial shock-like bore is created by the out-of-balance hydrostatic pressure thrust at the density interface, and this propagates inwards from the interface. Meanwhile, a circular rarefaction wave travels radially outwards. As the circular bore implodes at the centre, a clapotis forms, and the reflected bore propagates outwards with reduced strength towards the density interface. When this bore reaches the density interface, part is reflected back towards the centre and part travels through the interface into the denser liquid beyond. This process repeats itself, with the bores diminishing in strength, establishing a pattern similar to a shock diamond. Fluid motion exhibiting the shock diamond pattern is the supersonic jet. Photos of a supersonic jet can be found in Van Dyke (1982).

Figure 5.31 shows the 3-D $r$-$t$-$h$ representations of the wave diagram. The above view shows clearly the shock-diamond type structure whereas the side view gives visualisations of the free surface evolution along the diagonal of the domain. The bore partially propagates through the density interface into the denser outer liquid and there is also some partial reflection of the bore at the interface. The formation and dissipation of the first spike is very rapid which is observed as a sharp peak in the side view plot. By $t = 3$ s, the entire low-density region has
almost reached uniform depth. In the high-density liquid region, the rarefaction wave is followed by bores that emerge through the density interface.

Figure 5.32 displays the time history of the free surface at the centre of the domain. The depth at the centre remains almost constant at the initial value of 2 m up to \( t = 0.4 \) s. The free surface rises to a maximum of about 2.6 m at \( t = 0.6 \) s as the initial circular bore implodes, then falls almost to the equilibrium value, rises briefly to about 2.3 m at \( t = 1.5 \) s when the bore reflected from the contact surface reaches the centre. After the second rise, the free surface converges to the equilibrium.

### 5.5.4 Case CD4

Like case CD3, the initial hydrostatic pressure thrust inside the circular column is lower than that outside but with a ratio of 2:5. This case is a more severe than the previous one because the hydrostatic pressure thrust difference is much greater and therefore the resulting physical behaviour is much more distinct.

Figures 5.33 and 5.34 present 3-D free surface visualisations and profiles of depth and velocity along the centreline of the domain, at times \( t = 0.25, 0.5, 0.85, 1.1 \) and \( 1.4 \) s respectively. Figure 5.35 presents stacked \( x-t \) plots showing the evolution of the depth, depth-averaged speed and concentration distribution across the centreline of the domain from \( t = 0 \) s to \( t = 5 \) s plotted at 0.05 second intervals. Figure 5.36 shows the 3-D \( r-t-h \) representations of the wave diagram and Figure 5.37 displays the time history of the free surface profile at the centre of the domain.
The snapshots and the wave diagrams shown in Figures 5.33-5.37 of this case are very similar to the corresponding plots of the previous case except that all the physical features are much more pronounced due to the greater hydrostatic pressure thrust difference across the interface. As a result, the spike in the free surface and the shock-diamond structure are much more apparent and the time required to establish the equilibrium is longer.

5.6 Application Test

A more realistic situation is now considered whereby a river tributary carrying water and suspended sediment or debris joins a main river that carries water with negligible sediment content. The section of interest is the area close to, and slightly downstream of the junction between the two rivers. Examples of sediment-laden flows from tributaries into large rivers include debris-type flows into rivers joining the Upper Yangtze River, and hyperconcentrated loess (fine sediment) flows into the Middle Yellow River, in China.

The main river section considered here is 200 m long and 100 m wide, and is an idealised representation of a tributary of the Yangtze River for which field investigations have been undertaken by researchers at Tsinghua University (Cui et al., 2004 and He et al., 2005).

In the numerical model, the upstream and downstream boundary conditions of the main channel are both open, and transmissive. A constant inflow flux of 1 m³s⁻¹ is prescribed at the upstream boundary. Wall boundary conditions are closed, reflective. Initial values of the flow parameters throughout the main river channel are \( U = 1 \) m/s and \( h = 1 \) m. The junction between the tributary and main river channel is located from 60 m to 80 m downstream of the upstream edge of the computational domain. The tributary has length 100 m and width 20 m.
The initial value for the flow depth throughout the tributary is also $h = 1$ m and the initial value for the flow velocity $V$ is prescribed depending on the case considered. The tributary has a constant water-sediment mixture inflow flux of $1 \text{ m}^3\text{s}^{-1}$. The flow domain is shown in Figure 5.38. The bed friction is set to zero everywhere in both the main channel and in the tributary and both bed slopes are set to zero. Gravitational acceleration is $g = 9.81 \text{ m/s}^2$.

Three cases are studied: Case AP1, where $V = 1 \text{ m/s}$ everywhere in the tributary and the water-sediment mixture in the tributary is sufficiently dilute that it has the same density as that of the water in the main channel; Case AP2, where $V = 1 \text{ m/s}$ and the water-sediment mixture is hyperconcentrated in the tributary, such that its density is twice that of the water in the main channel; and Case AP3, where the tributary initially contains still water from the open interface with the main river to the section halfway along the tributary. The remaining upstream half of the tributary contains a hyperconcentrated water-sediment mixture flowing with $V = 1 \text{ m/s}$. In all three cases, a uniform grid of $200 \times 200$ cells and a time step of $0.05 \text{ s}$ are utilised. The limiter is chosen to be Minmod. Grid convergence tests reveal that this grid is adequate to model the flow behaviour properly.

5.6.1 Case AP1

In this case, the density of the water-sediment in the tributary is the same as that of the flow in the main river (i.e. dilute sediment concentration). Hence, the flow field has the same density everywhere, which is also constant with time. Figures 5.39 to 5.43 present free surface contours and 3-D visualisations at times $t = 5, 15, 30, 45$ and $60 \text{ s}$. The flow discontinuity at the junction causes something akin to a dyke break (but into the tributary and with a bore entering the main stream rather than a rarefaction).
Immediately after $t = 0$ s, a bore forms across the junction between the main stream and tributary, and then propagates up the tributary. Meanwhile, an approximately semi-circular weak bore forms within the main river, at the junction with the tributary. The flow in the main channel is clearly disturbed by this incoming weak bore. Separation takes place at the downstream corner of the junction between the main stream and tributary, leading to the development of a pronounced vortical structure by $t = 15$ s that migrates slowly downstream along the main channel close to its boundary (as can be seen by the position of the vortex at $t = 30, 45$ and $60$ s). The circular bore reaches the far wall and open boundaries of the main stream by $t = 30$ s, and reflects as can be seen by the 3D visualisation at $t = 45$ s. By $t = 60$ s, the free surface of the river flow is slightly raised everywhere (due to the incoming flow from the tributary), except at the major vortex downstream of the corner of the junction with the tributary. A part of the reflected circular bore enters the tributary, propagating in the upstream direction.

5.1.2 Case AP2

In this case, the density of the water-sediment mixture everywhere in the tributary has been increased to 2000 kg/m$^3$. The density of the water in the main river channel is 1000 kg/m$^3$. Figures 5.44 to 5.49 depict density and free surface contours and 3-D visualisations at times, $t = 5, 15, 30, 45, 60$ and $80$ s. Again, a bore forms immediately at the contact surface interface between the main stream and tributary, but is of much larger strength due to the difference in density between the two flows. The bore then travels into the main river section ahead of the contact surface, pushing up the free surface steeply (as is evident at $t = 5$ s). Immediately behind the bore is a trough corresponding to a weak rarefaction wave of opposite direction that travels upstream along the tributary. The contact surface at the interface between the high and low density liquids is located between the bore and rarefaction waves. Beyond the interface,
the higher hydrostatic pressure from the heavier sediment mixture causes water close to the contact surface to be squeezed upwards. As before, a vortex is created close to the downstream intersection point of the main river and its channel, and grows in strength with time. By time \( t = 15 \) s, the nearly circular bore has reached more than halfway across the main river channel, the rarefaction is moving up the tributary, and the vortex close to the downstream corner of the junction is clearly visible in the free surface visualisation as it gains strength. A step in the free surface is developing at the contact interface between the high and low density liquids. By \( t = 30 \) s, the bore has reflected at the opposite wall of the main river channel, and at the upstream flow boundary of the river, causing further nearly circular fronts in the free surface to develop.

The nearly circular main bore has its centre downstream of the entrance of the tributary, due to the advection effect of the main stream. The rarefaction wave continues to travel up the tributary, with an almost constant gradient in elevation. The contact surface is clearly evident as a step in both the density and free surface contour plots, and encompasses the major clockwise vortex down river of the downstream corner as well as a second vortex of anticlockwise sense that has sheared off from the upstream corner of the junction between the main stream and tributary. The results at \( t = 45, 60 \) and \( 80 \) s, indicate that the initial bore effects become less dramatic, as the reflected bore fronts interact with each other. Similarly, the rarefaction wave has reached the upstream (open) boundary of the tributary, and the depth along the tributary seems to be tending towards a constant (lower) value, compensating for the liquid being of higher density than that in the main channel. By contrast, the river level in the main channel has been pushed up everywhere beyond the contact surface. The contact surface itself delineates a mushroom structure with a pair of counter-rotating edge vortices that is continuously advected and distorted downriver by the main flow. At \( t = 60 \) and \( 80 \) s, there is evidence of successive weak bores running up the tributary due to partial transmission of reflections of the original circular bore across the contact surface and through the open junction.
5.1.3 Case AP3

In this case, the tributary initially contains still water of density 1000 kg/m\(^3\) between the junction with the main stream and the mid-point of the tributary. The upstream remainder of the tributary contains a hyperconcentrated water-sediment mixture of density 2000 kg/m\(^3\) flowing at an initial constant velocity \(V = 1\) m/s downstream towards the junction with the main river channel. The density of water in the main channel is 1000 kg/m\(^3\). Figures 5.50 to 5.55 present the predicted density and free surface contours and 3-D visualisations at times, \(t = 5, 15, 30, 45, 60\) and 80 s. The step differences in density and flow velocity at the middle section of the tributary cause the free surface to heap up immediately ahead of the contact surface (due to the effect of the denser upstream liquid on the otherwise still water in the tributary). By \(t = 5\) s, a noticeable hump has developed between the bore running towards the junction with the main stream and the contact surface. Both are characterised by steps in the free surface; the contact surface is however solely visible in the density plots. Immediately behind the contact surface, a depression can be seen in the free surface indicating the presence of an upstream propagating weak rarefaction wave. No effects are evident at the junction itself at this stage. At \(t = 15\) s, the bore front has just passed through the junction into the main river channel. The bore front is still quite straight, though is locally curved at the sides. The contact surface wave is advancing along the tributary towards the junction, while the very weak rarefaction moves upstream towards the open boundary of the tributary. The bore front develops into a near semi-circle by \(t = 30\) s, with its centre slightly downstream of the mid-point of the junction between the tributary and main stream. A strong vortex has formed immediately downriver of the downstream corner of the junction. The contact surface is about to reach the junction, and will then expand into the main flow, releasing a further rarefaction wave that starts propagating up the tributary. By \(t = 45\) s, the circular bore has reflected from the far side wall and open upstream boundary of the main river channel. The contact surface
has entered the main stream, and is sheared by the river flow. The rarefaction continues to progress up the tributary. As in the previous case, the main clockwise vortex near the downstream corner of the junction continues to grow in strength, but now no counter-rotating vortex is evident from the shear layer emanating from the upstream corner in this case. At later times \((t = 60 \text{ and } 80 \text{ s})\), it can be observed that the initial bore has undergone multiple reflections, and helped raise the overall level of water in the main river channel (outside the high density zone demarked by the contact surface). The contact surface shown in the density plots is deflected further and further downstream. One side of the contact surface curls around the main vortex. Its other side exhibits pronounced waviness, but does not roll up into localised vortices. This is also very evident in the free surface plots, where there is a step-like increase in free surface elevation at the interface between the two liquids, and wavy, vertical structures can be seen either side of the deflected mushroom-like downstream front. A secondary bore can be discerned running upstream along the tributary at \(t = 60 \text{ s}\) due to the passage of part of the reflected initial circular bore through the open junction.

The flow patterns shown for this specific case are similar to those observed in certain real debris flows. Figure 5.56 presents some stills of the video captured during a real debris flow (Cui et al., 2004), taken at \(t = 13, 15, 17\) and \(20 \text{ s}\). The width of the tributary is estimated to be in the order of 15-50 m which is comparable to the 20 m used in the numerical test. The depth of the sediment mixture taken in the video has a depth of 1-2 m (compared to the 1 m used in the numerical test). The tributary in the real debris flow has a slope that varies between 1/100 and 1/20 approximately. The numerically simulated flow process is slower than the observed debris flow but the timescale is of the same order of magnitude. The purpose of the simulation is merely to reproduce the main qualitative features of the flow. The common features appearing in the computationally simulated flow and the observed debris flow are the faster propagating bore and the ‘pit’ behind the contact interface of the water and the sediment.
mixture. The contact surface formed is at approximately half of the distance across the main river for the test case and the real debris flow. However, in the real debris flows, horizontal mixing starts to take place soon after the sediment mixture is disposed into the main river once the flow has steadied slightly (i.e. after \( t = 20 \) s in the video). Moreover, the rarefaction wave is usually not apparent in the real debris flow due to the slope and the turbulent conditions in the tributary.

5.7 Concluding Remarks

This chapter presents the 1-D analytical solutions for some idealised case and results obtained from certain idealised cases. Analytical approximations are obtained wherever possible so that the results from the parameter tests can be used to verify the model under variable density conditions.

Cases HB and SB that have continuous analytical steady state solutions remain in equilibrium with negligible discrepancies. This indicates that the flux gradient and source terms are correctly balanced and the model can simulate variable bed conditions. Furthermore, the subtraction of the constant density equilibrium from the analytical steady-state equilibrium as part of the balancing technique has given numerical results as predicted.

Cases A and B are dam breaks induced by a single discontinuity in the density. The initial conditions of the tests are tests exactly symmetrical about the centre of the domain and the numerical results of each case are mirror images of the other, which is as expected. Other properties such as the wave speeds and the speed of the contact surface are also in agreement with analytical predictions.
Cases DB1 to DB4 are parameter tests designed to investigate effects on flow hydrodynamics due to varying density ratio inside and outside of a liquid column. The numerically predicted height and width of the liquid column at equilibrium are close to the analytical approximation of the equilibrium height and equilibrium width of the liquid column. Results are interpreted as snapshots in time and also wave evolutions and compared to analytical approximation wherever appropriate.

Cases CD1 to CD4 are 2-D circular dam break tests induced by both density and depth differences on either side of the initial circular interface. Analytical equilibrium height and radius of the circular liquid column are obtained for each case. Numerical results are presented as snapshots in time, $x$-$t$ wave and 3-D $r$-$t$-$h$ diagrams. Physical interpretations of each case and analogy to special cases in fluid and gas dynamics are explained for each case.

Overall, the results for the above variable-density tests show that the model produces sensible results for variable density problems. As there are no published data for the type of tests carried out, numerical results are compared to analytical approximations from calculations. The approximate Riemann solver is robust and accurate in capturing shock fronts and contact surfaces. Flux gradient and source term balancing is achieved and symmetry is conserved.

For the idealised application case of a debris flow from a tributary into a main river, the potential of the variable-density model is demonstrated by the qualitative similarity between the simulated behaviour with that of real debris flows. The distinctive contact interface of the water and sediment mixture following the initial bore is simulated by the variable-density model but not by a conventional constant-density model.
Figure 5.1 Case HB: Initial steady state equilibrium and constant density equilibrium

Figure 5.2 Case HB: Time histories of depth error, non-dimensional velocity and density error
Figure 5.3 Case SB: Initial steady state equilibrium and constant density equilibrium

Figure 5.4 Case SB: Time histories of depth error, non-dimensional velocity and density error
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Figure 5.8 Case DB1: Stacked $x$-$t$ plots of the depth, velocity and concentration for $t \leq 50$ s
Figure 5.9 Case DB2: Results for the depth and velocity at $t = 1, 4, 12, 18, 30$ and $50$ s
Figure 5.10 Case DB2: Time history of the free surface position at the channel centre
Figure 5.11 Case DB2: Stacked x-t plots of the depth, velocity and concentration for $t \leq 50$ s
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Figure 5.13 Case DB3: Time history of the free surface position at the channel centre
Figure 5.14 Case DB3: Stacked x-t plots of the depth, velocity and concentration for $t \leq 300$ s
Figure 5.15 Case DB4: Results for the depth and velocity at $t = 1, 2, 4, 8, 30$ and $50$ s
Figure 5.16 Case DB4: Time history of the free surface position at the channel centre
Figure 5.17 Case DB4: Stacked $x$-$t$ plots of the depth, velocity and concentration for $t \leq 50$ s
Figure 5.18 Case CD1: Surface contours at $t = 0.35, 0.65, 1, 1.25,$ and $1.7$ s
Figure 5.19 Case CD1: Depth and velocity profiles at $t = 0.35$, 0.65, 1, 1.25 and 1.7 s
Figure 5.20 Case CD1: Stacked x-t plots of the depth, speed and concentration for $t \leq 5$ s
Figure 5.21 Case CD1: 3D $r$-$t$-$h$ representation of the wave diagram

Figure 5.22 Case CD1: Time history of the free surface elevation at domain centre
Figure 5.23 Case CD2: Surface contours at \( t = 0.55 \) and 0.7 s

(a) \( t = 0.55 \) s

(b) \( t = 0.7 \) s

Figure 5.24 Case CD2: Depth and velocity profiles at \( t = 0.55 \) and 0.7 s

(a) \( t = 0.55 \) s

(b) \( t = 0.7 \) s
Figure 5.25 Case CD2: Stacked $x$-$t$ plots of the depth, speed and concentration for $t \leq 5$ s
Figure 5.26 Case CD2: 3D r-t-h representation of the wave diagram

Figure 5.27 Case CD2: Time history of the free surface elevation at domain centre
Figure 5.28 Case CD3: Surface contours at $t = 0.3$, $0.6$, $1.05$, $1.5$ and $1.7$ s
Figure 5.29 Case CD3: Depth and velocity profiles at $t = 0.3$, 0.6, 1.05, 1.5 and 1.7 s
Figure 5.30 Case CD3: Stacked x-t plots of the depth, speed and concentration for $t \leq 5$ s
Figure 5.31 Case CD3: 3D $r$-$t$-$h$ representation of the wave diagram

Figure 5.32 Case CD3: Time history of the free surface elevation at domain centre
Figure 5.33 Case CD4: Surface contours at $t = 0.25, 0.5, 0.85, 1.1$ and $1.4$ s
Figure 5.34 Case CD4: Depth and velocity profiles at $t = 0.25, 0.5, 0.85, 1.1$ and $1.4$ s
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Figure 5.40 Case AP1: Free surface contour and 3-D visualisation at $t = 15$ s
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Figure 5.42 Case AP1: Free surface contour and 3-D visualisation at $t = 45$ s

Figure 5.43 Case AP1: Free surface contour and 3-D visualisation at $t = 60$ s
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Figure 5.47 (a) Case AP2: Free surface contour and 3-D visualisation at $t = 45$ s

Figure 5.47 (b) Case AP2: Density contour and 3-D visualisation at $t = 45$ s
Figure 5.48 (a) Case AP2: Free surface contour and 3-D visualisation at $t = 60$ s

Figure 5.48 (b) Case AP2: Density contour and 3-D visualisation at $t = 60$ s
Figure 5.49 (a) Case AP2: Free surface contour and 3-D visualisation at $t = 80$ s

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Figure 5.50 (b) Case AP3: Density contour and 3-D visualisation at $t = 5$ s
Figure 5.51 (a) Case AP3: Free surface contour and 3-D visualisation at $t = 15$ s

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Figure 5.52 (a) Case AP3: Free surface contour and 3-D visualisation at $t = 30$ s

Figure 5.52 (b) Case AP3: Density contour and 3-D visualisation at $t = 30$ s
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Figure 5.55 (b) Case AP3: Density contour and 3-D visualisation at $t = 80$ s
Figure 5.56 Snapshots of real debris flow from the upper Yangtze River into the middle Yellow River (photographed by researchers at Tsinghua University)
CHAPTER 6  CONCLUSIONS AND RECOMMENDATIONS

6.1  Conclusions

This thesis has presented a new mathematical formulation of the nonlinear shallow flow and species transport equations designed for variable horizontal density free-surface flows. The equation set involves mass conservation, momentum conservation, and species conservation. The ambient liquid has a benchmark density $\rho_w$ (usually that of water). The species can be either solid or liquid of given density $\rho_s$. The presence of species may cause the local density of the liquid-species mixture to vary according to the species concentration. The formulation deals with cases where the density difference in different flow regions is sufficiently great as to drive flows. In deriving the mathematical model, it is assumed that the liquid-species mixture is instantaneously fully mixed in the vertical direction, but can vary in the horizontal plane. A Godunov-type finite volume numerical scheme is then used to solve the variable-density nonlinear shallow flow equations in order to permit steep fronts to be modelled. The model is applicable to many environmental free surface flows, including hyper-concentrated sediment-laden flows in rivers, and debris flows.

The governing equations, derived from first principles, have been formulated as a set of hyperbolic conservation laws in order that they can be solved using a Godunov-type finite volume scheme that reproduces shock-like behaviour at steep-fronts. These conservation laws have been transformed into an equilibrium-corrected form that balances the flux gradient and source terms using the generalised flux gradient and source terms balancing technique derived by Rogers et al. (2003). The reformulation eliminates spurious oscillations.
and unphysical solutions when the bed is spatially non-uniform, while keeping the equations hyperbolic.

The correct structure of the equilibrium-corrected equations is confirmed because their eigen-structure is identical to that of the original unbalanced equations. The Jacobian matrix has four real eigenvalues, which verifies the hyperbolicity of the system (not strictly hyperbolic, because two eigenvalues are identical). Two of the eigenvalues are associated with characteristic speeds of the left or right shock/rarefaction wave, and the corresponding eigenvectors indicate the directions of propagation upstream and downstream. The two identical eigenvalues and corresponding eigenvectors represent the speed and direction of the intermediate shear wave at contact discontinuity. The solver based on the equilibrium-corrected equations was simple to implement without requiring explicit manipulation of numerical balancing algorithms. The equilibrium being subtracted is the constant density quiescent equilibrium which is calculated from the total volume of the mixture such that $h^{eq} + z_h = \text{constant}$ and $u = v = 0$. This is simpler and more straightforward to obtain than other equilibrium states, such as the steady-state no-flow equilibrium.

In the numerical solver, the inter-cell fluxes were obtained using either Roe's approximate Riemann solver or the HLL approximate Riemann solver. For the majority of cases, Roe's approximate Riemann solver was selected because of its ability to capture discontinuities, and its robustness. One of the problem areas associated with the Roe solver occurs in cases with a dry/wet bed front, where errors arise in estimating the front speed due to singularities encountered in evaluating the Roe's averages across the wet-dry interface. The HLL solver can deal with dry bed problems but does not properly capture the intermediate contact waves.
Taking the limit in the mathematical equations, as the species density tends to the ambient liquid density or *vice versa*, the variable density nonlinear shallow water equations reduce to the conventional (constant-density) nonlinear shallow water equations, with an extra equation describing passive transport of a marker species. The present model has therefore been validated for constant density shallow flows, for which a wide range of benchmark tests is available. The tests included: uniform flow in a channel, seiching in a rectangular basin, steady transcritical flow over a 1-D hump, wave propagation over a 2-D hump, dam break simulation, 2-D pure diffusion and 2-D advection diffusion. In all cases, close agreement was obtained between the numerical predictions and analytical or nearly analytical solutions of the constant-density shallow water equations. For 1-D wet-bed tests, it was found that the HLL solver gave slightly more accurate results than obtained using the Roe solver. Results from the dry-bed tests using the HLL solver were satisfactory, with very close agreement with analytical solutions except at the wet/dry fronts where more evident deviations from the analytical solutions could be discerned.

Using the full 1-D variable-density nonlinear shallow flow and species transport equations, analytical steady-state solutions were derived for certain idealised cases with a horizontal and a sinusoidal bed and these cases were used to help validate the numerical solver. Predictions were made of the steady-state depth and density distributions along a channel for a variable-density liquid-species mixture, where the bed was either horizontal or sinusoidal. The results were in almost exact agreement with the analytical solutions.

Further predictions were made for variable-density cases analogous to 1-D dam breaks, where the flow was driven by initial discontinuities in density, and 2-D circular dam breaks, where the flow was driven by initial discontinuities in both density and depth. For these cases, equilibrium values such as the equilibrium depth, the equilibrium width and the
equilibrium radius were calculated from mass conservation and the hydrostatic pressure thrust balance. The numerical predictions in these cases converged to equilibrium values in agreement with approximate analytical solutions based on mass conservation. Detailed parameter studies were undertaken to examine the effects of varying initial density or/and initial depth in the regions on either side of the initial interface.

The first 1-D parameter test was undertaken for two liquids, one occupying the left-hand side, the other the right-hand side of a rectangular tank. Both liquids were initially of the same depth, but had different densities. It was found that a shock-type bore propagated from the initial interface between the two liquids into the lower density liquid (which corresponded to the lower initial $\rho h^2$ value). A contact wave followed the bore propagating in the same direction as the bore. A rarefaction wave propagated simultaneously in the opposite direction into the higher density liquid. The test was run for two cases with initial conditions that were the mirror image of each other. The numerical results were also symmetrical about the axis of symmetry (i.e. the tank centre), as would be expected. The wave structures from this test were found to be similar to those that occur in shock tube gas dynamics (examples given by e.g. Liepmann and Roshko, 1957).

A second 1-D parameter study considered the motions induced by an initial liquid column of different density than the surrounding ambient liquid. The initial depth was the same everywhere in the tank, and therefore the $\rho h^2$ value depended solely on the density. The liquid motions were characterised according to whether the column had higher, the same or lower density than the surrounding liquid.

- For cases where the density of the column was higher than that of the surrounding liquid, the transient flow behaviour was similar to that of a conventional wet-bed dam
break. Bores propagated from the density interface into the low-density surrounding liquid as rarefaction waves propagated in the opposite direction into the high-density liquid of the central column. Reflection of the rarefaction waves caused a sudden drop in free surface elevation at the centre. In establishing equilibrium, the high-density central region underwent a series of readjustments counteracting overshoots in the free surface motions.

• When the density was the same either side of the interface, the system remained stationary, as would be expected.

• For cases where the density is lower inside than that outside of the column, bores initiated from the interface propagated inwards into the low-density region while rarefactions propagated outwards. At equilibrium, a peak is formed at the centre by the superposition of the inwards propagating bores.

A 2-D parameter test was also carried out to examine the effect of setting different initial $\rho h^2$ values for liquids inside and outside an initially circular interface. In all these cases, the initial depth of the liquid inside the column was higher than that of the surrounding liquid. Results were obtained for cases corresponding to the liquid in the initial circular column having a $\rho h^2$ value that was higher, the same or lower than that of the surrounding liquid.

• It was found that when the initial central liquid column had a higher $\rho h^2$ value than that of the surrounding liquid, the resulting flow behaviour was similar to that of a conventional dam break. A radial bore and a radial rarefaction were initially created at the interface, each travelling in opposite directions, with the bore heading outward
from the interface. The free surface at the centre fell to a minimum as the rarefaction focused, and this was then immediately counteracted by a secondary radial bore that propagated outward from the centre.

- When $\rho h^2$ had the same value either side of the interface, the system remained essentially in equilibrium (i.e. stationary), except for small perturbations due to grid-related errors, even when the initial density and depth values were different either side of the interface.

- When the initial central liquid column had a lower $\rho h^2$ value than that of the surrounding liquid, the behaviour was as follows. First, a circular bore propagated inwards as a circular rarefaction wave propagating outwards from the interface. The bore focused at the centre, creating a transient spike of liquid that then travelled radially outward until being partly reflected and partly transmitted at the density interface. The central column of liquid then continued to experience bore interactions of decaying amplitude as equilibrium was approached. The wave diagram had a planar pattern similar to that of a shock diamond caused by the repeated bore interactions in the central column. Analogous shock diamond features are well known in supersonic jet flows, photos are reproduced by Van Dyke (1982).

In short, the parameter study showed that free surface flows analogous to dam breaks can be driven by local density differences, even in the absence of a depth change across the interface between two adjacent liquids. A theoretical analysis showed that the factor that controls such flows is the product of the initial density and the initial depth squared i.e. the
\( \rho h^2 \) value, which can be interpreted as the depth-integrated hydrostatic force per unit width in the vertical directions \( \frac{1}{2} \rho gh^2 \).

After validating the variable-density model using the tests mentioned above, an idealised application case of debris flow from a tributary into a main river is considered. The results from the variable-density model show qualitatively similar behaviour to that observed in real debris flows, which include the distinctive contact interface of the water-sediment mixture following the initial bore. This result showing the intermediate contact wave, i.e. the propagation of the contact surfaces can not be simulated using a conventional constant-density model.

6.2 Recommendations

This thesis represents a start at modelling variable density fluids in environmental flows, there remains much future work.

- *Extension of the present mathematical model formulation*

The most important extension is to deal with heavy fluid running beneath light fluid and vice versa and in case of a strong mean flow where the violent vertical and horizontal mixing take place. This is required to overcome the stable vertical density gradient as light fluid runs over heavy fluid as the strong mean flow drives very strong vertical mixing.

In the present work, viscous and turbulence terms have not been included in the mathematical formulation. The assumption of zero viscosity and zero eddy viscosity are
restrictive, as all real liquids are viscous and environmental free surface flows are invariably
turbulent. It is therefore recommended that the momentum equations be extended to include
diffusion-like terms in the horizontal dealing with viscosity and additional turbulent terms,
bearing in mind that the effect of variable density should be carefully incorporated.

Further work on model validation would be required, of course, perhaps by comparison
against standard separated flow problems (e.g. topographic wind-induced gyres in a circular
basin, re-circulating flow past a side-wall expansion, etc.). It is recommended that further
parameter studies take place to examine the influence of adding viscous and turbulence
terms. A further useful extension could be achieved by generalising the treatment of
viscosity, so that the model would apply to non-Newtonian flows (such as occur in hyper-
concentrated sediment transport and debris flows).

For application to fluvial hydraulics, the equation set should be extended to incorporate a bed
defformation equation based on continuity of bed material. Empirical sediment transport
equations could couple the variable density non-linear shallow water equations to the bed
deformation equation. This extended model would permit further physical insight into the
processes of bed deposition/erosion and associated morphodynamic processes. Bed
deformation modelling is important for relatively high-velocity flows over mobile (erodible)
beds. The present model would be particularly well suited to hyper-concentrated sediment-
laden flows. It should be noted that previous experience (Huang, 2005) has shown that small
fluctuations in the velocity field can cause large differences in species concentration that
then have a subsequent impact on the velocity field.
• Numerical investigation into molecular diffusion, Coriolis and surface stress

Molecular diffusion, Coriolis and surface stress terms in the mathematical formulation should be studied further and included whenever these terms are significant to the problem being modelled. Although benchmark tests are not available for variable-density conditions, the model can be verified against constant density tests such as wind-induced circulation in a basin, or Coriolis-induced flow in a tank. There is a need for further cases with analytical solutions by which to check that each term in the mathematical governing equations has been accurately discretized.

• Higher order scheme in curvilinear coordinates

The present model is a second-order Godunov type scheme based on finite volume discretisation on a uniform grid. Investigations into the accuracy and efficiency of higher order schemes, e.g. by Falconer and Liu (1995), should be carried out with the aim of improving the numerical model. For complicated geometries, the model may benefit from being sited on boundary-fitted curvilinear, unstructured, or hierarchical grids. For example, adaptive quadtree grids used by Rogers et al. (2001) and Liang et al. (2004) offer considerable promise for representing complex evolving localised flow features within complicated natural domains. Cartesian approaches, such as uniform rectangular grids and quadtree hierarchical grids lead to problems at curved or irregular boundaries, where spurious reflections can occur. This drawback can be overcome by the use of cut cells, such as suggested by Yang et al. (2001) and Causon et al. (2000). Another method is to use mappings (such as curvilinear coordinates) to fit the grid to the domain boundaries. Curvilinear coordinate grid systems have been used by Lin and Falconer (1995), Borthwick and Akponasa (1997) and Fujihara and Borthwick (2000). Mappings have the advantage of
properly modelling the boundary curvature, but have the drawback of introducing additional terms in the equation set. To some extent, this can be offset by using orthogonal curvilinear grid approaches. In the future, it should be possible to solve the variable density non-linear shallow water equations on curvilinear quadtree grids, thus combining the best features of boundary-fitted mappings with an easy to adapt hierarchical grid structure. An alternative approach would be an unstructured mesh solver such as an unstructured triangular finite volume algorithm developed by Namin et al. (2004).

- **A complete 3-D variable-density shallow flow and species transport model**

The present model is depth-averaged and so is limited to nearly horizontal flows with pressure that is hydrostatic. Although most shallow flows can be assumed to be nearly horizontal, there are cases where the local flow field is quite three-dimensional. It would be clearly advantageous to develop a complete 3-D variable-density shallow flow and species transport model in order to obtain a proper picture of the flow and density processes. In the literature, researchers have developed 3-D constant density models with non-hydrostatic pressure. Examples are those by Stansby and Zhou (1998), Namin et al. (2001) and Koçyigit et al. (2002). However, extension to three-dimensions comes at considerable computer cost.
REFERENCES


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National Climatic Data Centre (2005)
http://www.ncdc.noaa.gov/oa/reports/chinaflooding/chinaflooding.html

National Climatic Data Centre (2005)


Stoker, J.J. (1992) “Water Waves, the Mathematical Theory with Applications”, John Wiley and Sons


