Plan of Action

Quantifying numerical diffusion and dispersion in D-Flow Flexible Mesh using a lock-exchange experiment

by

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1 Introduction

Due to temperature and salinity differences density driven currents can occur. Because important water systems such as the drinking water supply and large coastal systems in the Netherlands are strongly influenced by these currents it is important to understand these phenomena. With the use of D-Flow FM, a software package by Deltares, the mixture of salt- and fresh water can be numerically approximated. However, a side effect of these numerical flow models is the occurrence of numerical diffusion and dispersion caused by characteristics of the numerical discretization scheme that is used.

Numerical diffusion is sometimes referred to as “numerical viscosity” since the associated approximation errors mimic the effect of an increase in viscosity, i.e. the solution is overdamped. Since viscous properties of a fluid decrease the amplitude of the diffusivity rate in advection-diffusion flow problems. Additionally, numerical dispersion is related to unrealistic oscillations in an approximation of an advection-diffusion problem that may occur if stability of the solution is not ensured. Because avoiding such errors requires contrasting measures a quantification of their responses to certain modelling parameters is desirable. [4, 9]

In order to quantify the numerical diffusion and dispersion terms in the D-Flow FM model, and thus get an idea of the model’s sensitivity to certain parameters, a lock-exchange experiment will be set up which serve as the basis for a sensitivity analysis. After an initial qualitative analysis of the terms and settings found during an explorative setup of the basic D-Flow FM model, a stable basis for the parameter variations will be defined. In this basic model the desired boundary conditions, the lenght and timescale of the simulation and the constant parameters and modelling characteristics will be determined. Herafter the creation of such basic model will be automated so that the data required for the sensitivity analysis may be generated.

The required data consist of the numerical errors produced while changing the grid resolution, the timestep size and parameters related to the flow model. Subsequently the sensitivity S of a parameter P is defined as the relative change of a state variable per change of this parameter: $S = (\delta x/x)/(\delta P/P)$. The state parameters are defined as the difference between the approximation and the analytical solution at predefined monitoring points, also known as the accuracy of the approximation. Prematurely three state parameters are defined; the flow velocity error, the density error and wave speed error.

During the explorative model setup and the data generation phase, the observed data is analyzed and compared to certain indicator parameters in order to explain the observed phenomena. These indicators have previously been found to characterize the significance of certain modelling parameters [7] of a discretization scheme and the associated error or are composites of important model parameter. Finally the leverage of parameters, forcing functions and submodules of the model are assessed based on the observed sensitivity for which a possible explanation in terms of the indicators and model characteristics will be sought.

This document describes the research questions and hypotheses in the first chapter, subsequently it will describe the research strategy explained above in further detail in chapter two. Lastly, in the appendix a planning for this research project can be found.

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Research Question & Hypothesis

2.1. Research questions

1. How much numerical diffusion and or dispersion does the D-Flow FM model produce when simulating a 3D lock-exchange experiment dependent?

    1. What is the order of errors produced by D-Flow FM as a result of numerical diffusion and/or dispersion?
    2. How sensitive is the accuracy of the D-Flow FM model to time, space and numerically related parameters?
    3. What sort of errors are produced given different parameters?
    4. What parameters in the D-Flow FM model have the largest influence on errors related to numerical diffusion and dispersion?
    5. Are there indicators that predict the occurrence of numerical diffusion and dispersion in D-Flow FM?

2.2. Hypotheses

1. There is significant numerical diffusion and negligible numerical dispersion in the D-Flow FM model when performing a lock-exchange experiment.

    1. The order of errors is of 10E-4
    2. It is very sensitive to time and space related parameters and can be slightly improved by flow model parameters.
    3. Mostly numerical diffusion errors are produced except when more elaborate advection schemes are applied.
    4. The time step size, grid resolution and viscosity have the larges influence leverage on the accuracy of the model.
    5. Examples of such indicators are the dimensionless Reynolds and Froude numbers or the ratio between the net diffusivity coefficient in the model and the eddy

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Model Exploration

In order to provide a solid basis for the sensitivity analysis the basic model has to be applicable to the research objective and sufficiently robust to enable all parameters to be explored. To ensure a working model first most default settings will be used to set up the lock-exchange model, this will already require a minimal definition file where general settings, physics, geometry, flow and numerical parameters are set.

Thereafter possibly more realistic physical properties, boundary conditions, a more relevant geometry and specifics of the flow model such as bed friction and the will be defined. This should be done with the research objective in mind thus possibly requires setting up three different models for three different mesh grids in order to enable stable testing, at the cost of consistency between models. These trade-offs with respect to the research applicability and generalizability will have to be made.

Further on the post-processing of the generated model will be performed, in this way the results of the basic model can be qualitatively assessed with respect to basic indicators.

Finally, monitoring points have to be set up at logically sound locations and the basic models and subsequent post-processing have to be automated as much as possible.

In short the following parts of the model should be explored:

- General settings
- Physics
- Geometry
- Flow
- Numerics
- Post-processing
- Automation

3.1. Boundary conditions

Choosing the correct boundary condition for the lock-exchange model may be of significant importance considering the different boundary conditions that can be chosen within D-Flow. These boundary conditions can be divided into three groups and can all be related to the lock-exchange quite well: - Boundary conditions that complement the governing equations; continuity and momentum conservation. - Supplementary boundary conditions that impose additional constraints at a boundary. E.g. the weir at t=0 and the sidewalls and possibly the free surface [1]. - Boundary conditions for constituents, such as salinity.

3.2. Hydrostatic characteristics

The model is hydrostatic thus vertical accelerations are not taken into account. The pressure is assumed to vary linearly at each cell along the vertical direction depending on the density state of the cell, related to the temperature and salinity. [3, p.121]

The horizontal stresses resulting from the vertical stress profile however are included in the model. This should be further looked into.

3.3. Bed level type

Certain different bed level types may be specified that are either piecewise constant (1,2) or piecewise linear (3-6).

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Data Generation

In the third phase of the research, the research strategy is completely developed and provides a way to generate the data required to test the hypotheses, which is threefold and dependent on given parameter ranges: - Analytical (exact) reference data at monitor points

- Results obtained from the model

- Indicator parameters based on the results and input parameters

4.1. State variables

In order to define the sensitivity of the model to certain parameters, the sensitivity S of a parameter P is defined as the relative change of a state variable per change of this parameter: S = (δx/x)/(δP/P).

It seems that possibly one state variable would be enough which would be the velocity. Yet it would be interesting to see if there is significant molecular diffusion and thus measure the density as a state variable. Also the negative and positive wave of the fluid with a higher density will have a wave speed that might be to analyze because of it's possible relation to the tide induced translatory wave in the Rhine-Muese delta. - Flow velocity error

- Density error

- Wave speed error

It is also important to notice that it is still unknown how the analytical solutions at the monitor points can be calculated.

4.2. Spacial sensitivity

A very important parameter in the flexible mesh is the resolution of the grid and the sort of mesh used. In order to get a complete analysis of numerical diffusion and dispersion errors in D-Flow FM this should be elaborately evaluated. With respect to the grid three evaluation criteria can be seperately evaluated to assess the applicability of the results obtained from a model.

* Is the solution converging with an acceptable Residual RMS Error (< 10E-4)

* Are the imbalances of the results sufficiently small (< 1%)

* Achieve grid independence

4.2.1. Convergence & grid independency

Results obtained from the D-Flow FM model are the results of a numerical approximation specific to the mesh grid defined in the posed problem. Therefore the convergence of the solution and the independency of it's results to the mesh grid needs to be analyzed.

With respect to convergence of the model the output can be analyzed according to three points:

- Residual Mean Squared Error
- Gradient at monitor points (and observed parameters)
- Imbalance of the computation (Global sum of a parameter

A grid independence study is well depicted by plotting number of cells vs. value at monitoring points. However it may be expected that a relatively acceptable tolerance might not be attained given the limitations the numerical model poses on the grid size in combination with the timestep and the viscosity.

4.3. Numerical sensitivity

Another major parameter is the time step size of the approximation. The discretized advection-diffusion equation can be found on page 43 of Del [3], which uses an implicit and explicit scheme. Because of the explicit time integration of the momentum diffusion there is a limitation on the time step, however, in D-Flow this is implemented as a limitation on the eddy viscosity coefficient.

In general the turbulence and diffusion model parameters seems to have a great influence on the calculation complexity of the model. Therefore in appendix A an elaborate explanation of diffusion and turbulence modelling is given including the way D-Flow FM deals with this. Because turbulence, shear stresses and viscosity are similar processes all expressed in diffusivity terms they are grouped in the appendix for brevity.

In general the following parameters of the numerical model can be evaluated: * Timestep (Δt)

* Viscosity

* Flow model parameters

    * Entrainment (mixing terms)

    * Turbulence parameters

* Numerical parameters

    * Max. degree

    * Conditioner

    * Advection scheme

4.3.1. Numerical scheme

A short description of the numerical solving process implemented by D-Flow can be explained as follows. The discretized PDE's are solved by Gaussian elemination up to a maximum degree, a parameter that can be set, after which the resulting diagonally dominant, symmetric matrix is solved by the Conjugate Gradient method. Before the CG method is applied the matrix is preconditioned in order to assure a fast convergence of the CG method. Two methods can be used for this preconditioning: - Using the Jacobi preconditioner the diagonally dominant matrix is preconditioned by a matrix consisting only of the diagonal of the original matrix. - Using the LU decomposition preconditioner lower- and upper triangular matrices (L, U) are formed that enable a solving the matrix by Ux = y and Ly = b. However these matrices may be a lot less sparse then the original matrix which would cause an increase in memory usage. To overcome this problem the maximum degree parameter in D-Flow may be set.

[3, p.21]

(Possibly incomplete LUD is applied where L and U are matrices with a same sparsity pattern as the original matrix are formed such that LU ≈ A. The matix M = LU is then used to precondition (L, U). The matix M = LU is then used to precondition the original matrix before CG is applied.)

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Data Analysis

5.1. Indicator parameters

From phase 2 onwards the indicator parameters will be compared to the obtained result in order to get insight into the model and how it behaves. The following parameters will be used as indicators:

* Reynolds number

* Froude number

* Diffusivity and viscosity ($\eta = \rho \cdot D = \rho \cdot \mu$)

5.2. Numerical conditions

In order to analyze the numerical results and qualitatively be able to explain why certain behaviour is observed the numerical schemes will be analyzed according to common conditions and parameters used to asses the consistency, stability and convergence of numerical methods and schemes.

5.2.1. Consistency, stability and convergence of finite differences

1. If the local truncation error goes to zero in the limit of Δx a finite difference scheme is called consistent.

2. If there exists a constant C independant of Δx such that the norm of matrix A stays smaller than C if Δx goes to zero, a finite differences scheme is called stable.

3. If the global truncation error goes to zero as Δx goes to zero a scheme is called convergent. This happens if the scheme is both consistent and stable.

[8]

5.2.2. Condition number

The condition number K of a matrix A is defined as the ratio between the relative error in the approximation ($\Delta w/w$) given a relative error in the right hand side of the matrix equation ($\Delta f/f$). For symmetric matrices this number is equal to the magnitude of the maximum eigenvalue divided by the magnitude of the minimum eigenvalue: $K = |\lambda max|/|\lambda min|$. This range of eigenvalues can be estimated using Gershgorin circle theorem [8, p.107].

Using a more realistic estimation of the relative error in the approximation one can obtain the effective condition number defined as: K-eff = $1/\lambda min \cdot |f|/|w|$.

5.2.3. Other conditions

The conditions below will be discussed further if they turn out to be relevant.

* Von Neumann condition (Amplification factor)
* CFL condition (Positive numerical diffusion, domain of influence)
* Computational stability (Domain of influence)
* Heuristic stability
* Monotonicity

[9]

5.2.4. Spectral analysis

If significant numerical dispersion is observed a spectral analysis may be performed as proposed by Ruano et al. [6].

5.2.5. Interval analysis

To deal with uncertainties in model parameters an interval analysis may be done. Also to attain a range of values for certain parameters.

5.3. Variable leverage

Eventually after the data analysis the sensitivity of the numerical diffusion and dispersion produced by the model to a number of chosen parameters can be produced. A distinction will be made between model parameters, forcing and submodels in order to separate the grounds on which conclusions can be drawn.

* Parameters

* Forcing

* Submodels

A

Appendix A

A.1. Modelling of flow and transport

A.1.1. Molecular diffusion

As emphasized by [2, p194]: "..molecular diffusion is irrelevant in civil engineering practice, where turbulent diffusion and dispersion are dominant..".

In this case however it could be relevant because of the specific experiment. Still with the goal of modelling the Rhine-Maas delta in mind emphasis may be put on diffusion and dispersion processes related to turbulence.

A.1.2. Turbulent diffusion

To describe the turbulent diffusion the fluctuating quantities are averaged over a certain time and lenght scale. Because of gravity the concentration gradient is positive in the downward z-direction. From the averaging of the turbulent motion and the gravity induced concentration gradient it follows, as quoted from [8, p.197], that: "..turbulent fluctuations cause a mean transport in the direction of decreasing values of the mean concentration, as in a diffusion process."

Because the fluctuating quantities cause such net transport processes, the resulting motion and turbulent properties need to be quantified. To this end Prandtl [5] defined the concept of mixing lenght that defines the lenght over which the fluctuations cause a deviation from the average state and correspond to the average distance the turbulence eddies travel. For example, velocity fluctuations can be related to the velocity of the turbulent eddies. Further the turbulence induced transport processes are found to be proportional to the concentration gradient, also called the turbulence diffusivity. It has the order of magnitude of the eddie velocity times the mixing lenght.

For vertical diffusion in free surface flows the mixing lenght changes over the depth since it is induced by the bed friction expressed in the bed shear stress (τ-b). Using his an estimate of the particle velocity can be made by the so-called shear velocity which together with a parabolic variation of the mixing length over the depth gives a measure for the turbulence diffusivity: $\varepsilon t = K \cdot u \cdot L = K \cdot u \cdot z \cdot (1 - z/d)$. Where K is the Von Karman coefficient which was previously empirically determined.

In exactly this manner horizontal momentum can be vertically distributed through so-called Reynolds shear stress (τ-xz). Thus, in this case it is not a concentration (c) but a momentum per unit volume (ρu) that is diffused, an effect referred to as eddy viscosity. In a simple free surface flow [8, p.199] shows how this leads to a logarithmic velocity profile.

A.2. Turbulence modelling in D-Flow FM

A.2.1. Reynold stresses

In the D-Flow FM model the total horizontal viscosity can be divided into three contributing parts: - sub grid scale turbulence - 3D turbulence - dispersion for depth averaged simulation

Horizontal eddy viscosity
Modelling horizontal eddy viscosity has three seperate parameters that determine the total viscosity as follow: μ-H = μ-sgs + μ-v + μ-H-back.

These three parameters account for the following: - Horizontal turbulent viscosity may be underestimated because of the sub-grid scale turbulent motions, i.e. turbulence on a scale smaller than the meshgrid. This can be resolved by the sub-grid scale viscosity: μ-sgs - With Reynolds averaged shallow water equations horizontal eddy viscosity might not accounted for (enough) either thus D-Flow introduces the μ-v. - If extra constant or spatially dependant viscosity is desired the background viscosity μ-back may be added.

With respect to the 3D viscosity resulting from three-dimensional turbulence a closure model is used [3, p.26]. For specific closure models one can even account for unresolved mixing through an ambient background mixing coefficient μ-V-back. Eventually the vertical eddy viscosity is thus calculated by a combination of the 3D viscosity μ-v and μ-mol, the latter being the kinematic viscosity of water, as follows: μ-v = μ-mol + max(μ-v, μ-v-back).

In D-Flow FM four turbulence closure models can be chosen, the first being user defined and the latter three based on models by Kolmogorov and Prandtl, all are explained in further detail in [3, p.112-120]; - Constant coefficient - resulting in a parabolic vertical velocity profile - Algebraic eddy viscosity closure model - based on the Von Karman constant (κ), the bed friction (Cf), without including transport processes, computing mixing lenght (L), the shear velocity and the vertical turbulent viscosity μ-v. - K-ε turbulence model - involves solving a non-linear coupled system of equations describing turbulent kinetic energy (K) and energy loss (ε) including diffusivity coefficients (D), a turbulent kinetic energy production term (P), a Buoyancy flux (B) and a variation of kalibration terms (c1-3). Thereafter the vertical eddy viscosity μ-v is determined as proportional to the ratio K^2/ε and the mixing lenght. Still, this coupled system has to be discretized in terms of advection and diffusion which is done explicitly by a first order upwind scheme and implicitly, respectively. Accordingly the production and buoyancy term are discretized while conserving the diagonally dominant matrix (ensuring positivity). Finally this leads to two tri-diagonal matrices for K and ε that can be solved using Thomas algorithm, which may be seen as the tri-diagonal LU-decomposition, by using specific boundary conditions. - K-τ turbulence - Where τ is a typical timescale of the turbulent eddies and the eddy viscosity is proportional to K·τ. Coupled by a system of convection diffusion equations including diffusivity, production and buoyancy terms. The resulting advection equation is discretized with an first order upwind difference scheme and the vertical diffusion term is discretized implicitly by a temporal discretization scheme. Again this leads to two tri-diagonal matrices that can be solved by the Thomas algorithm using specific boundary conditions.

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