

Multi-scale modelling of effluent dispersion in the marine environment

PhD thesis written by

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Declaration

I confirm that all work described within this thesis that was not performed by me has been properly acknowledged. No portion of the work referred to in this thesis has been submitted in support of an application for another degree or qualification of this or any other university or institute of learning.

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Abstract

This research aimed to investigate whether the unique numerical methods available within CFD model software Fluidity could progress the state-of-the-art in various aspects of modelling effluent dispersion within the marine environment. Fluidity contains a large library of models and numerical methods that enable modelling of flow processes at a wide range of scales. It has been proven to perform well when used for massively-parallel simulations (i.e. it scales well), and it has the un-common facility of unstructured mesh adaptivity, which has the prospect of significantly increasing the efficiency of CFD simulations when guided skillfully.

This research also forms part of a longer-term project to create a coupled (or even single) model of effluent dispersion that represents influencing factors from a wide range of scales (from tidal currents down to turbulent eddies) entirely using CFD techniques. As such, one aspect of the research was to validate the numerical methods available within Fluidity for use in modelling effluent dispersion. To facilitate this validation, some of the model studies investigate aspects of effluent dispersion modelling from a hypothetical outfall site off the North-East coast of the United Kingdom.

Studies were performed in a series of stages in which key aspects of effluent dispersion modelling were addressed. CFD models were created of near-field jet dispersion, tidal motion, and far-field plume dispersion. Idealised test cases were also performed to investigate the performance of advection-diffusion solver methods. At each stage the aim was to investigate the benefit of novel numerical modelling techniques and compare their accuracy and efficiency to existing methods.

A set of near-field buoyant jet dispersion CFD models were created, one representing conditions associated with power, and combined power and desalination plants, and one representing conditions typically associated with desalination discharge. These CFD models utilised a mesh adaptivity algorithm to optimise mesh resolution during the course of the simulation. Model predictions were compared with published laboratory data and the predictions from validated integral models. An assessment was made of when CFD offers a benefit over other modelling options, and when it might be sufficient to use cheaper tools. There was also a discus-

sion of the effectiveness of mesh adaptivity in increasing model efficiency, together with advice for how and when it is best to use mesh adaptivity when modelling buoyant jet dispersion. Model results showed that with modest parallel computing resources and expertise, high-resolution simulations of jet dynamics can be achieved with reasonable accuracy using CFD modelling.

A model was created of tidal flow within the European continental shelf and results were compared to a large database of tide gauge measurements. This model took advantage of recently published methods for ocean model meshing and coastline resolution reduction. The purpose of this study was to confirm that these methods offered a benefit to model accuracy and efficient, and also that Fluidity could be used to accurately generate the tidal forcing boundary conditions for a far-field model of effluent dispersion at a hypothetical outfall site.

The predictions of M_2 tide amplitude in the vicinity of the outfall site had an average error of 10.1% compared with tide gauge measurements. The predictions of S_2 tide amplitude in the vicinity of the outfall site were even closer to tide gauge measurements, with an average error of 3.7%. The speed of the model solve showed a vast improvement over a previous comparison model study, with 37 days of tidal motion being simulated in 15.2 hours (58.4 seconds of simulation for each second of solving), compared to the comparison simulation with a similar level of accuracy, which simulated 2 seconds of tidal motion for every second of solver time.

A series of simplified test cases were run to assess a commonly-used advection-diffusion solution method from the library of those available within Fluidity. This work was intended to give general confidence that the numerical methods available within Fluidity are suitable for modelling coastal processes and so give confidence in later multi-scale results. The test cases chosen were relevant to coastal dispersion, including those testing tracer advection, diffusion, point sources and stratification. The method compared well with results published using world-leading free surface modelling software, Open TELEMAC.

A model was created of the dispersion of neutrally-buoyant dissolved pollutant from a hypothetical outfall. The assumed effluent is typical of that released from a manufacturing plant. The aim of this modelling was to validate the use of Fluidity for modelling effluent dispersion within the coastal zone, and also investigate the benefit of using 2-d horizontal mesh adaptivity to optimise model mesh resolution during the course of

the simulation. It was shown that the use of mesh adaptivity improved model efficiency, significantly lowering the effect of numerical diffusion.

Finally, a short outline was given of a prospective strategy for producing a coupled-model of effluent dispersion, using as a basis the techniques developed within this thesis. The proposed coupled model of effluent dispersion would include a near-field jet model two-way (i.e. “fully-coupled”) to a far-field plume model. Tidal forcing would be provided by a one-way coupled tidal model. Fluidity is capable of modelling all of these processes and so third party coupling software would be unnecessary.

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1 Introduction

1.1 Effluent dispersal in the marine environment

As of 2009, about 40% of the world's population lives within 100 kilometres of the coast (United Nations [2009]). Living by the sea is highly desirable for a variety of reasons. Significant tourism is drawn for the water sports, atmosphere and pleasures that can be derived from the coastline. Additionally, many industries benefit from the shipping access and plentiful water supplies available from being based near to the sea. This in turn creates employment that can sustain a large coastal population.

As industries and tourist destinations fall in and out of favour, the requirements of a particular section of coastline can shift through time. A land owner or property developer will naturally want to adapt their infrastructure to cope with these changes. But the coastline is a sensitive natural environment, and every change to infrastructure has complex consequences for its surroundings. Before a significant coastal development can be implemented, the local government usually mandates that an Environmental Impact Assessment (IAIA [1999]) is performed. This confirms the adherence to local regulations and guidelines, and requires decision makers to account for environmental values in their decisions and to justify those decisions in light of detailed environmental studies, and public comments on the potential environmental impacts (Holder [2004]).

A common by-product of coastal development is effluent, which is usually discharged through an outfall into the ocean. Examples include cooling water from power stations, brine from desalination plants, and treated sewage effluent from wastewater treatment facilities. This effluent may be diluted with sea water before being discharged, or treated (depending on its content and the cost-effectiveness) to lower its toxicity. For sewage, this treatment can either be primary: removing settleable solids, grease, oil and floatables; or more sophisticated secondary or tertiary treatments: removing biochemical oxygen demand (BOD), nutrients, pathogens and other biology. The discharged effluent can have a different temperature or salinity than the receiving water, and, depending on the process, it may also contain residual chemicals or pathogens. This can cause harm to sea

flora & fauna, or indeed the public. It also has the potential to interfere with nearby infrastructure that have intakes in the same receiving water (see Figure 1.1 for an aerial photo of sewage discharge spreading over a large area). Despite this, the relative volume of the discharged effluent is usually small compared to the size of the receiving waters and will typically be harmless once dispersed, only having the capacity to damage the local environment whilst still relatively concentrated.



Figure 1.1: pollutant discharge into the Mediterranean Sea, Greenpeace Philippines.

A typical outfall consists of a submarine pipeline placed offshore; in shallow water it is buried under rock armour (“rip-rap”) for wave protection, and at greater depths it is laid on the ocean floor with ballast rock on either side. At the outlet there is often a diffuser section – a manifold with many relatively small holes (ports) to distribute the flow over a large distance (Koh and Brooks [1975]). Typically the overall length of an outfall pipeline is an order of magnitude larger than the depth, which in turn is an order of magnitude larger than the pipe diameter and port spacing, which again are an order of magnitude larger than the typical port diameters. Some photographs of a typical outfall pipeline being laid are shown in Figure 1.3. A schematic of a typical pipeline once in place is shown in Figure 1.4



Figure 1.2: Photograph of a coastal outfall diffuser port, COAST [2011].



(a)



(b)



(c)

Figure 1.3: The laying of a typical coastal outfall pipeline, Krah Pipes.

As effluent leaves an outfall diffuser, flow is typically dominated by its initial buoyancy and momentum. It discharges from the diffuser in a jet-like manner (see Figure 1.2), rising towards the sea surface or sinking to the seabed, depending on its relative density. Once it has arrived at either the seabed or free-surface, effluent spreads laterally and momentum is quickly dissipated. The near-field refers to the region where the outfall characteristics and effluent characteristics dominate flow development and the far-field refers to the region where the ambient conditions dominate. In some scenarios, such as strong cross-flow, the distinction between the near- and far-field is less easily defined.

On leaving the near-field region, as momentum dissipates, effluent becomes more plume-like, and the environmental conditions begin to have a greater influence on flow development. The range of influential environmental physical phenomena can be wide, with local tidal currents, water depth, wave-induced currents, precipitation and flows from nearby estuaries and rivers potentially having a role in dispersion. This region of effluent dispersion is called the far-field. In reality, flow influences are not always this simply segregated and on some occasions the influences of the outfall design, effluent characteristics and environmental conditions have significant overlap. This is particularly true if currents are relatively weak. But this distinction between near- and far-field is often useful in separating what is inside an outfall designer's control, and what is not. Roberts et al. [2010] stresses that for sewage effluent dispersion, effective outfall design has a far greater influence on environmental impact than pre-treatment.

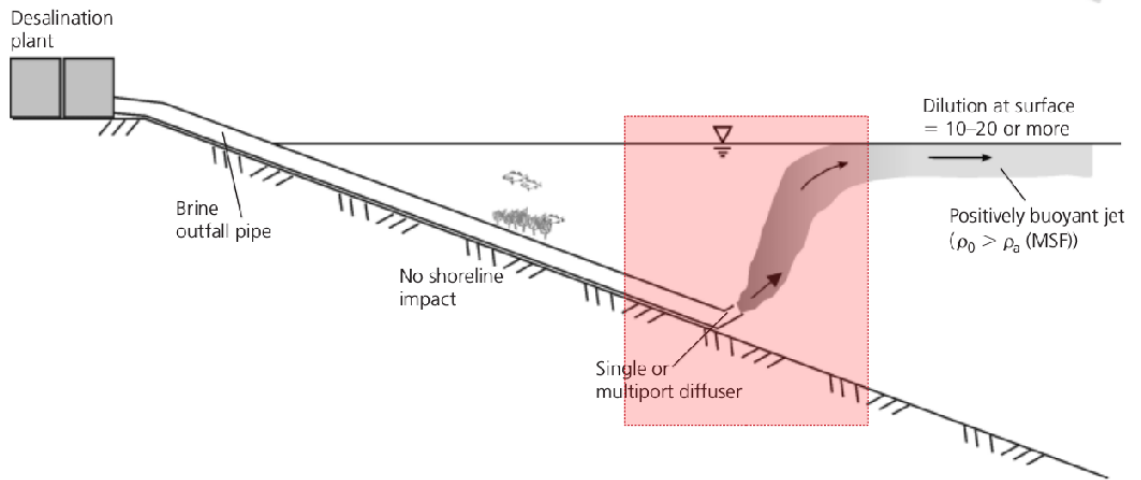


Figure 1.4: Schematic of a typical coastal outfall, showing the approximate near-field region in red. This image has been extracted and edited from Bleninger [2006].

The regulation of effluent dispersal varies from country to country. International guidance comes from the World Bank Group, which published the General Environment, Health, and Safety Guidelines (World Bank Group [2007a,b]). Europe has the European Union Water Framework Directive (European Union [2010]) which sets out agreed aims for legislation within European Union (EU) member states. Then, within the UK, say, this informs The River Basin Management Plans (RBMP).

For the Middle East, examples of legislation include, for Saudi Arabia, the National Ambient Water Quality Standards (Presidency of Meteo-

rology and Environment [2012]), for Oman, the Ministerial Decision No: 159/2005 (promulgating the bylaws to discharge liquid waste in the marine environment, Sultanate of Oman [2005]), and the Trade Effluent Control Regulations for United Arab Emirates [2010].

The USA has state-by-state regulation, with notable mentions for the California Ocean Plan (California Environmental Protection Agency [2012]), and the Ocean Outfall Legislation for Florida (Miami-Dade Water and Sewer Department [2013]), which have been influential in the formation of other international guidelines.

Each of the specifics of these guidelines are different, but most specify limits for the relative concentrations of the main effluent constituents, including fats, oils & greases, trace metals, pH imbalance, floatables, suspended solids, Biochemical Oxygen Demand (BOD), temperature, salinity (or Total Dissolved Solids), and pathogens (although usually limited to indicator organisms such as intestinal enterococci and faecal streptococci).

The effectiveness of environmental quality standard was reviewed by Ragas [2000]. A “combined approach” is typical of most developed nations, with an effluent standard (ES) “end of pipe” regulation limiting against acutely toxic conditions, and an ambient standard (AS) regulation applying to pollution quantities outside a “mixing zone”. This mixing zone is a regulator-defined limited area within which concentrations are allowed to exceed the AS regulations. Depending on the regulator, this zone may be defined as a length, an area, or a volume of the water body. A discussion of mixing zone definition for effluent discharge into EU waters was published by Bleninger and Jirka [2011].

Once a new coastal development has been proposed and the relevant regulations have been determined, a key step in the design process is to model the proposed development within its expected coastal environment. The effect that a proposed development has on the coastal zone (and vice-versa) can be modelled and used to inform practical designs that can withstand exposure to the forces of nature whilst causing minimal impact to the environment, people and ecology. It can be very difficult, if not impossible, to predict the effect of the physical environment at the early design stage, using only desk calculations. Once more expensive physical or computer modelling is employed, the design can undergo many iterations, as the possible environmental impact is managed alongside cost, material resources, construction constraints (often dictated by the weather) and durability / maintenance implications.

Accurate modelling, that takes into account key relevant physical processes, whilst also delivering answers in a practical time-scale, is imperative for reliably producing effective outfall design.

1.2 Modelling best practice and state-of-the-art

The accurate modelling of effluent dispersion is not straight-forward. The dispersion of effluent typically occurs over a wide range of spatial and temporal scales (at least six orders of magnitude). The mixing processes associated with the near-field are governed by the initial characteristics of the effluent and the outlet, with both the spatial and temporal scales being relatively short. Further away from the outfall, where mixing and dilution of the discharge becomes largely due to the underlying ambient conditions, spatial and temporal scales associated with mixing are usually much larger. If all these processes were to be resolved within a single model, the computational time-step and mesh resolution would need to be very small (hundredths of a second and centimetres, respectively), while the duration of the simulation and the size of the domain must be very large (days and tens of kilometres). Even with the rapid advancement of computing technology, this is generally prohibitively expensive. Consequently, the prediction of dispersion and dilution is typically carried out using nested or coupled computational models that are each specifically built to model features of the discharge at the different spatial scales, using turbulence models to account for sub-grid scale mixing (a description of current modelling techniques is given by Roberts et al. [2010]). These models are usually run independently and information is only shared at discrete points in space and time. In the case of outfall discharge modelling, a local near-field model is usually created to represent the rapid mixing close to the outfall, and a larger scale far-field model is then used to model the wider dispersion of the plume, including the effects of time- and spatially-varying water depths and currents.

Near-field modelling is most commonly performed using either length-scale or integral models such as NRFIELD (Roberts et al. [1989a,b,c]) or CORMIX (Jirka et al. [1996]). Length-scale models categorise discharge regimes based on key non-dimensional numbers, including fluxes of volume, buoyancy, and momentum. Once categorised, the steady-state behaviour of the discharge field is then predicted, using relationships calibrated to measured data. Integral models solve the conservation equations of mass and momentum along the jet centreline. They assume that jets are “self-similar” (i.e. there is no radial variation in velocity profile)

and that the jet profile is axisymmetric and Gaussian. Both these sets of models make significant assumptions about flow development that can limit their applicability, but they solve very quickly (of the order of seconds to minutes) and have been extensively validated against physical data for a range of commonly occurring scenarios.

Far-field modelling is usually performed using hydrodynamic models (sometimes known as ocean or free-surface flow models). Commonly used examples include Delft3D (Deltares), MIKE (DHI) and Open Open TELEMAC. These models can solve either the two-dimensional Shallow Water Equations, or if necessary, the three-dimensional Navier-Stokes equations on an extruded two-dimensional mesh. The three-dimensional models can include the effects of stratification and vertical mixing, but this comes at extra computational cost. The Boussinesq assumption, Vallis [2006], is usually assumed, together with an assumption that the pressure is hydrostatic; this means that flow is incompressible, and that density differences are sufficiently small to be neglected apart from in the buoyancy term in the underlying momentum equation. Hydrodynamic models might, depending on applicability, include the effects of tides, water depth, wave-induced-currents, evaporation, atmospheric effects, and Coriolis forces, but do not resolve individual waves and rarely resolve turbulent eddies less than a few metres wide.

1.3 Fluidity

Fluidity is an open source, general purpose, multi-phase CFD code capable of solving numerically the Navier-Stokes on a fully three-dimensional (3-d) unstructured mesh, using a range of finite element and control volume based discretisations. It can include models of turbulence, tidal forcing, Coriolis effects, density variations and associated buoyancy forces. Fluidity has been shown to scale well when run in parallel on large numbers of cores (8,000+ Guo et al. [2013]). It also has an anisotropic adaptive mesh capability which allows local control over mesh resolution and solution accuracy throughout the domain. This combination means that through appropriate use there is more potential for accuracy to be achieved without excessive time costs, with the unstructured mesh adjusting to efficiently concentrate computational effort only on those regions of the flow that are deemed to be important at a given time. The momentum and continuity equations solved by Fluidity can be either single or multi-material / phase, compressible or incompressible, they can use the linear-momentum formulation, or simplified using

the Boussinesq approximation for density, or depth-averaged using the shallow-water approximation.

Fluidity has been in development since 1999. As of June 2015, there are 54 people with developer status within the Fluidity user community, from a range of institutions across the globe, submitting multiple code updates per day. In order to manage code updates, the AMCG group uses the Git distributed version control system, hosted online by Github. The Github site allows access to the source code repository of all current and (most) past versions of Fluidity. This includes the “head” (i.e. latest) version of the trunk (also known as the base or master version of Fluidity), all extant branches, and most past versions of either the trunk or branches. Developers use Git to “clone” a Fluidity source code repository, create their own branch, and then edit and develop it as they see fit.

The AMCG group has created a bank of tests that is used for validation and verification of the code. This bank contains a total of over a thousand tests, falling into four categories of length: unit tests, verifying individual sub-routines, and running for a few seconds; short tests, running Fluidity and taking up to a minute to complete; medium tests, modelling shorter test cases, and taking up to 20 minute to run; and long tests, taking hours to run and often run in parallel. Each test confirms that Fluidity can perform a particular task, or model a particular physical phenomenon accurately.

If a developer wishes to merge their branch into the master version of Fluidity, they must submit a merge request through Github. An independent developer is then nominated to review the code and check that it is clear and robust. The Fluidity manual is updated, and suitable new tests are created to verify the code development. It is confirmed that the branch passes all unit, short and medium tests. The branch is merged with the master only once the reviewer is satisfied and has given approval. Since the development team adopted Github in late 2009, there have been over 8000 new code commits to the Fluidity trunk.

Alongside this protocol, AMCG uses Buildbot, a continuous integration system, to automatically rebuild and test the master after each merge, or after a set amount of time has passed. Buildbot builds the master in a wide range Linux environments, including workstations and clusters, using GCC and Intel compilers. All short and medium tests are run in each environment. Message Passing Interface (MPI) tests are also performed in parallel on workstations and High Performance Computing clusters. When a branch is merged with the master, the tests created by

the developer to verify their code edits are added to the existing bank of tests to ensure functionality is maintained in future versions of Fluidity.

The use of automated verification and validation, drawing on such a wide range of tests, ensures that the master version of Fluidity has a high level of robustness and continuity of performance. However, it is possible that during testing by Buildbot, the master will fail one or more of the validation and verification tests (if say, for instance, there was a significant difference between a submitted branch code before and after merging). At that point the latest master version available to the user would not be guaranteed to work satisfactorily. For users that require a more stable version of Fluidity, the AMCG group also have a “release” version that is created roughly once every six months. Unlike the master, a particular release of Fluidity is given a version number, and is static (the current release number is 4.1.11). A release of Fluidity has been shown to pass all available tests (crucially including the long tests, which are not guaranteed to pass for the master version). An inevitable limitation of the release version is that it does not contain the latest functionality of the master.

A full description of the methods used by the Fluidity research group to verify and validate Fluidity were published in Farrell [2011]. For the simulations performed within this research, where possible, the latest master version of Fluidity has been used. Some examples of the application of Fluidity solving on three-dimensional fully-unstructured meshes may be found in Vire et al. [2012], Parkinson et al. [2014] and Jacobs et al. [2014]. Some multi-scale coastal ocean examples may be found in Mitchell et al. [2010], Oishi et al. [2013] and Martin-Short et al. [2014].

1.4 Structure of Thesis

This research aimed to investigate whether the unique numerical methods available within CFD model software Fluidity could progress the state-of-the-art in various aspects of effluent dispersion modelling within the marine environment. Fluidity contains a large library of models and numerical methods that enable modelling of flow processes at a wide range of scales. It has been proven to perform well when used for massively-parallel simulations (i.e. it scales well), and it has the un-common facility of unstructured mesh adaptivity, which has the prospect of significantly increasing the efficiency CFD simulations when guided skillfully.

The dispersion of effluent within the marine environment typically occurs

over a wide range of spatial and temporal scales. Close to the outfall, mixing processes are governed by the initial characteristics of the effluent and the outlet (the near-field), and both the spatial and temporal scales associated with mixing are relatively short. Further away from the outfall, mixing and dilution of the discharge becomes largely due to the underlying ambient conditions (the far-field). Spatial and temporal scales associated with mixing are usually much larger in this region. If all these processes were to be resolved within a single model, the computational time-step and mesh resolution would need to be very small, while the duration of the simulation and the size of the domain must be very large. Even with the rapid advancement of computing technology, this is generally prohibitively expensive. Therefore, a local near-field model is usually created to represent the rapid mixing close to the outfall, and a larger scale far-field model is then used to model the wider-area dispersion of the plume.

This research forms part of a longer-term project to create a coupled (or even single) model of effluent dispersion linking near- and far-field models to represent influencing factors from a wide range of scales (from tidal currents down to turbulent eddies) entirely using CFD techniques. As such, one aspect of the research was to validate the numerical methods available within Fluidity for use in modelling effluent dispersion.

Studies were performed in a series of stages in which key aspects of effluent dispersion modelling were addressed. CFD models were created of near-field jet dispersion, tidal motion, and far-field plume dispersion. Idealised test cases were also performed to investigate the performance of advection-diffusion solver methods. At each stage the aim was to investigate the benefit of novel numerical modelling techniques and compare their accuracy and efficiency to existing methods.

Chapter 2 describes a set of CFD near-field buoyant jet dispersion models. The use of a fully three-dimensional CFD model for the near-field modelling is considerably more expensive than the integral or length-scale model alternatives, but it does avoid some of the assumptions that these simpler models make. As CFD models solve a more general form of the Navier-Stokes equations, they do not require the existence of a steady-state solution, nor need to assume jet profile self-similarity. They also allow open, prescribed, free-slip, or no-slip boundaries to be defined as required, which means that boundary interactions can be simulated directly. CFD models make fewer assumptions, and resolve more of the relevant physics, but consequently require far greater flow resolution than simpler models. As a result, despite its advantages, if a model requires the

inclusion of far-field influences, CFD modelling for the near-field effects has generally been considered a practical impossibility or an unnecessary expense. The near-field modelling performed within this research aims to lower the cost implications of CFD using Fluidity’s mesh adaptivity algorithms and parallel scaling.

Two standard test cases are modelled and compared to published physical and numerical data. This assessment of the modelling results include a discussion of when CFD offers a benefit over other modelling options, and when it might be sufficient to use cheaper tools. This is the first detailed study of a CFD model utilising mesh adaptivity which has been used to model jet dispersion. The discussion of model results offers an appraisal of the effectiveness of mesh adaptivity in increasing model efficiency for jet dispersion modelling, together with guidance for how and when it is best to be applied for modelling buoyant jet dispersion.

Chapter 3 presents the validation of a European continental shelf tidal model, using Fluidity. The aim was to confirm that Fluidity can accurately model tidal motion, and could be used to accurately define input tidal forcing constituents for far-field modelling of effluent dispersal. The model solved the non-conservative form of the shallow-water equations on a Cartesian mesh created using the Universal Transverse Mercator (UTM) coordinate system (i.e. flat, not spherical). This offered significant speed-up over previous Navier-Stokes solving simulations performed using Fluidity (Wells [2008]). The mesh was then generated using a combination of Quantum Geographic Information System (QGIS) and GMSH (Geuzaine and Remacle), using methods described in Avdis et al. [2015b]. The model results were compared against tide constituents calculated from over a thousand tide gauges, provided by the National Oceanography Centre (NOC). This is the first validation of this modelling technique using such comprehensive tide gauge data from the European continental shelf. Three-dimensional far-field hydrodynamic modelling is now more commonplace when the physical scenario being modelled requires it.

Chapter 4 describes the results of a series of test cases used to validate the use of Fluidity for modelling tracer advection & diffusion. The test cases described are a subset of those published by the developers of the world-class open-source free surface flow solver Open Open TELEMAC, chosen for their relevance to effluent dispersion modelling. This work was intended to give general confidence that Fluidity is suitable for modelling far- and near-field effluent mixing and dispersion. Several of the test cases model active tracer, with a state equation included to account for

the effects of buoyancy.

The Fluidity develop team has created many full-scale CFD-type test cases to assess the performance of the advection-diffusion solver, but none are as simple as the test cases described here. The advantage of these test cases are that they are simple enough to allow a quick and isolated assessment of each aspect of the solving process. These test cases gave the first comparison between the performance of the advection-diffusion solver available within Fluidity and that available within Open TELEMAC.

Chapter 5 describes the modelling of effluent dispersal from a hypothetical outfall off the east coast of the UK. The modelling investigated the possible advantages of using 2-d horizontal unstructured mesh adaptivity to improve the efficiency of coastal effluent dispersion modelling. This is the first time this modelling technique has been used to model effluent dispersal in the coastal zone. An assessment is made of the benefits of using 2-d horizontal mesh adaptivity for effluent dispersion modelling, together with guidance for its successful application.

Chapter 6 describes current model coupling methods used for modelling effluent dispersion within the marine environment, and outlines a prospective method for creating a coupled model using Fluidity.

2 Near-field buoyant jet modelling

2.1 Introduction

When effluent is released from a coastal outfall, the flow dynamics are initially dominated by the outfall characteristics and outlet conditions. Eventually, as the effluent moves far from the outfall, the outfall characteristics become less influential and ambient conditions begin to dominate. The “near-field” is defined as the region where the outfall characteristics and effluent properties dominate. This can be approximately quantified by the jet-to-plume length, Equation 2.5.

Near-field mixing processes are characterised by the relative influence of momentum and buoyancy effects. Discharges form “jets” when their behaviour is largely dominated by momentum (see Figure 2.1), and “plumes” when buoyancy dominates (see Figure 2.2). The initial flow from many outfalls shares a proportion of influence from both momentum and buoyancy forces (for example, thermal-saline discharges from desalination plants). In such cases, the discharges form “buoyant jets”. In either case, as a jet or buoyant-jet develops, it will eventually become a plume as the initial momentum is dissipated.

For a single round jet, three fluxes can be used to roughly apportion the influence from momentum and buoyancy forces: the specific volume flux,

$$Q = \frac{1}{2}\pi D^2 u, \quad (2.1)$$

the specific momentum flux,

$$M = \frac{1}{2}\pi D^2 u^2, \quad (2.2)$$

and the specific buoyancy flux,

$$B = g \frac{\Delta\rho_0}{\rho_A} Q, \quad (2.3)$$

where u is the discharge exit velocity, D is the diameter of the outlet, g is acceleration due to gravity, ρ_A is the ambient density and $\Delta\rho_0$ is the initial density difference between the effluent and the ambient fluid.



Figure 2.1: A water cannon salute, showing jets (in air) rising under their initial momentum before the formation of falling plumes [photograph by the US Navy].

These three terms are often combined to define two characteristic path-lengths: L_Q , a characteristic length-scale from the outfall exit,

$$L_Q = \frac{Q}{M^{1/2}}, \quad (2.4)$$

and L_M , the jet-to-plume transition length-scale,

$$L_M = \frac{M^{3/4}}{B^{1/2}}. \quad (2.5)$$



Figure 2.2: Soufriere Hills volcano erupting, showing plume-like flow in air [Photograph by Voight].

As a buoyant jet leaves an outfall, there is an initial zone of flow establishment where only the outer edges of the jet are directly influenced by the ambient fluid. The shear layer at the edge of the jet then grows inwards until it reaches the core of the jet. The length L_Q is a measure of the distance at which the volume flux of the entrained ambient fluid becomes approximately equal to the initial flux, Q . For distances greater than L_Q , which is proportional to the jet diameter, the effects of the initial jet volume flux become negligible in influencing the flow behaviour. The length, L_M , is the distance over which the buoyancy generates momentum that is approximately equal to the initial momentum flux, M . The jet behaviour will thus be momentum dominated for distances greater than L_Q and less than L_M , but will be controlled by the buoyancy flux

at distances much greater than L_M away from the source (Wright [1984]; Roberts et al. [1997])

The densimetric Froude Number, F , is also a key parameter in the near-field behaviour of a jet. This is defined as

$$F = \frac{L_Q}{L_M} = \frac{QB^{1/2}}{M^{5/4}} = \frac{u}{(g'D)^{1/2}}, \quad (2.6)$$

For all practical prototype-scale scenarios the flow will be highly turbulent. The transition to turbulence is dependent on the outfall Reynolds Number, Re_D , which for a round outlet is defined as

$$Re_D = \frac{uD}{\nu}, \quad (2.7)$$

where ν is the effluent kinematic viscosity. Flows transition to turbulence at a Reynolds Number of approximately 2000, which is at least two orders of magnitude smaller than typical outfall conditions. For experimentation or numerical models to represent prototype conditions, they must also have a Reynolds Number that places them in the turbulent region.

Some of the limitations of standard near-field modelling approaches are discussed in more detail in Section 2.2.3, and a more detailed description of the different model methodologies, including their advantages and disadvantages, is given by Roberts et al. [2010].

A potential solution to some of the limitations of near-field modelling lies in Computational Fluid Dynamics (CFD). As computing power increases, CFD is becoming a viable alternative to high-fidelity modelling in situations where standard near-field models may not be applicable, or there is considerable two-way interchange between the near- and far-field regions of mixing. CFD is more computationally expensive than standard modelling approaches, and its limitations are discussed further in Section 2.2.4.

This chapter describes a validation study for the use of CFD code Fluidity in modelling near-field buoyant jet dispersion. Two standard test

cases for jet dispersion were simulated: the buoyant jet (which is associated with power, and combined power and desalination plants), and the dense jet (which is typically associated with desalination discharges). Jets were discharged into stagnant, homogeneous (unstratified) ambient receiving water. These CFD models utilised a mesh adaptivity algorithm to optimise mesh resolution during the course of the simulation. Predictions were compared with published laboratory data, or the predictions of validated integral models.

The assessment of the modelling results will include a discussion of when CFD offers a benefit over other modelling options, and when it might be sufficient to use cheaper tools. There will also be a discussion of the effectiveness of mesh adaptivity in increasing model efficiency, together with advice for how and when it is best to use mesh adaptivity when modelling buoyant jet dispersion.

This chapter is an extended version of Robinson et al. [2015].

2.2 Review of jet modelling state-of-the-art

2.2.1 Physical modelling

Field measurement of pollutant discharge concentrations around outfalls is expensive and cumbersome. Natural variations in ambient conditions can make collection and analysis of data difficult. Consequently, laboratory experiments have been the primary source of our understanding of jet behaviour, as they allow accurate measurement and control of the jet and ambient conditions (a typical experimental set-up is shown in Figure 2.3).

Currently, the best technologies for measuring tracer concentration and velocity within lab experiments are Planar Laser-Induced Fluorescence (PLIF), introduced by van Cruyningen et al. [1990], and Particle Image Velocimetry (PIV), introduced by Simoens and Ayrault [1994]. Wang [2000] compared results using both PIV and PLIF.

Useful reviews and discussion of early experimental data were published by Fischer et al. [1979], Chen and Rodi [1980], and List [1982]. They highlighted several disagreements within the available data, mainly due to limitations in the size of the experimental tanks used. The later experiments of Dai et al. [1997], Shabbir and George [1992] and Sangras et al. [1999a,b] were able to take measurements at far greater distances

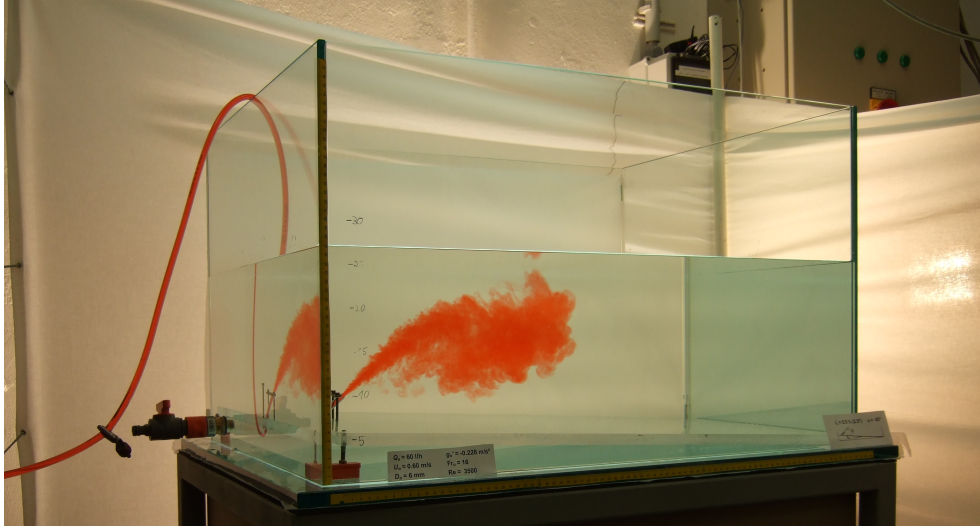


Figure 2.3: Photograph of a physical model experiment measuring jet dispersion, Bleninger and Jirka [2010].

downstream from the jet source and showed a significant improvement in their data as a result.

Lipari and Stansby [2011] published a more recent summary paper comparing the physical data taken from buoyant jet experiments published by Wygnanski and Fiedler [1970], Panchpakesan and Lumley [1993], Papanicolaou and List [1988], Hussein et al. [1994], Xu and Antonia [2002], Shiri and George [2008] and Wang and Law [2002].

The majority of the papers published up until the turn of the century concentrated on buoyant jets, as the majority of marine discharges were historically buoyant (coastal freshwater discharges from wastewater treatment plants, and thermal discharges from power station cooling water outfalls). As desalination and Liquefied Natural Gas regasification become more common, the number of marine outfalls discharging dense effluent has increased. With this, there has been a rise in dense jet research to aid understanding. Summaries of recent experimental studies are provided by Wood and Mead [2008] and Palomar et al. [2012]. The Ph.D theses of Oliver [2012] and Crowe [2013] both contain useful discussions of the published physical data for negatively buoyant jets.

2.2.2 Length-scale modelling

Length-scale models categorise discharge regimes based on key non-dimensional numbers, including fluxes of volume, buoyancy, and momentum. Once categorised, the steady-state behaviour of the discharge field is then predicted, using relationships calibrated to measured data.

Length-scale models come to a solution very quickly (typically seconds) but can be sensitive to user input data when the flow categorisation is close to the boundary between two regimes. Small adjustments in the input data can result in large differences in flow predictions, requiring Monte-Carlo-type testing and user experience to interpret the influence of input factors. Predictions can be inaccurate if using length-scale models outside of the parameter-space on which they have been calibrated (Zhao et al. [2011]).

Commonly used length-scale models include NRFIELD, of Roberts et al. [1989a,b,c] and CORMIX (Jirka et al. [1996]). Some of the flow classifications used by CORMIX are shown in Figure 2.4.

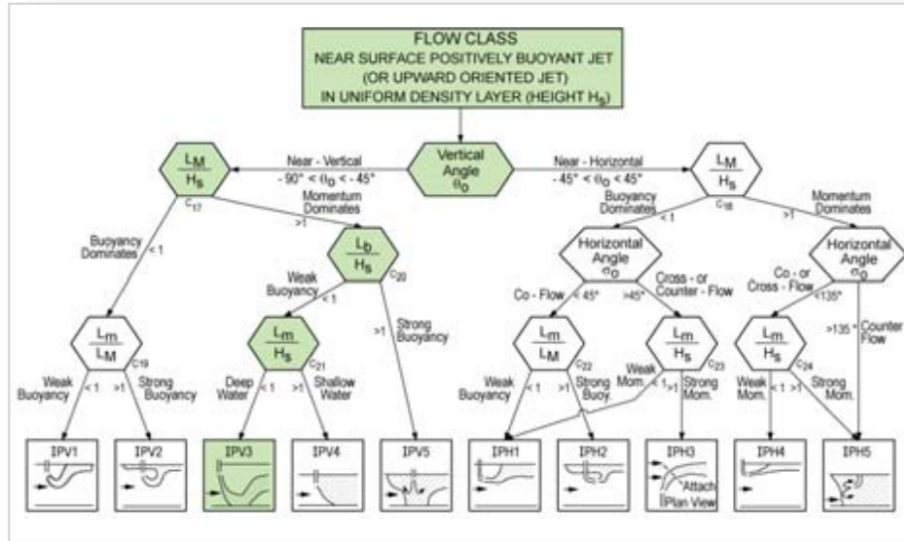


Figure 2.4: Some of the flow classifications used by CORMIX, Jirka et al. [1996].

2.2.3 Integral modelling

Integral models solve the conservation equations of mass and momentum along the jet centreline. They assume that jets are “self-similar” (i.e. can be described by non-dimensional terms) and that the jet profile is axisymmetric and Gaussian.

General first-order jet integral models were first published by Abraham [1963] and Turner [1969] based on the jet diffusion approach, and by Morton et al. [1956] and Fan [1967], based on the jet entrainment closure approach. Second-order integral models have been developed by Wang and Law [2002], Yannopoulos [2006], and Jirka [2004]. Popular commercial software packages incorporating integral models include Vis-jet (Cheung et al. [2000]), Visual Plumes (Frick [1984]) and CORMIX (Jirka et al. [1996]). CORMIX incorporates the integral model, CorJet, developed by Jirka [2004].

Standard integral models are less applicable if:

- the discharge is significantly affected by lateral or horizontal boundaries, Jirka [2004],
- the near-field region is unstable, with re-entrainment of partially-diluted effluent back into the jet (Jirka et al. [1996]),
- there is significant re-entrainment of partially diluted effluent from the mid- and far-fields back into the near-field region over successive tidal cycles (Nash and Jirka [1996]),
- or the initial momentum and buoyancy of the discharge act in opposite directions, leading to edge instabilities, as is observed on the underside of inclined dense jets (Kikkert et al. [2007] and Shao and Law [2014]).

2.2.4 CFD modelling

CFD modelling of jet dynamics can potentially overcome all of the problems of parameter-based approaches, but presents its own new range of challenges. It is not trivial to create a CFD model of jet mixing that is suitably accurate, stable, and provides a solution in a practical amount of time. CFD codes are necessarily large (i.e. expensive) and complex, requiring considerable training to use effectively. In order to trust and

interpret the results that a CFD code produces, a thorough validation and verification procedure is necessary (see Stern et al. [2001] for further reading).

It is rarely possible to resolve all turbulent length scales within a CFD simulation and so most simulations are dependent on a turbulence model to parameterise at least some proportion of the mixing. If used inappropriately (i.e. for representing physical scenarios for which they have been shown to be invalid) turbulence models can provide stable but unphysical solutions. This makes validation especially important for confidence.

Even with the aid of a turbulence model, the mesh resolution required to give a stable solution is often high. This can make CFD modelling very expensive. Even with modern computing techniques, accurate CFD models of near-field mixing may require simulation times in the order of several days. This is significantly more expensive than the simulation times for simpler parameter-based approaches, which typically produce results in minutes or seconds. For more complex outfall cases (e.g. merging jets from multiport outfalls) CFD models are theoretically possible but, to produce accurate solutions, may require prohibitively high computational effort. Therefore, a key goal of the present research was to develop models using adaptive meshing and parallel computing, which can reduce simulation times.

The choices of field discretisation and advection schemes for CFD modelling also involve compromise. There are trade-offs between differing degrees of stability, numerical diffusion, conservation, boundedness and cost. A more complete discussion of this is given by Wilson [2009]. As these choices can significantly affect predicted tracer concentrations, their consideration is particularly important for jet and plume modelling.

Despite these complications, once created, a fully validated and verified CFD model can produce a high resolution, fully 3D representation of jet dynamics, not necessarily restricted to the assumptions of integral modelling. As CFD models solve a more general form of the Navier-Stokes equations, they do not require the existence of a steady-state solution, nor need to assume jet profile self-similarity. They also allow open, prescribed, free-slip, or no-slip boundaries to be defined as required, which allow consider flexibility in simulation set-up.

Many published studies of jet modelling using CFD codes concentrate on the choice of turbulence model, as this greatly affects the accuracy of model predictions. Oliver et al. [2008] used the standard $k - \varepsilon$ tur-

bulence model (Launder and Spalding [1974]) to model dense jets, with experimental adjustment of the Schmidt number for scalar diffusivity. They found limitations in the predictions of bulk parameters and the cross-sectional distribution of tracer.

Worthy et al. [2001] and Brescianini and Delichatsios [2003] compared a range of $k - \varepsilon$ turbulence model formulations when modelling the near-field mixing regions of dense and buoyant jets, respectively. Brescianini & Delichatsios concluded that the Reynold Stress Transport Model (Malin and Younis [1990]) and the Algebraic Stress Model (ASM, Davidson [1990])) showed no improvement over the standard model, but the Generalised Gradient Diffusion Model (GGDM, Daly and Harlow [1970]) showed a slight improvement in the accuracy of the turbulent stream-wise mass flux. Worthy et al found that combining the GGDM and ASM gave an improvement on the standard model but this required the inclusion of the Richardson correction term (Rodi [2000]) in order to be of any benefit (which the modelling of Brescianini and Delichatsios [2003] did not include). Both studies concluded that due to the level of noise within the experimental data available, it was difficult to discern with confidence any advantage between any particular $k - \varepsilon$ turbulence model formulation.

Basu and Mansour [1999] used a dynamic Large Eddy Simulation (LES) turbulence model to simulate buoyant jets. Computed velocity fields were compared with experimental data, and the authors found that their predictions lay within the scatter of the available data. The study highlighted the difficulties in obtaining definitive data for comparison with predictive models, as the intensity of turbulence within a jet is strongly dependent on the way the fluid is introduced to the domain.

Devenish et al. [2010] compared LES simulations of vertical buoyant jets rising into stratified ambient water to results obtained using integral models developed and validated by Morton et al. [1956] and Bloomfield and Kerr [2000]. The LES simulations differed significantly from the validated integral model results in their prediction of jet penetration and overturning.

Worthy [2003] gave a comprehensive account of buoyant jet modelling using LES. However, simulations were only carried out using low Reynolds numbers (50 and 1300), and therefore comparisons with turbulent buoyant jet data is not possible.

In summary, $k - \varepsilon$ models have been shown to successfully predict results that lie within the scatter of published experimental data, but do not

resolve the details of turbulence that can be influential to jet dynamics. In contrast LES models resolve turbulence but require considerably more computational expense (or compromising model assumptions) for them to solve in a practical amount of time.

This study uses both the standard $k - \varepsilon$ turbulence model and the Smagorinsky LES model as these have been shown in the above references to compare favourably with experimental data. In contrast to previous studies, this study aims to overcome the cost implications of the different turbulent closure approaches using Fluidity’s mesh adaptivity algorithms and parallel scaling to both reduce computational cost and increase scalability.

2.3 Validation test cases

The test cases were based on published physical models: dense jet experiments published by Nemlioglu and Roberts [2006], and buoyant jet experiments published by Wang and Law [2002]. The test configurations are summarised in Table 2.1. Buoyant jets were generated using horizontally discharged effluent with a salinity deficit relative to the receiving water. In this configuration, the jet trajectory is initially horizontal but, as momentum dissipates to the ambient, the jet deflects upwards under its buoyancy. The model domain for these simulations was $4\text{ m} \times 1\text{ m} \times 1\text{ m}$, with the outlet nozzle placed at the centre of the rear wall, protruding 0.05 m into the domain. The predicted centreline trajectories and velocities were compared with the validated integral model, CorJet, of Jirka [2004]. As centreline velocity decays is related in part to the rate of dilution, this measure also compares the rate of entrainment into the jet with that predicted by the integral model.

Dense jets were generated by discharging effluent at an angle of 60° to the horizontal, with a salinity excess relative to the receiving water. This is a commonly used configuration in the design of marine outfalls for dense discharges (such as those from desalination plants). A jet is generated that initially rises under its momentum, before sinking back to the bed under its (negative) buoyancy. As has been found by many authors (e.g. Zeitoun et al. [1971]), a 60° angle maximises the jet’s path length (and therefore dilution) before impact with the seabed. The model domain for these simulations was $6.5\text{ m} \times 1\text{ m} \times 1\text{ m}$, with the outlet nozzle located at one end, protruding at an angle of 60° to the horizontal, and with the tip located 0.035 m above the bottom.

Table 2.1: Summary of parameters used in the two jet test-cases

Parameter	Horizontal buoyant jet	Angled dense jet
Inlet velocity (m/s)	0.57	0.68
Inlet diameter (mm)	9.4	3.3
Inlet salinity (g/l)	2.6	42.4
Ambient salinity (g/l)	41.2	1.5
Inlet angle (°)	0	60
Densimetric Froude no., F	10.7	21.3
Reynolds Number	6000	2500
Parameters comparison	Centreline trajectory mean axial velocity decay	Centreline terminal rise height bottom impact distance minimum impact dilution
References for comparison	CorJet integral model, Jirka [2004]	experimental data summarised by Wood and Mead [2008] and Palomar et al. [2012]

Densities for both sets of tests were calculated assuming standard room temperature (21 °C) fluid, with a uniform temperature distribution through the domain.

The limited performance of standard integral models for angled dense discharges has been widely reported, for example Kikkert et al. [2007] and Shao and Law [2014]. This is due to the non-Gaussian concentration profile that develops downstream, due to the buoyancy-induced instability of the lower edge of the dense jet. For the angled dense jet, the predicted centreline terminal rise height (Z_t), centreline impact distance downstream (x_i) and centreline impact dilution (S_i) were compared with formulae derived from several experimental studies, which are summarised by Wood and Mead [2008] and Palomar et al. [2012]. These depend on the nozzle diameter, D , and the densimetric Froude number, F :

$$Z_t = k_1 \cdot D \cdot F; \quad x_i = k_2 \cdot D \cdot F; \quad S_i = k_3 \cdot F.$$

Values of the coefficients k_i derived from each of the studies are shown in

Table 2.2. These coefficients are used in the model comparisons presented in Section 2.5. For comparison, equivalent predictions from the CorJet integral model are also presented. The published measurements of the characteristic lengths presented in Table 2.2 have a large range. The jet dynamics are very sensitive to the test set-up, and the resulting noise in the results of the laboratory experiments is the prime reason why it is necessary to compare against a wide cross-section of published results to gain confidence in model accuracy.

Table 2.2: Dense jet data summary

	$k_1 = Z_t/DF$	$k_2 = x_i/DF$	$k_3 = S_i/F$
Zeitoun et al. [1971]	—	3.19	1.12
Roberts et al. [1997]	—	2.4	1.6 ± 0.12
Nemlioglu and Roberts [2006]	—	3.25	1.7
Cipollina et al. [2005]	1.77	2.25	—
Kikkert et al. [2007]	1.6	2.72	1.81
Papakonstantis et al. [2011a,b]	1.68	2.75	1.68 ± 0.1
CorJet, Jirka [2004]	1.85	2.28	0.77 ± 0.1
Gildeh et al. [2014] ¹	1.49–1.80	2.66–4.60	0.81–1.21
Jiang et al. [2014] ¹	—	3.00	1.42

¹ It should be noted that the two recent references (Gildeh et al. [2014] and Jiang et al. [2014]) used jets angled at 45 degrees to the horizontal, whereas the present tests have been carried out using 60 degree angles.

2.4 Model details

2.4.1 Continuity, momentum and turbulence modelling

The jet test cases being modelled are all turbulent. The outflowing energy of the jets is cascaded from larger to smaller and smaller eddies, until it reaches the smallest eddies, at which point it is converted to heat energy (see Figure 2.5). The eddies with the largest energy are the size of the integral wave number, κ_I , which is approximately the size of the definitive length-scale of the flow. The smallest eddies, where turbulent energy is converted to heat energy, are of the Kolmogorov length-scale, which is,

$$\eta_K = \left(\frac{\nu^3}{\varepsilon} \right)^{1/4}. \quad (2.8)$$

The associated Kolmogorov time-scale is,

$$\tau_K = \left(\frac{\nu}{\varepsilon} \right)^{1/2}, \quad (2.9)$$

and the Kolmogorov velocity-scale is,

$$v_K = (\nu\varepsilon)^{1/4}, \quad (2.10)$$

where ν is the fluid viscosity and ε is the average rate of dissipation of turbulence kinetic energy per unit mass. Resolving all the turbulence within a simulation (known as the Direct Numerical Solution, DNS) would require the mesh edge lengths to be as small as the kolmogorov length-scale, which would be prohibitively expensive for most practical flows. The jet models described in this research reduce costs by using eddy viscosity turbulence modelling to model (rather than resolve) some (or all) of the energy dissipation due to turbulence. An eddy viscosity, ν_T , is calibrated to dissipate energy at the same rate as the turbulence it is modelling.

For eddy viscosity models, the velocity vector field, u_i , is decomposed into a resolved component, U_i , and a modelled component, $\overline{u'_i}$, such that

$$u_i = U_i + \overline{u'_i}. \quad (2.11)$$

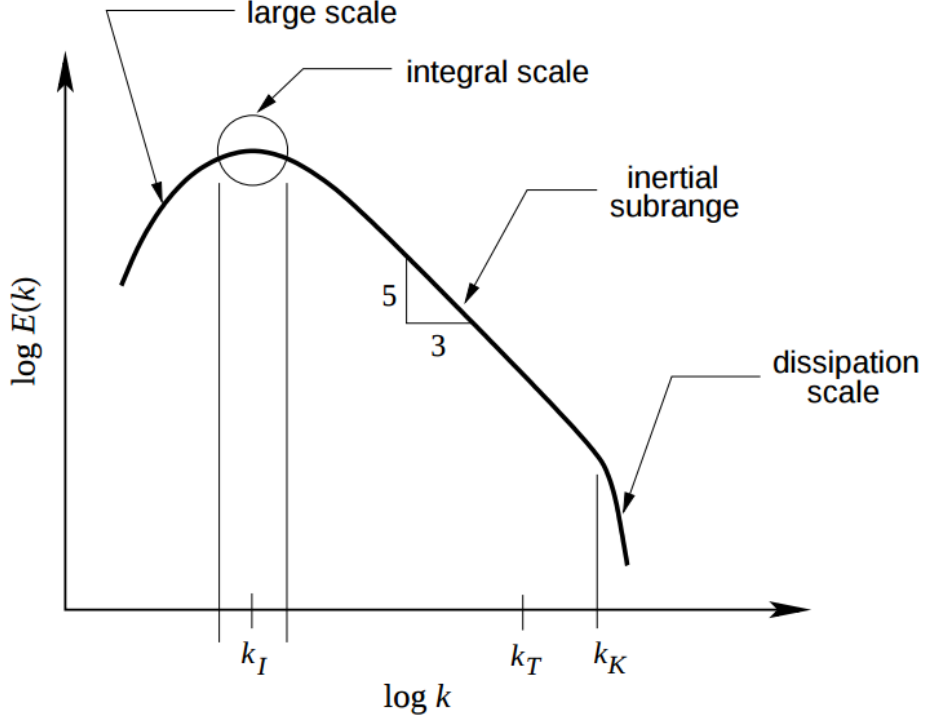


Figure 2.5: Von Karman Spectrum, describing the energy cascade in turbulent flow, McDonough [2004], where l is eddy length-scale, $\kappa = \pi/l$ is the wave number and $E(\kappa)$ is the energy present at that wave number.

The Boussinesq form of the continuity equation (for both resolved and modelled flow) is

$$\nabla \cdot u = 0 \quad (2.12)$$

and the associated momentum equation is showing (respectively) the unsteady, convection, pressure, viscous and gravitational terms:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p'}{\partial x_i} + \frac{\partial}{\partial x_j} \left\{ \nu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right\} + \rho' g_i \quad (2.13)$$

where ρ' is the perturbation density ($\rho' = \rho_{\text{ref}} - \rho$), t is time, p is pressure, ν is the molecular kinematic viscosity, ρ is density, p' is the perturbation pressure ($p = -\rho_{\text{ref}}gz + p'$), p is pressure, and g_i is gravitational acceleration vector.

Incorporating Equation 2.11 into Equation 2.13 to gives:

$$\frac{\partial U_i}{\partial t} + \frac{\partial}{\partial x_j} (U_i U_j + \overline{u'_i u'_i}) = -\frac{\partial p'}{\partial x_i} + \frac{\partial}{\partial x_j} \left\{ \nu \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \right\} + \rho' g_i, \quad (2.14)$$

which can be re-arranged into its most recognisable form:

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{\partial p'}{\partial x_i} + \frac{\partial}{\partial x_j} \left\{ \nu \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \overline{u'_j u'_i} \right\} + \rho' g_i. \quad (2.15)$$

This equation is similar to Equation 2.13 but for the $\overline{u'_j u'_i}$ term within the momentum equation. This term is commonly named the “Reynolds Stress” and represents the momentum loss due to unresolved eddies.

Eddy viscosity models assume that the Reynolds Stress can be modelled as:

$$-\overline{u'_i u'_j} = \nu_T \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} k \quad (2.16)$$

where δ_{ij} is the Kronecker delta. The final term in this equation produces an isotropic (or spherical) stress that does not contribute to momentum transport, behaving instead like an additional pressure term. This term is typically dropped (as described here) on inclusion in the momentum equation, and so is implicitly included in the pressure term.

This allows the momentum equation to be rewritten as:

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{\partial p'}{\partial x_i} + \frac{\partial}{\partial x_j} \left\{ [\nu + \nu_T] \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \right\} + \rho' g_i \quad (2.17)$$

The eddy viscosity, ν_T , varies in space and time, and its calculation is the crux of eddy viscosity modelling. All eddy viscosity models share Equation 2.17, but the meaning and calculation of ν_T is not the same for each model. There are a range of categories for eddy viscosity turbulence modelling, each defined by how much of the turbulence is being modelled by the ν_T term.

For Reynolds–Averaged Navier–Stokes (RANS) turbulence models, ν_T models all turbulence. ν_T is raised such that only the non-turbulent

fluctuations remain, resulting in an ensemble-averaged velocity field that is laminar-like in appearance. Depending on the particular RANS model, ν_T is calculated using dimensional analysis, relating ν_T to any two of the following key parameters of turbulence: k , the turbulent kinetic energy, ε , the rate of turbulent kinetic energy dissipation, ω , the specific rate of turbulent kinetic energy dissipation, l , the Prandtl mixing length.

The most common RANS models are:

- $k - \varepsilon$, where $\nu_T = C_\nu \frac{k^2}{\varepsilon}$, Launder and Spalding [1974],
- $k - \omega$, where $\nu_T = C_\nu \frac{k}{\omega}$, Wilcox [1994],
- and $k - l$, where $\nu_T = C_\nu k^{1/2} l$, Prandtl [1945].

C_ν is a constant that varies between turbulence models, but for each model there is a standard value that has been accepted by the user community.

The smoothing of the velocity field caused by ν_T modelling decreases its curvature. This means that when using a RANS turbulence model, a much coarser mesh will achieve mesh convergence when compared to models that allow resolution of some (or all) of the turbulence, which makes it relatively cheap. A constraint of RANS modelling is that the damping of fluctuations can have an adverse effect on the modelling of non-turbulent oscillations in flow (e.g. vortex shedding). As a consequence, RANS models are less accurate if the flow is not steady-state.

A general drawback of modelling turbulence, that is particularly true of RANS models, is that flow developments that are dependent on variations in turbulence may not be captured accurately. Flow separation and instabilities such as salt-fingering, Kelvin-Helmholtz instability, Rayleigh-Taylor instability and Richtmyer-Meshkov instability, can be poorly predicted by inappropriate turbulence models as often they are triggered by the variations in shear created by turbulence.

For Large-Eddy Simulation (LES) turbulence models, turbulence is “filtered” such that ν_T only models sub-grid turbulence. The turbulent energy cascade has a linear decay within the sub-inertial range (see Figure 2.5). In this region, the turbulent kinetic energy is assumed to be proportional to the inverse of the eddy length-scale. Within a given element, assuming edge lengths are all within the sub-inertial range, the rate of turbulent dissipation can be estimated from the size of a representative

edge length.

Edge lengths within the sub-inertial range can be very small, especially near no-slip boundaries, so the required mesh resolution for LES modelling can be very high. Several intermediate forms of eddy viscosity turbulence model use the RANS definition of ν_T near walls, and transition to the LES definition in the free stream. Turbulence that follow this concept, with varying methods for controlling the transition from RANS to LES, include the Detatched-Eddy Simulation model (Spalart et al. [1997]), the Hybrid LES-RANS model (Rodi and Furey [2002]), the Partially-Averaged Navier-Stokes model (Girimaji [2006]), the Delayed-Detatched-Eddy Simulation model (Shura et al. [2008]) and the Scale Adaptive Simulation model (Menter and Egorov [2010]). These models allow resolution of turbulence in the free-stream without the expense of resolving turbulence close to no-slip boundaries. Because the turbulence within boundary layers are not resolved, these turbulence models are less accurate at predicting flow phenomena that are triggered by boundary layer turbulence, such as separation points along curved surfaces and hydraulic jumps.

For the modelling described within this research, two turbulence models were used: the standard $k - \varepsilon$ turbulence model (described by Launder and Spalding [1974]), and the Large-Eddy Simulation turbulence model (using the Smagorinsky model developed by Benthall [2003], which allows for an anisotropic eddy viscosity that gives better results for flow simulations on unstructured grids).

For the $k - \varepsilon$ turbulence model, turbulent kinetic energy, k , and the turbulent dissipation, ε , fields were solved for using the advection-diffusion equation:

$$\frac{\partial k}{\partial t} + U_j \frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j} \left\{ \frac{\partial k}{\partial x_j} (\nu_T + \nu) \right\} + \nu_T \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial U_i}{\partial x_i} - \frac{\nu_T}{\rho'} g_i \frac{\partial \rho'}{\partial x_i}, - \varepsilon \quad (2.18)$$

$$\begin{aligned} \frac{\partial \varepsilon}{\partial t} + U_j \frac{\partial \varepsilon}{\partial x_j} = & \frac{\partial}{\partial x_j} \left\{ (\nu_T + \nu) \frac{\partial \varepsilon}{\partial x_j} \right\} \\ & + C_{\varepsilon 1} \left(\frac{\varepsilon^2}{k} \right) \left\{ \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial U_i}{\partial x_i} - C_{\varepsilon 3} \nu_T g_i \cdot \frac{\partial \rho'}{\partial x_i} \right\} \\ & - C_{\varepsilon 2} \frac{\varepsilon^2}{k}, \end{aligned} \quad (2.19)$$

and then used to calculate the turbulent eddy viscosity:

$$\nu_T = C_\nu \frac{k^2}{\varepsilon}, \quad (2.20)$$

where:

$$C_{\varepsilon 1} = 1.0, \quad C_{\varepsilon 2} = 1.0, \quad C_{\varepsilon 3} = 1.0, \quad \text{and} \quad C_\nu = 0.4.$$

For the Large Eddy Simulation (LES) model, the eddy viscosity is calculated using an indicative length from the adaptivity process, $\mathcal{M}^{-1}$ (see Pain et al. [2001]), and the Smagorinsky coefficient, C_s , which is usually taken to be 0.1.

$$\nu_T = 4C_s^2 \left[\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial U_i}{\partial x_j} \right]^{1/2} \mathcal{M}^{-1} \quad (2.21)$$

2.4.2 Advection–diffusion and state equations

Salinity, S , was calculated using the advection–diffusion equation,

$$\frac{\partial S}{\partial t} + \frac{\partial}{\partial t}(u_i S) = \frac{\partial}{\partial x_i} \left\{ D \frac{\partial S}{\partial x_i} \right\}, \quad (2.22)$$

with linear equation of state used to calculate the density, ρ ,

$$\rho = \rho_{\text{ref}}(1 - \beta(S - S_{\text{ref}})). \quad (2.23)$$

A saline contraction coefficient of $7 \times 10^{-6} \text{ l/g}$ was used, which is appropriate for the range of salinities being tested. The reference density, ρ_{ref} , and reference salinity, S_{ref} , were defined on an case–by–case basis, depending on the properties of the fluids being simulated.

The diffusivity, D , was determined by assuming a turbulent Schmidt number, Sc_t of unity, Omstedt [2015]:

$$\text{Sc}_t = \frac{\nu_t}{D}. \quad (2.24)$$

2.4.3 Boundary conditions

All tank and nozzle walls were assumed to be free–slip,

$$\mathbf{u} \cdot \mathbf{n} = 0, \quad (2.25)$$

and the water surface was modelled using a free-surface boundary with a simple Dirichlet pressure boundary condition $p = 0.0$; This is a kinetic boundary condition which is derived by forcing a fluid particle following the flow at the free surface, to remain at the free surface:

$$\frac{\partial \eta}{\partial t} = \frac{\mathbf{u} \cdot \mathbf{n}}{\mathbf{n} \cdot \mathbf{k}} \quad (2.26)$$

where $\mathbf{k} = (0, 0, 1)$ is the vertical normal vector, η is the free surface height, $\mathbf{n}$ is the surface normal vector.

The nozzle velocity boundary condition was assumed to have a one-seventh power law profile, as an approximation to fully-developed turbulent pipe flow (Chant [2005]). For the VLES simulations, synthetic noise was introduced using methods described by Jarrin et al. [2006] and a Reynolds Stress profile defined using the methods of Panton [1997].

2.4.4 Discretisation

The incompressible Navier-Stokes equations were discretised on an unstructured tetrahedral mesh using a simple $P_1 - P_1$ (piecewise-linear continuous representation of momentum and pressure) finite element discretisation (Piggott et al. [2008]).

A control volume discretisation was used for the advection-diffusion of k , ε and salinity fields, as recommended by Hiester [2011] to minimise numerical diffusion. An implicit time discretisation was used for all fields, with an adaptive time-step calculated to give a maximum Courant number of 2.0 anywhere in the domain.

2.4.5 Domain

The model domain was the same size as the experimental tank used in the comparison physical model (see Table 2.1). Outfall pipes are assumed to be 16-sided extrusions, to avoid excessive resolution from the adaptivity algorithm.

2.4.6 Mesh adaptivity

Unstructured anisotropic adaptive remeshing was used to optimise the mesh during the course of the simulations. The aim of using adaptive meshing was to produce a mesh that efficiently described the solution fields as flow develops in time. The suitability of the mesh was regularly re-assessed by the algorithm and the distribution of mesh resolution was optimised to increase simulation efficiency.

A flow chart showing the calculation steps of the adapt meshing algorithm is shown in Figure 2.6. The process can be split into three stages:

- The formation of a metric that describes the ideal distribution of mesh resolution,
- the optimisation of the mesh in order to produce this resolution,
- and the projection of the solution fields from the old mesh to the new.

The first stage (the metric formation) aims to define an ideal mesh for simulating the flow development from the current time until the next time at which the mesh will be adapted. It is assumed that the ideal mesh resolves all flow features evenly, with an even spread of error between the finite element description of the fields and the exact solution.

For a piece-wise linear continuous field on a continuous mesh, the error in approximating a field on a finite element mesh (i.e. the interpolation error, ϵ) is dominated by the second order term (based on a Taylor Series expansion of the field at a node). The interpolation error for a given field, ϵ_ψ , is given by:

$$\epsilon_\psi \leq \mathbf{v}^T |H_\psi| \mathbf{v}, \quad (2.27)$$

where H is the field Hessian (i.e. field curvature) on a mesh with edge lengths, $\mathbf{v}$.

The desired geometrical properties of the mesh needed to describe field, ψ , can be expressed by a tensor field “metric”, M_ψ . There are several methods for defining M_ψ , each incorporating in some way the field Hessian and a target interpolation error, $\hat{\epsilon}$ (see Pain et al. [2001] and Castro-Diaz et al. [1997]). For this modelling, the absolute error p -metric (developed by Loseille and Alauzet [2011]) was used:

$$M_\psi = \frac{|H|}{\hat{\epsilon}} \det|H|^{-\left\{\frac{1}{4+n}\right\}} \quad (2.28)$$

Hiester [2011] showed that a value of $n = 2$ (meaning that the metric was based on the L_2 norm) gives the most efficient response from the meshing algorithm. The exponential term in the equation encourages a skew in the error metric which encourages resolution in areas of both low and high curvature.

The metric, M_ψ , can be defined for any number of fields. The resulting set of M_ψ can then be consolidated into an overall M that incorporates all resolution requirements, by taking the minimum across all input field metrics. The desired edge lengths, l , within the mesh can then be determined by the eigenvalues, λ , of the metric, M :

$$l_i = \frac{1}{\sqrt{\lambda_i}} \quad (2.29)$$

Several geometrical constraints were applied to the mesh adaptivity algorithm to control the quality of the resulting mesh. A cap was applied to the maximum edge length that could be produced, and a lower limit applied to the minimum edge length. This was implemented by assigning limits to the size of the metric eigenvalues:

$$\lambda_i = \max\{\lambda_i, \lambda_{min}\}, \quad (2.30)$$

$$\lambda_i = \min\{\lambda_i, \lambda_{max}\} \quad (2.31)$$

The maximum edge length cap was dictated by the dimensions of the domain. A cap of approximately one third of the height of the domain was applied to avoid impractically large edge lengths. Close to the inlet pipe, the cap was lowered to be approximately half the inlet diameter, in order to avoid high aspect ratio elements in this region. The minimum edge length cap limited the size of edge lengths at areas of especially high field curvature. This avoided impractically small edge lengths being caused by sharp steps within a field.

Element anisotropy was constrained by capping the aspect ratio, a , of the eigenvalues:

$$\lambda = \max \left(\lambda, \frac{1}{a^2} \max(\lambda) \right) \quad (2.32)$$

where “i” is the index of the eigenvalue that is being filtered, and the second term with the “j” index is the maximum eigenvalue of the tensor.

A gradation algorithm was used to smooth sharp changes in the metric. The growth rate of edge lengths along an edge was capped to be less than 1.3. This is imposed by looping over all node pairs in the mesh and altering the edge lengths to meet the constraint (Li [2003]). Both the limit on aspect ratio and gradation rate were put in place to avoid a deterioration in mesh quality

Finally, metric advection is used to estimate the resolution requirements in the intervening timesteps between the current time and the next mesh adapt (Wilson [2009]). The advection–diffusion equation is solved for each component of the metric, using the velocity field output from the solved momentum equation.

Once a metric has been formed, the stage of optimising the existing mesh begins. Rather than perform the very expensive process of re-meshing the entire domain from scratch, the method used at this stage was to incrementally improve the existing mesh. This was performed using optimisation library libadaptivity (Pain et al. [2001]). A functional is defined which measures the degree to which the mesh satisfies the metric, M . The mesh is then assessed in clusters of elements, with trials performed for a series of local mesh operations, to calculate how to best alter the existing mesh to meet the new requirements.

The mesh can either undergo:

- vertex movement,
- edge splitting, a new vertex is created at the centre of an edge,
- edge collapsing, a vertex is removed and surrounding elements are merged,
- edge swapping, where adjacent elements have edges swapped, without changing the number of vertices,
- face and edge swapping, converting a convex interior face to an edge,
- edge and face swapping, the reversal of the above operation,

Once the mesh optimisation process is complete, the final stage is to map the fields from the old mesh to the newly adapted mesh. This was performed using consistent interpolation, which uses the mesh basis function to estimate the field values at the new vertex positions. This method is standard amongst the adaptive meshing community. It is non-conservative but bounded, and considerably cheaper than the alternative, Galerkin projection, which requires the creation of a super-mesh of the old and new mesh, together with a further finite element solve.

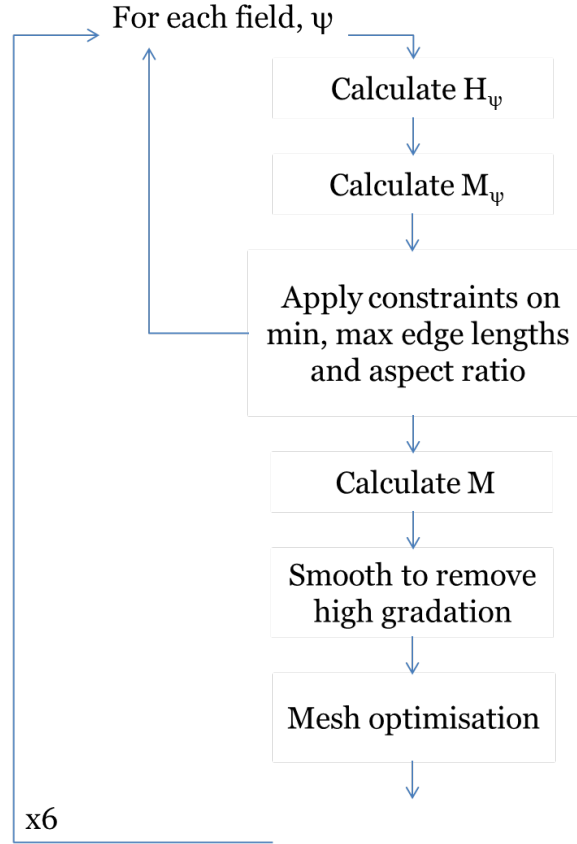


Figure 2.6: A flow chart showing a calculation stages of the mesh adaptivity algorithm

2.4.7 Domain partitioning

The simulations described in this chapter were all solved using parallel processing. Fluidity has been developed to offer both Zoltan (Devine et al. [2002]) and SAM (Gorman et al. [2009]) load-balancing algorithms. These algorithms divide the model domain into partitions that (ideally)

exert an equal computational load on the specified number of processors. This operation is performed once at the start of a simulation, and then again after every mesh adapt. Zoltan is the default partitioner when using Fluidity, as it offers a wide range of partitioning libraries (ParMETIS, PT-Scotch, as well as its own graph and hypergraph partitioners), and can partition high-order, discontinuous and control volume elements.

SAM partitioner can only partition piece-wise linear elements using the ParMETIS library, and so has limited application. An advantage of its simplicity is that it requires fewer halo elements at partition boundaries. During mesh adaptivity, halo elements are necessarily fixed in their position. If the proportion of fixed nodes to free nodes becomes too high, the mesh adaptivity algorithm will struggle to deliver a suitable mesh. The SAM partitioner can offer a benefit if flow patterns are likely to result in long-thin partitions (such as jet modelling), where this ratio is most high. Sam partitioning was used for the jet simulations described within this research. At the current time, neither Zoltan nor Sam partitioning allow constraint of the shape of partitioning.

It is worth noting that AMCG is currently developing PRAgMaTic (Parallel anisotropic Adaptive Mesh ToolKit, Gorman et al. [2012]), an alternative to Zoltan and SAM, which will provide 2-d and 3-d anisotropic mesh adaptivity for the meshing of simplexes. One of the design goals of PRAgMaTic is to develop highly scalable algorithms for clusters of multi-core and many-core nodes.

2.5 Results

2.5.1 Horizontal buoyant jet

Three different adaptive meshes were tested with resolution effectively doubled between each test to establish mesh convergence. Simulations were run for ~20 seconds to allow the jet to develop and establish approximate equilibrium. Speeds and salinities predicted using the finest mesh are shown at the end of the simulation along a vertical slice through the jet centreline in Figure 2.7.

Time-averaged results were used to derive properties along the jet centrelines. A comparison with CorJet is shown in Figure 2.8. The predicted centreline trajectories and decay of velocity for each of the Fluidity predictions match closely with each other, which suggests that mesh

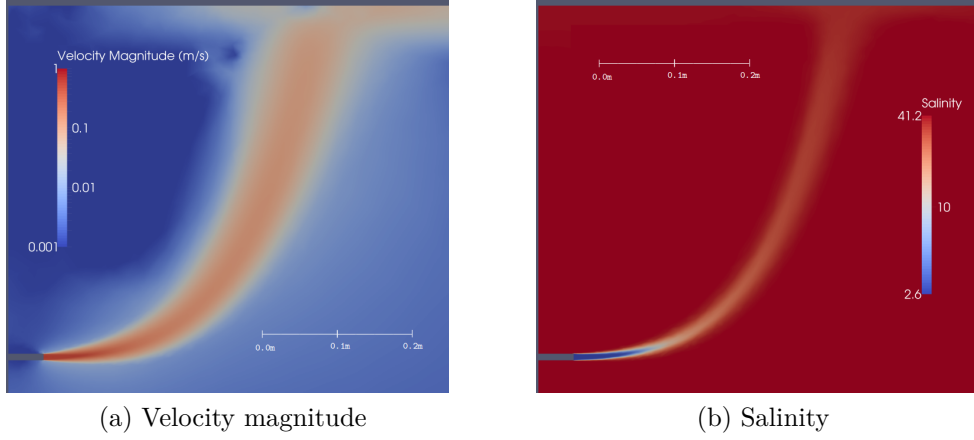


Figure 2.7: Buoyant jet model results on a 2-d plane through the domain. $k - \varepsilon$ turbulence model and finest mesh

convergence has been achieved. The Fluidity predictions are in reasonable agreement with those of CorJet, although there appears to be a tendency for Fluidity to dissipate momentum more rapidly, close to the nozzle, compared with CorJet. This is apparent from the tail-off of the centreline velocity that begins at around $x/d = 5$ for Fluidity, whereas the CorJet centreline velocity begins to tail off at $x/d = 7$. This region is within the so-called zone of flow establishment, which typically lies 5–10 nozzle diameters downstream (Jirka [2004]). It might be expected that some small differences would be observed between the two models in this region.

2.5.2 Angled dense jet

Tests with a dense jet have also been carried out using $k - \varepsilon$ turbulence closure schemes and V-LES, with simulation lengths of over 20 s, as was performed for the buoyant case. Testing of the dense jet is still underway, and so far mesh convergence has yet to be established. Results of the finest mesh tests are presented here, and mesh convergence will be established and reported separately.

Speeds and salinities predicted by the $k - \varepsilon$ test are shown along a vertical slice through the jet centreline in Figure 2.9.

Time-averaged results were used to derive the following along the dense jet centrelines: terminal rise height, bed impact distance and minimum bed impact dilution. A comparison of the predictions with experimen-

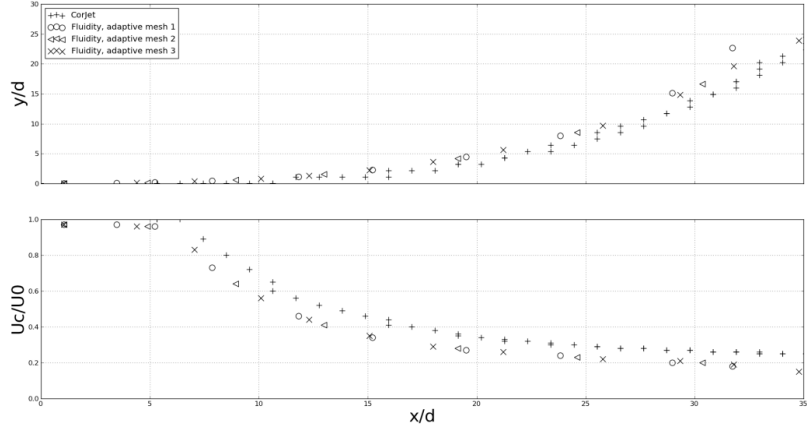


Figure 2.8: Buoyant jet comparisons: normalised centreline trajectories (top) and normalised centreline velocity decay with distance downstream (bottom). Adaptive mesh 1 is the coarsest and 3 is the finest.

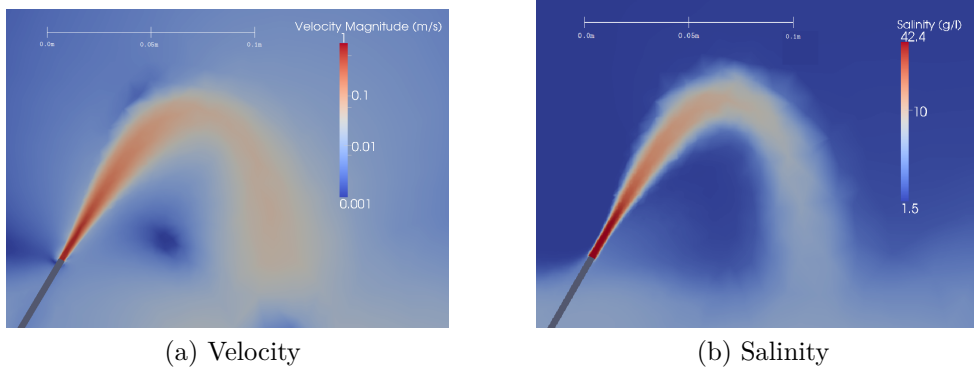


Figure 2.9: Dense jet model results on a 2-d plane through the domain. $k - \varepsilon$ turbulence model and finest mesh (convergence not established)

tal data is shown in Figure 2.10. The preliminary predictions notably under-predict the terminal rise height, impact distance and minimum impact dilution when compared with the experimental data. This indicates that too little ambient fluid is being entrained into the jet and, as a result, the simulated jet is more concentrated (and denser) than it should be. The V-LES simulation compares somewhat more closely with the experimental data than the $k - \varepsilon$ simulation. This is likely due to numerical diffusion in the solution, leading to higher entrainment, due to the relatively low spatial resolution of the preliminary V-LES simulation. Future simulations will investigate the role of mesh resolution in controlling the rate of entrainment in both cases.

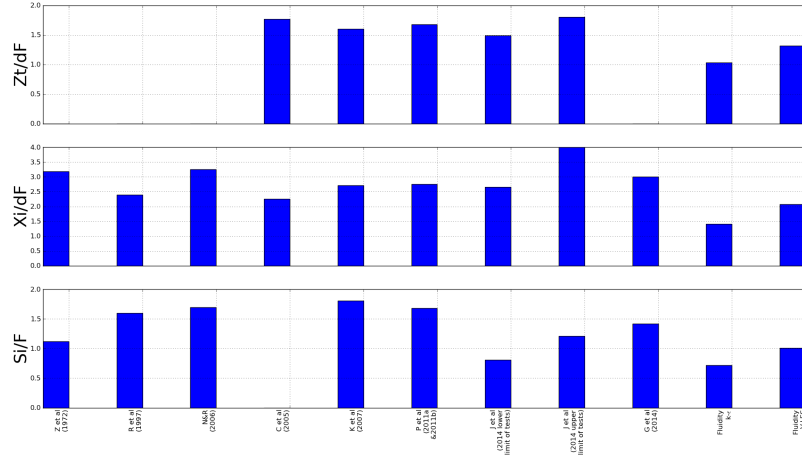


Figure 2.10: Dense jet comparisons: normalised centreline terminal rise heights (top), impact points (middle) and impact dilutions (bottom)

2.6 Discussion

2.6.1 Accuracy of results

This chapter has presented the results of testing to assess the suitability of the Fluidity CFD software (and the associated mesh adaptivity tools) for modelling the near-field mixing of jets. Two standard test-cases for jet dispersion were simulated: the buoyant jet (often associated with power station, or combined power and desalination discharges), and the dense jet (commonly associated with desalination plant discharges). Test conditions were based on release into stagnant homogeneous ambient receiving water. In each case predictions were compared with published laboratory data, or the predictions of validated integral models.

Centreline predictions for the buoyant jet compared well with the integral model CorJet. Further work will investigate different discharge flow rates, buoyancies and ambient currents. The preliminary results here are encouraging, and suggest that the software is a suitable tool for simulating the near-field mixing of buoyant jets.

2.6.2 Impact of mesh adaptation for jet modelling

Mesh adaptivity offers a way to achieve a user specified accuracy at minimum computational cost. While the benefit may be marginal for

relatively simple problems, it is a critical numerical method for problems with strong multi-scale features, whether they be transient or time independent.

A mesh is usually generated using a mesh generator that in general knows nothing of the numerical requirements of the model. When using a mesh generator, a user has to make judgements of which regions require fine resolution, and which regions do not. This judgement requires some *a priori* knowledge of the flow in order to account for the resolution requirements during the course of the simulations. This can require several iterations of the mesh (and re-running of the simulation) to get right for more complicated flow. Usually the metric for success is a stable solution that looks plausible. This heuristic methodology is inherently flawed, and some regions will be un-necessarily resolved whilst others (possibly more problematically) will be under-resolved. This can be addressed by reviewing errors after a simulation is complete, as well as performing mesh sensitivity testing, but it is still rarely easy to manually generate a suitable and efficient mesh for modelling complex flow. The user experience for mesh generation is important; The user should feel confident that they are reliably generating a suitable and efficient mesh for use within their model.

Mesh adaptivity simplifies and automates the entire process by basing mesh resolution on the generation of formal error metrics. Local modifications to the mesh are made during the simulation to control spatial discretisation errors.

For a representative jet simulation, Figure 2.11 shows the calculated velocity field at a point during the simulation, and the mesh produced by the mesh adaptivity algorithm. It can clearly be seen that away from the jet mixing the mesh edge lengths are relatively large, whereas within the areas of high mixing, and so high field curvature, the edge lengths are relatively short.

The main draw-back of mesh adaptivity is its effective use. The mesh adaptivity algorithm requires the user to prescribe parameters defining the ideal distribution of mesh resolution. In practice, the definition of this ideal distribution requires patience, experience and skill. The inclusion of a mesh adaptivity algorithm adds a non-linear operation to the solving of the already non-linear partial differential equations. Typically, numerical models are a balance between stability, speed and accuracy (you rarely get all three). Particularly when using mesh adaptivity, it can be difficult to keep control of all of these three parameters simultaneously. Also,

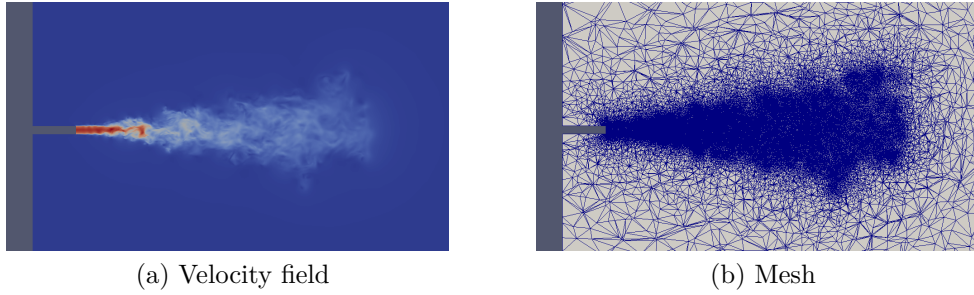


Figure 2.11: The velocity field for a neutrally-buoyant jet simulation, and the resulting mesh produced by the mesh adaptivity algorithm.

the extra layer of complexity makes error diagnosis considerably more difficult, because the symptoms of model failure are not always easily relatable to an underlying cause.

Many features have been added to the mesh adaptivity algorithm available within Fluidity, so that the user can constrain several of the mesh properties, and so control the quality of the output mesh. Also multiple error messages have been added to the algorithm, to assist in the diagnosis of failures. For the modelling described in this chapter, it was necessary to go through several iterations of model design in order to create a configuration that usefully drove the algorithm to produce a suitable mesh (advice for how to do this is given in the next section).

The proportion of time that is spent in solving the adaptivity algorithm can be changeable, but indicative numbers when using Fluidity were published by Hiester [2011], showing that it was typically between 20–30 %. The aim of using mesh adaptivity is that this time is more than offset by the resulting drop in the number of nodes necessary to achieve a given resolution (compared to a mesh generated manually).

Whilst it is difficult (if not impossible) to quantify guidelines, my experience from the modelling performed for this chapter is that mesh adaptivity offers less benefit to the efficient running of a CFD model if:

- the user can easily identify and describe the regions of the domain that require high resolution (in which case multi-scale mesh generation may be useful),
- flow features requiring higher resolution are steady and stay in generally the same place within the domain during the course of the simulation,
- enough computational resources are available so that having some areas of unnecessarily high resolution is not restrictive, and
- you have a good enough mesh generation capability.

The simulations described within this chapter had readily predictable and simply describeable mesh requirements. The benefits of the mesh adaptivity for these simulations were less than would possibly would occur for jet simulations of more complex ambient conditions or outfall designs. It would be an interesting extension of this work to investigate the benefits for more complex outfall configurations.

2.6.3 Best-practice guidelines for combining turbulence modelling, parallel processing, and mesh adaptivity for jet modelling

The jet simulations described within this chapter combined parallel processing, turbulence modelling, and mesh adaptivity to bring down run times. Each of these methods required some expertise to use effectively. When used in combination they influenced each other, and this added significant further complexity to their effective use.

When starting-off with a new simulation where one hopes to combine these tools, it is important that the first simulations are conservative. Using mesh adaptivity, parallel processing and turbulence modelling all at once will create far too much opportunity for user error, and make error diagnosis almost impossible.

The first simulations to be attempted are advised to have the same scale and flow rates as the final scenario to be modelled, but with considerable simplification. They should:

- use a relatively high-resolution static mesh,
- if possible be two-dimensional, in order to lower the number of degrees-of-freedom that need to be solved, allowing quick iteration of important parameters,
- use no more than a moderate number of partitions (i.e. greater than 10,000 degrees of freedom per partition). Mesh adaptivity usually requires that nodes sitting on partition boundaries are kept stationary. Too few nodes per partition can cause the mesh adaptivity algorithm to return a bad quality mesh;
- and have no turbulence model. A constant eddy viscosity should be used that gives a $Re_D \sim 100$ (see Equation 2.7). This is outside of the turbulent regime, but not too viscous that the pressure field becomes unstable.

This initial set of simulations provides the user with some trust that the domain, boundary conditions, discretisation and solver methods are appropriate for the problem at hand. Once this has been confirmed, it is recommended that one change be made at a time, e.g. a turbulence model should be introduced, whilst maintaining at first a relatively low Reynold Number. Also, it is advised that mesh adaptivity be first introduced to the 2-d simulation (before progressing to three dimensions), to allow easier calibration of the target interpolation errors.

For simulations with multiple active fields, such as the jet simulations described in this chapter, there is the option to adapt to more than one field (see Section 2.4.6). This choice of which fields to include and what interpolation error to prescribe to each is not straight-forward. An assessment needs to be made of the relative influence of each field's resolution on the overall accuracy and stability of the simulation. Often, when using mesh adaptivity, it has been considered sufficient to adapt only to the velocity field. This has the benefit that it simplifies the use of the mesh adaptivity algorithm, with only one term controlling resolution (and needing calibration). This simplification makes the assumption that curvature of the remaining fields are either small, or a mesh that sufficiently resolves velocity is also sufficient for the other fields.

Unfortunately, these last two assumptions are rarely true for free surface (or multi-phase) flow, tracer advection, or simulations with fields related

to eddy viscosity (k , ε , ω , etc.). For the jet simulations described within this chapter, it was found that the resolution of the k , ε and salinity fields were significantly influential on the final accuracy and stability of the solution, and that the curvature of these fields was not well approximated by the curvature of the velocity field.

In order to improve stability and produce a mesh that more evenly resolved all the influential fields, for the simulations described in this chapter, the target interpolation error for u , v , w , k , ε and salinity were set to be equal. This calibration of relative target interpolation errors will most likely not be appropriate for all turbulent simulations. Generally speaking, it is advisable to compare the regions of high curvature in all active fields to assess which fields need to be accounted for by the mesh adaptivity algorithm. Ideally, to create an optimally efficient mesh, a convergence test could be performed for each field in turn, to establish their relative influence on model accuracy. It might often be sufficient to perform this assessment on a simplified 2-d version of the simulation, if run-times are large in 3-d. Sometimes, in especially coarse simulations, it was found that although some fields had lesser influence on the accuracy of indicative flow quantities, it was necessary to maintain a minimum smoothness to the field in order to keep solver stability. This was particularly the case during these jet simulations for k and ε , which had high field curvature near the jet nozzle but relatively low curvature elsewhere in the domain. A minimum interpolation error was necessary for these fields in order to avoid divergence when solving their respective advection-diffusion equations.

The interval between adapts has an influence on the effectiveness of mesh adaptivity. Adapting regularly means less of the domain needs to be highly resolved, as regions of complexity requiring additional resolution will migrate less far between adapts. This benefit needs to be balanced against the expense of calling the mesh adaptivity algorithm, which will increase for regular adapts. A further disadvantage of adapting the mesh is that the interpolation of fields between meshes introduces numerical diffusion, which can have a significant effect on model accuracy if performed too frequently. Generally speaking, adapting the mesh regularly can be efficient when the simulation contains quickly moving fronts (especially if the rest of the domain is fairly benign), but will not be a benefit for simulations with relatively steady features (say, flow over a bump), or large areas of interest (say, flow within pumping stations). During the jet simulations described within this chapter, the mesh was adapted once every 10 timesteps, with metric advection (described by Wilson [2009]) used to predict resolution requirements between adapts.

Metric advection uses the velocity field from the current timestep to predict the mesh resolution requirements between the current timestep and the next mesh adapt. The error metric is effectively “pushed” ahead of the flow to avoid regions of high curvature becoming badly resolved between mesh adapts.

In the immediate vicinity of the inlet, all fields have a very high curvature perpendicular to the flow direction and a relatively low curvature in the direction of flow. If left unconstrained, this would lead the mesh adaptivity algorithm to return very long–thin elements running parallel to the flow, with a high gradation perpendicular to the flow. The resulting pressure matrix would be ill–conditioned (or “stiff”), which would either cause a significant increase in the number of solver iterations needed to converge (increasing run time rather than lowering it) or more often cause a fatal divergence of the solver. It was found that limiting the element aspect ratio to be less than 2.0 and the edge length gradation to be less than 30% was necessary to limit the ill–condition of the pressure matrix.

Parallel processing allows a numerical model to be partitioned and solved simultaneously by multiple processors. The aim is to speed–up the time taken for a simulation to complete by sharing the workload. Ideally, the speed–up of a simulation solve by parallel processing is linearly related to the increased number of processors. However, inter–processor communication will generally mean that perfect parallel efficiency is not achieved, i.e. adding extra processors does not linearly increase the speed of solving. This lack of linearity will degrade further with the addition of more processors for a fixed problem size. Consequently, for any given simulation there will be an optimum number of processors for solving most quickly. When using parallel computing, it is usual to perform a quick assessment of the optimum number of processors, solving a few timesteps of the simulation on a range of possible processor numbers, and comparing their speed.

The use of mesh adaptivity together with parallel processing adds further constraint to the optimum number of processors. For each iteration of the mesh adaptivity algorithm the elements on partition boundaries (halo elements shared by partitions) are fixed in place. The partition boundaries are re–drawn with each iteration, so halo elements will be adapted, but still, as the number of partitions increases, the number of fixed nodes within the mesh increases. For a given partition, if the ratio of fixed to free nodes too high, then the adaptivity algorithm will fail, or produce a low quality mesh. This affect is particularly acute for long–thin partitions, where the surface to volume ratio is relatively high. Because

of the inherent shape of jet flow, these long–thin partitions are particularly common for these simulations. This may create a upper limit for the number of partitions that is less than that predicted to be optimal by scaling analysis.

Pressure matrix preconditioning is also affected by adaptivity and partitioning. The jet simulations described in this research have used the geometric agglomerated algebraic multigrid (GAMG) preconditioner because this is better at handling meshes with a large range of edge lengths. Despite the advantages of the GAMG preconditioner, it does not perform solution smoothing across partitions. This means that solver iterations may increase significantly as the number of partitions is increased, especially where those partitions are long and thin.

2.6.4 Future Work

More work is required on the dense jet test case; simulations so far have under–predicted the rate of entrainment, leading to the over–prediction of concentrations in the rising and falling phases of the jet. On–going work is examining the importance of the computational mesh in governing the rate of entrainment, and the revised predictions will be validated against data and reported separately. It would also be preferable to make direct comparisons with the recently published studies of Gildeh et al. [2014] and Jiang et al. [2014].

Further work is required to establish whether the Fluidity offers suitable solutions in cases where standard near–field models are less applicable (e.g. unstable mixing). This could include work to investigate different discharge flow rates, buoyancies and ambient currents.

2.7 Conclusions

This preliminary work has shown that with modest parallel computing resources and expertise, high–resolution simulations of jet dynamics can be achieved with reasonable accuracy using CFD modelling. Clearly, standard parameter–based near–field models are less computationally expensive, and for scenarios that lie within the limits of their validity, they offer suitably accurate predictions of key jet parameters.

3 Tidal modelling of the North–West European Continental Shelf

3.1 Introduction

Tides within the ocean are generated by the gravitational interaction of the ocean, Earth, Moon and Sun. The Moon orbits the Earth, the Earth rotates about its axis, and the Earth orbits the Sun. These rotations cause cyclical variations in the gravitational forces acting on the ocean, which in turn generate a series of the long period, long wavelength waves that perpetually travel the globe.

Tidal models predict the motion of tides within the ocean. Because tidal waves have such long periods and large wavelengths, tidal models must represent large sections of the ocean, if not the whole globe, and simulate several days, if not months of wave propagation. Regional ocean flow models at smaller scales typically account for tides by using elevation and / or velocity boundary conditions derived from larger scale tidal models.

This chapter presents the validation of a European continental shelf tidal model, using open–source CFD code Fluidity. The purpose of this validation study was to confirm that Fluidity could accurately generate the tidal forcing boundary conditions for a far–field model of effluent dispersion from a hypothetical outfall situated off the coastline of the North–East of the United Kingdom, in the North Sea.

This chapter presents a model of tidal flow within the European continental shelf, with a comparison of results to a large database of tide gauge measurements. This model took advantage of recently published methods for ocean model meshing and coastline resolution reduction. The purpose of this study was to confirm that these methods offered a benefit to model accuracy and efficient, and also that Fluidity could be used to accurately generate the tidal forcing boundary conditions for a far–field model of effluent dispersion at a hypothetical outfall site.

The position of the hypothetical outfall was assumed to be 53.97°N latitude, -0.10°E longitude, which is approximately 3 km from the UK coastline. A map of the United Kingdom showing the position of hypothetical outfall is shown in Figure 3.1. This section of coastline is highly industrialised and as such outfalls in this area are very common.

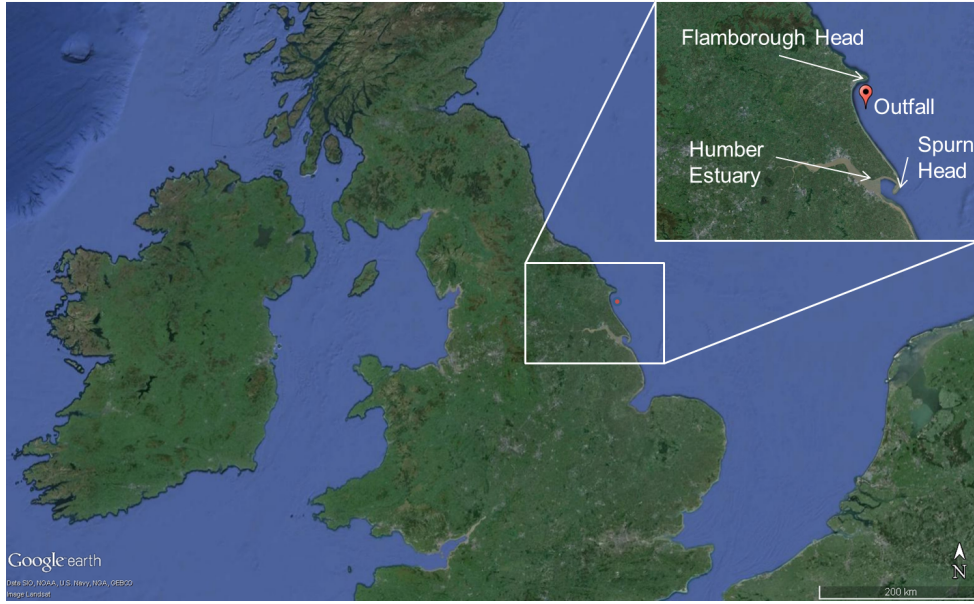


Figure 3.1: Assumed position of the hypothetical outfall, off the coastline of the North-East of the United Kingdom, in the North Sea, Google Earth [2015]

In order to understand the forces that generate tides, we need to first start with Newton’s Law of gravitational attraction, which states that the gravitational force, Φ , between two objects is given by:

$$\Phi = G \frac{m_1 m_2}{r^2}, \quad (3.1)$$

where the gravitational constant $G = 6.67 \times 10^{-11} \text{ N m}^2 \text{ kg}^{-2}$, m_1 and m_2 are the masses of the two objects in kilograms (say, for the purposes of our example, the Earth and Moon), and r is their distance apart in metres.

This gravitational force is a conservative vector field, and so can be written as the gradient of a scalar potential. The gravitational potential is the work required to move a unit mass from its current position to a position an infinite distance away. Then, if we assume that the Earth is

spherical, this potential can be written as a function of the distance from the centre of the Earth, r :

$$\Phi = -\nabla\Omega \quad (3.2) \quad , \text{ where } \Omega = -G\frac{m_2}{r}. \quad (3.3)$$

If point P is an arbitrary point on the Earth's surface, at an angle ϕ , relative to a line between the Earth and Moon, the potential at point, P , can be written:

$$\Omega_P = -G\frac{m_2}{R} \left[1 - 2\left(\frac{r}{R}\right)\cos\phi + \left(\frac{r}{R}\right)^2 \right]^{-1/2}, \quad (3.4)$$

where R is the distance between the Earth and Moon. A schematic is shown in Figure 3.2.

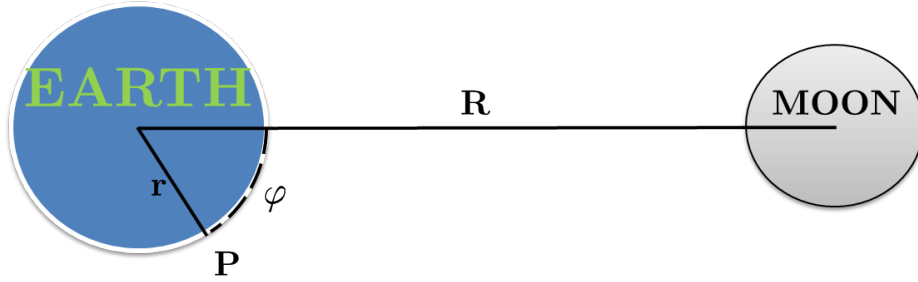


Figure 3.2: A schematic of tide force.

The terms in the brackets can be expanded-out using a Taylor series expansion of the Legendre polynomials, P_n , defined via:

$$\frac{1}{\sqrt{1-2xt+t^2}} = \sum_{n=0}^{\infty} P_n(x)t^n, \quad (3.5)$$

giving,

$$\begin{aligned} \Omega_P = & -G\frac{m_2}{R} \left[1 + \left(\frac{r}{R}\right)P_1(\cos\phi) \right. \\ & \left. + \left(\frac{r}{R}\right)^2 P_2(\cos\phi) + \left(\frac{r}{R}\right)^3 P_3(\cos\phi) + \dots \right], \end{aligned} \quad (3.6)$$

where the Legendre polynomials are:

$$\begin{aligned}
P_1(\cos\phi) &= \cos\phi, \\
P_2(\cos\phi) &= \frac{1}{2}(3\cos^2\phi - 1), \\
\text{and} \quad P_3(\cos\phi) &= \frac{1}{2}(5\cos^3\phi - 3\cos\phi).
\end{aligned}$$

The distance between the centre of the Earth and Moon is approximately 60 times the radius of the Earth ($r/R \sim 1/60$), meaning that terms beyond P_3 can be reasonably neglected. Remembering that it is the gradient of this potential that produces the tide, the first two terms produce a zero and constant force, respectively. The zero force term clearly results in no force. The constant term describes the force keeping the Earth and Moon about a common centre of mass (and so does not generate tides). This leaves the third term alone describing the tidal generating potential:

$$\Omega_P = -\frac{1}{2}Gm_2\left(\frac{r^2}{R^3}\right)(3\cos^2\phi - 1) \quad (3.7)$$

The derivatives of this potential with respect to r and ϕ give the local vertical and horizontal components of the gravitational force experienced by the ocean:

$$F_P^{\text{vert}} = -\frac{\partial\Omega_P}{\partial r} = Gm_2\left(\frac{r}{R^3}\right)(3\cos^2\phi - 1), \quad (3.8)$$

$$F_P^{\text{horiz}} = -\frac{1}{r}\frac{\partial\Omega_P}{\partial\phi} = -\frac{3}{2}Gm_2\left(\frac{r}{R^3}\right)\sin(2\phi). \quad (3.9)$$

Both these terms imply that the gravitational pull of the Moon will create two bulges in the Earth's ocean, one at the closest point to the Moon ($\phi = 0^\circ$) and one at the furthest point ($\phi = 180^\circ$), with a ring of ocean between the two having a low water level. A similar set of bulges is generated by the gravitational pull of the Sun on the ocean.

A time dependency now needs to be added to these equations because the Earth, Moon and Sun are not stationary. To include the time varying aspects it helps to re-form the angle, ϕ , into constituents:

ω = the latitude of P

θ = the angle between the Moon and the equator, and

α = the angle between the Moon and the Greenwich Meridian (perpendicular to the equator).

ϕ can then be re-formed as: $\cos\phi = \sin\omega\sin\theta + \cos\omega\cos\theta\cos\alpha$

substituting this back into the potential equation gives:

$$\Omega_P = -\frac{Gm_2}{r} \left[\frac{1}{2}C_0(3\sin^2\theta - 1) + \frac{1}{3}C_1\sin(2\theta) + \frac{1}{3}C_2\cos^2(\theta) \right] \quad (3.10)$$

where:

$$C_0 = \frac{3}{2} \left(\frac{r}{R} \right)^3 (\sin^2\theta - 1/2), \quad (3.11)$$

$$C_1 = \frac{3}{4} \left(\frac{r}{R} \right)^3 \sin(2\theta)\cos\alpha, \quad (3.12)$$

$$C_2 = \frac{3}{4} \left(\frac{r}{R} \right)^3 \cos^2\theta\cos(2\alpha). \quad (3.13)$$

This explanation of the forces that generate tides was based on that published by Pugh [1987]. His book gives a thorough and clear explanation of tidal forces and motion, and includes useful advice for tidal modelling.

Equations (3.10) - (3.13) describe the gravitational forces that the ocean experiences, but not the motion that happens in reaction to those forces. In practice this motion is extremely complex, mainly because the Earth is not completely covered in ocean, and some of the ocean is not very deep. This means that the land “gets in the way” of the tides, causing tidal flow to be heavily distorted in some areas of the ocean. Also, the speed of tidal waves is limited, particularly in shallow water, causing a lag in reaction to the changing gravitational force that can be difficult to predict.

The tide at any particular point in the ocean is often assumed to be constructed of many super-imposed constituents, each having a sinusoidal variation in time, with a given period and amplitude. The three terms, C_0 , C_1 and C_2 , are responsible for three categories of tidal constituent. The first term, C_0 , is only a function of θ , which varies as either the Earth

orbits the Sun, or the Moon orbits the Earth. This happens over a period of order weeks to years, so this term represents the “long-period” tides. The second term, C_1 , also varies with θ , but includes α , which is dependent on the daily rotation of the Earth about its axis. It appears in the form $\cos\alpha$ so varies once daily, and represents the “diurnal” tides. The third term, C_2 , again contains θ and α , but this time α appears in the form $\cos(2\alpha)$ and so varies twice daily, and represents the “semi-diurnal” tides.

A further fourth set of tidal constituents is generated by the higher harmonics of the tidal constituents from the three previously mentioned categories. In areas where the tidal range is a significant proportion of the water depth (i.e. in shallow water), non-linear effects generate natural frequency modes of the dominant tidal constituents (in a similar way that playing a note on a musical instrument generates overtones of that note). So, for example, the M_2 tide (the lunar semi-diurnal tide) gives rise to constituents M_4 , M_6 and possibly M_8 (having a frequency two, three and four times the fundamental mode, respectively), with the amplitude of each subsequent tide being much smaller than its parent. The amplitude of shallow water overtides within the European continental shelf was investigated by Andersen [1999], using satellite altimetry.

The major diurnal tides are named O_1 , K_1 , M_1 , S_1 , P_1 and Q_1 . The major semi-diurnal tides are named M_2 , S_2 , N_2 and N_2 . Each of these tidal constituents are created by physical properties of the Earth, Sun, Moon and ocean, such as the elliptical orbits of the Moon and Earth, and their eccentric rotation about their axes. A list of the major constituents is given in Table 3.1, together with their period and a representative amplitude at site within the North Sea.

The tides created by the Sun and Moon have slightly different periods because of the direction and angular velocity of the Earth and Moon’s orbits. Relative to a fixed point in space (say, a distant star), the Earth rotates about its axis once every 23 hours, 56 minutes and 4 seconds. This is called a “sidereal” day. Because the Earth is also orbiting the Sun (in the same direction that the Earth spins), we see the Sun pass through the sky at a slightly longer period, exactly 24 hours (the S_1 period). The Moon is also orbiting the Earth (in the same direction that the Earth spins), but at a faster angular velocity, and so we see the Moon pass overhead at a slightly longer period, approximately 24 hours and 50 minutes (the M_1 period).

The tide in most areas of the ocean is dominated by the M_2 and S_2 tides.

The super-position of these two tides gives the effect of one tide, whose period is the average of the M_2 and S_2 periods, and whose amplitude varies between the summation and difference of the M_2 and S_2 amplitudes, with a period that is the product of the M_2 and S_2 periods. This later period is referred to as the Spring–Neap cycle, and is essentially the period between times when the Sun and Moon’s gravitational force work in the same direction.

The relative amplitude of tidal constituents varies across the Earth, especially at coastlines. The variation of the amplitude of the M_2 tide across the globe is shown in Figure 3.4. When constructing an ocean scale model which will be forced by tidal constituents, Pugh [1987] states that the choice of which tidal constituents to include is a “dark art”. Typically, models are tidal–forced by the constituents that have the greatest amplitude in the region of interest. The “ F ratio” is often used as a measure of which set of tides dominate for a given site:

$$F_{\text{RATIO}} = \frac{K_1 \text{amplitude} + O_1 \text{amplitude}}{M_2 \text{amplitude} + S_2 \text{amplitude}} \quad (3.14)$$

For places where $F_{\text{RATIO}} < 0.25$ the tides are considered predominantly semi-diurnal, for places where $0.25 < F_{\text{RATIO}} < 3.0$ then the tides are considered mixed, and for places where $3.0 < F_{\text{RATIO}}$ then the tides are considered diurnal. A map of the globe showing the predominance of diurnal and semi-diurnal tides is shown in Figure ?.

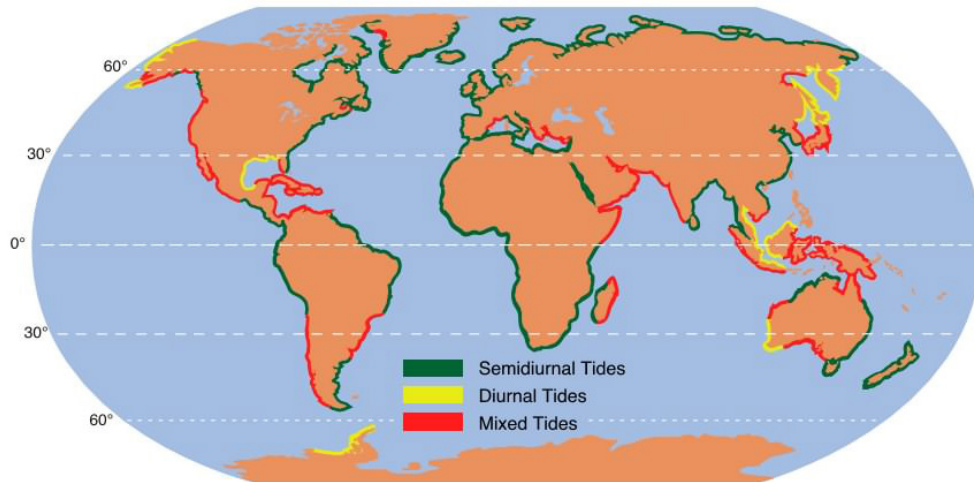


Figure 3.3: A map of the globe showing the predominance of diurnal and semi-diurnal tides, Pidwirny [2006]

Table 3.1: Tide constituents (NOAA)

	Symbol	Period	Example Amplitude (m)*
Principal lunar semi-durnal	M_2	12.42	0.274
Principal solar semi-diurnal	S_2	12.00	0.078
Major lunar elliptic semi-diurnal	N_2	12.66	0.057
Luni-solar declinational semi-diurnal	K_2	11.97	0.021
Principal lunar diurnal	O_1	25.82	0.029
Luni-solar declinational diurnal	K_1	23.93	0.021
Smaller lunar elliptic diurnal	M_1	24.84	0.006
Smaller solar elliptic diurnal	S_1	24.00	0.01
Principal solar diurnal	P_1	24.07	0.007
Major lunar elliptic diurnal	Q_1	26.87	0.015
Shallow water overtides of principal lunar	M_4	6.21	0.018
Shallow water overtides of quarter diurnal	MS_4	6.10	0.010

* Constituent amplitudes at a representative tide gauge from the middle of the North Sea, NOC.

3.2 A review of tidal modelling state-of-the-art

When constructing a model of effluent dispersion in the marine environment, the tidal boundary conditions are often derived from a tidal model of the surrounding region. This regional tidal model will be a much larger than the dispersion model, typically covering the whole of a continental shelf or an ocean. The boundary conditions for this regional tidal model can be defined using a global tidal model, which give low-resolution predictions of tides throughout the globe.

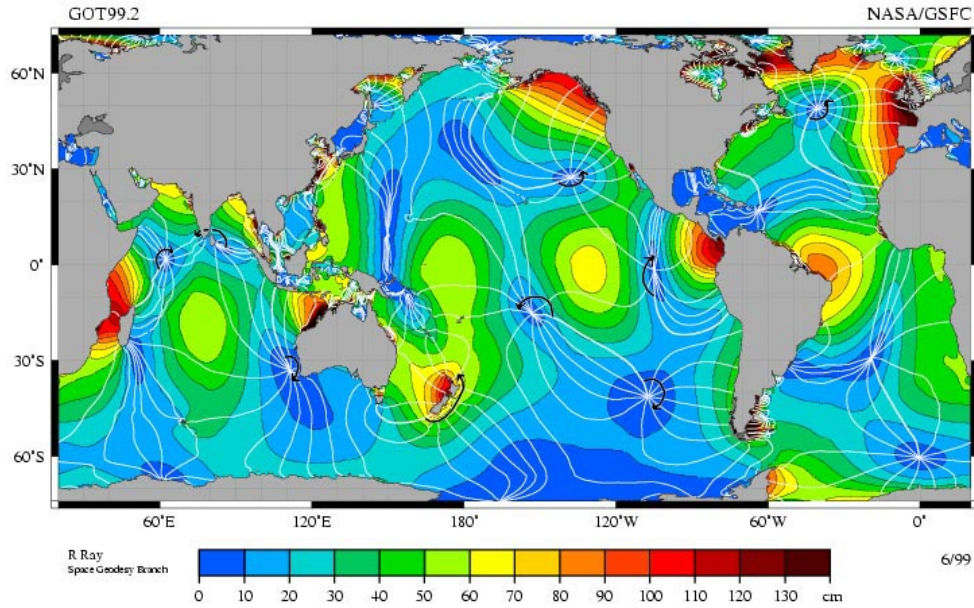


Figure 3.4: A map of the globe showing the variation in the amplitude of M2 tide Accad and Pekeris [1978] and NIWA. The amplitude is shown by colour, with blue indicating areas of low tidal range, and red showing areas of large tidal range. The white lines show hourly co-tides (lines of equal phase). The points where co-tides meet are known as amphidromes. At these points the tidal range for this constituent is nil. Tidal waves rotate about these points in the direction shown by the black arrows.

Global tidal models have been developed by several research groups, and are typically created in one of three ways (Zahran et al. [2011]):

- Empirical models interpolated from satellite altimetry data (Goddard Ocean Tide model, Ray [1999]).
- Purely hydrodynamical models with no data assimilation: FES1994 (Lefèvre et al. [2000]) and Fluidity(Wells [2008]).
- Mixed models with a hydrodynamical base but also assimilating data from satellite altimetry and / or tide gauges; TPXO (Egbert and Erofeeva [2002]), NAO (Matsumoto et al. [2000]), and FES2004 (Lyard et al. [2006]).

When creating a regional tidal model, the user must decide on suitable data for describing the coastline and bathymetry, and an appropriate mesh that leads to an efficient resolution of both. Coastline

and bathymetry information for a site-specific dispersion study is often bought from commercial sources such as SeaZone, as publicly available data is too coarse to create a suitable model. For larger tidal models such as the one described here though, publicly available data such as GEBCO and Wessel and Smith [1996] is usually suitable (more information on these data sets is given in later sections).

The optimal mesh resolution has been investigated by a number of researchers. Jones and Davies [2005] used TELEMAC to investigate an optimal mesh resolution for computing the M_2 tide in a region of significant geographical extent. Calculations showed that solutions at offshore tide gauges were not significantly affected by the choice of nearshore water depths (i.e. the water depth that defined the position of the coastline), or coastal grid refinements, however a water-depth based dependent criterion for determining element size gave an optimal distribution over the majority of the region. In shallow water, the wave speed is $\sqrt{gh}$ and so, if one is to aim for a uniform Courant number, then the mesh resolution should be proportional to the square root of the water depth. Le Provost et al. [1995] found that for a tidal period, T_P , the optimal grid requirement was,

$$\delta x \leq \frac{T_P \sqrt{gh}}{n} \quad (3.15)$$

where n , the number of vertices per wavelength, needed to be greater than thirty. Legrand et al. [2007] created a mesh refinement strategy based on this constraint, defining a suitable metric based on a privileged direction that runs perpendicular to bathymetry gradient. This inevitably leads to finer resolution in coastal areas, where the water is shallowest.

Greenberg et al. [2007] investigated resolution issues in numerical models of oceanic and coastal circulation and reported a list of issues that can effect the adequacy of model solutions. They highlighted the importance of keeping $\delta h/h$ small (≤ 0.3) in order to properly resolve shelf-breaks.

Shoreline databases typically come in uniform levels of resolution, which is not necessarily efficient for modelling purposes. Ideally, the coastline near to areas of interest and influence are given higher resolution than those that are not. The algorithm published by Douglas and Peucker [1973] for reducing the number of point required to represent a digitized line is the most common method used for modifying coastline resolution. This method though can create a coastline that is difficult to mesh without producing poor quality elements. The shoreline data used within this

study was simplified using the methods described in Avdis et al. [2015b], using Principal Component Analysis (PCA) to create a smoothed representation of the coastline.

The work described within this chapter is a re-investigation of a study published by Wells [2008]. The modelling described here solved the 2-d shallow water equations (rather than the more expensive method of solving the 3-d Navier–Stokes equations on a mesh one element deep used by Wells), with a more efficiently described coastline and mesh, and making use of parallel processing. Previous studies looking at tidal motion within the North–West European Continental Shelf were performed by Pingree and Griffiths [1981], Kwong et al. [1997], and Sinha and Pingree [1997].

3.3 Brief description of the tidal flow within the North–West European Continental Shelf

The North–West European Continental Shelf is a broad platform of bathymetry in the north-west of Europe (a Google Earth image is shown in Figure 3.5). It has an average depth of ~ 100 m, compared to depths in the surrounding Atlantic Ocean of > 500 m. The exception being the Norwegian Trench, which is a ~ 500 m deep elongated depression running along the Norwegian coast. This forms the main connection to the Atlantic Ocean from the shelf. The shelf includes the seas to the west of the United Kingdom (UK), the Irish Sea (running between the UK and Ireland) the North Sea (between the UK and France, Germany, and Scandinavia), the English Channel (connecting the Atlantic Ocean to North Sea), and the Baltic Sea & Gulf of Bothnia (enclosed by Scandinavia and the Baltic countries). The continental slope, defining the western edge of the shelf, runs from the South of France, around the UK, and northwards parallel to the coast of Norway.

Both the M_2 and S_2 semi-diurnal tides follow similar patterns. Tidal waves enter west, from the Atlantic Ocean, and travel quickly over the west coasts of Ireland and Scotland, before entering the North Sea along the east coast of Scotland. The tide then slows as it takes an anti-clockwise journey down the east coast of England, along the northern coastline of continental Europe, and then back up toward Norway. The tide that arrives from the Atlantic Ocean towards the South of Ireland, bifurcates between the English Channel and the Irish Sea. Maps of the M_2 tidal amplitudes and phases throughout North–Western European



Figure 3.5: A map of Europe showing the European Continental Shelf, Google Earth [2015]

continental shelf, as published by Wells [2008], are shown in Figures 3.6 and 3.7, respectively.

Amphidromic points, where the M_2 tidal range is nil, within the European continental shelf are in:

- the North Channel, between Northern Ireland and Scotland,
- the Southern North Sea, between East Anglia and the Netherlands,
- and the Eastern North Sea, near Denmark.

“Degenerate” amphidromic points (where the point appears to be over land, rather than in the sea) are in:

- the East Irish Coast, west of Cardigan Bay,
- the English Southern coast, near to the Isle of Wight,
- and the Southern Norwegian coast.

Tidal amplification occurs in several places around the North–Western European continental shelf around sheltered areas, channels and contractions. Notably, within the Bristol Channel, on the Northern coast of France, on the East coast of Scotland and England (especially within The Wash), and on the West coast of England (North of Wales).

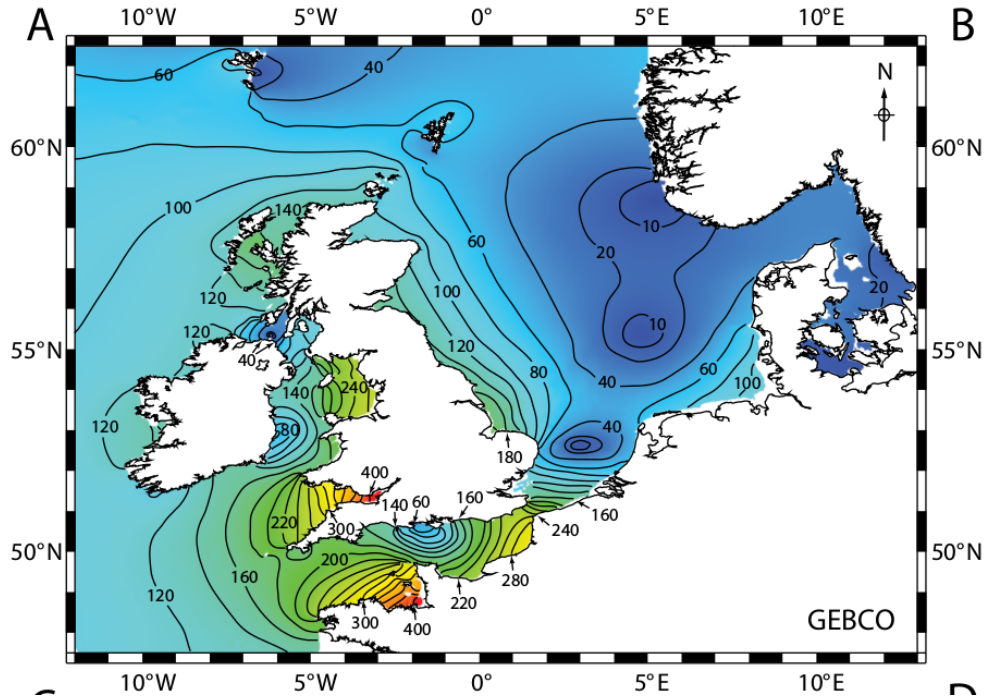


Figure 3.6: A map of the M_2 tidal amplitudes within the North–Western European continental shelf, as published by Wells [2008]

3.4 Model details

3.4.1 Model equations and their discretisation

The continuity and momentum were solved using the Shallow–Water equations, discretised on a $P_{1DG} - P_2$ finite element (piecewise–linear

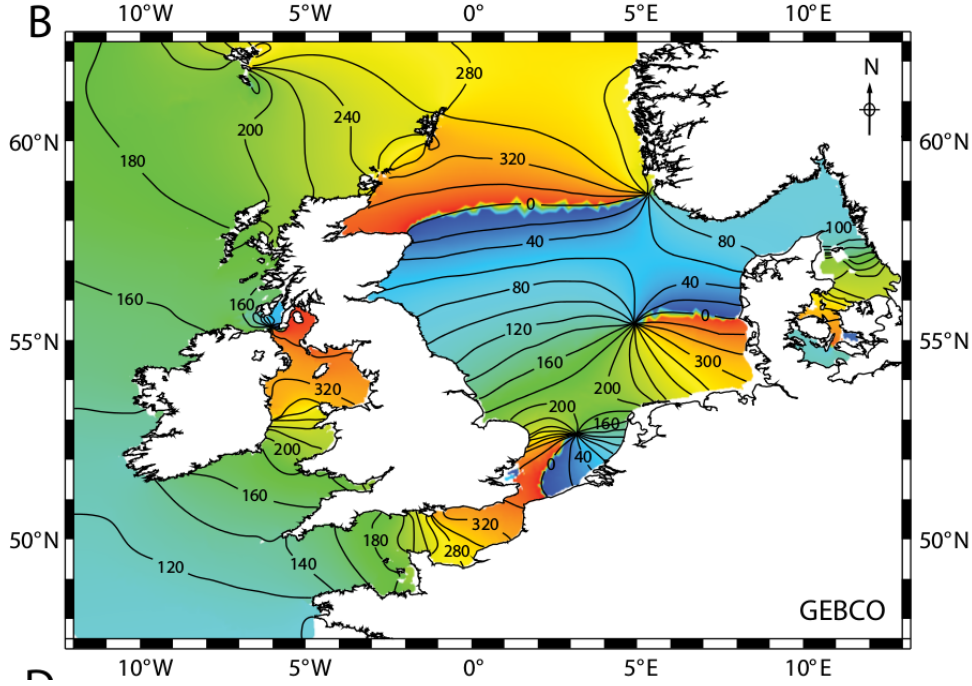


Figure 3.7: A map of the M_2 tidal phases within the North–Western European continental shelf, as published by Wells [2008]

discontinuous representation of velocity and piecewise–quadratic continuous free–surface).

Geostrophic balance is the balance between the horizontal pressure gradient and Coriolis accelerations. This element pair has the property that all geostrophically balanced states which strongly satisfy the boundary conditions have discrete divergence equal to zero and hence are exactly steady states of the discretised equations. This means that the finite element pair has excellent geostrophic balance properties (Cotter et al. [2009]). The higher degree of accuracy in the free–surface field minimises the error in the pressure gradients resulting from buoyancy and Coriolis accelerations. This gives a second–order accurate, LBB–stable discretisation without spurious pressure modes (Ladyzhenskaya [1969], Babuska [1971] and Brezzi [1974]).

The Shallow–Water equations assume a depth-averaged velocity, $\bar{\mathbf{u}}$, taken to represent the integral of the horizontal component of velocity, $\bar{\mathbf{u}}_H$ divided by the total water depth, h :

$$\bar{\mathbf{u}} = \frac{1}{h} \int_{z=b}^{z=\eta} \bar{\mathbf{u}}_H dz \quad (3.16)$$

leading to the continuity and momentum equations:

$$\frac{\partial \eta}{\partial t} + \nabla(h\bar{\mathbf{u}}) = 0 \quad (3.17)$$

$$\frac{\partial \bar{\mathbf{u}}}{\partial t} + \bar{\mathbf{u}} \cdot \nabla \bar{\mathbf{u}} + g \nabla \eta + C_D \frac{\|\bar{\mathbf{u}}\| \bar{\mathbf{u}}}{h} = 0 \quad (3.18)$$

where η is the free surface perturbation from the still water level, and C_D is the bottom drag coefficient (in this case set to 0.0025, as used in other tidal applications of Fluidity, Kramer et al. [2014]).

The shallow water equations make the assumption that flow is depth-averaged. This assumption is only valid if horizontal velocities are much greater than vertical velocities. This requires that wave are in “deep” water, i.e. wavelengths are greater than 20 times the water depths, and also that bathymetry gradients are small.

3.4.2 Time discretisation, time step, and simulation length

Model equations were solved with a timestep of 100 seconds, using a Crank–Nicolson (Crank and Nicolson [1947]) time discretisation. This gave a Courant number throughout the simulation of less than 1.0.

In order to independently resolve the M_2 and S_2 constituents, the simulation was run for greater than their “synodic period”, T_{syn} , which is the length of time required for the oscillations of period T_1 and T_2 to be separated by at least a complete period over the length of the simulation.

$$\frac{1}{T_{\text{syn}}} = \frac{1}{T_1} + \frac{1}{T_2}. \quad (3.19)$$

Thus, to determine M_2 and S_2 independently in an analysis requires 355 hours, or just over 14 days, of simulation time.

This tidal model simulated 37 days of tidal motion, with a spin-up time of 48 hours allowed for during time series analysis to account for the settling of the free-surface dynamics.

3.4.3 Domain

The model domain encompassed the majority of the seas within the European continental shelf, including the North Sea, the Irish Sea, and the English Channel. An image of the model domain is shown in Figure 3.9. It was defined on its western side by a tidal–forced boundary given by the 500 m depth contour of the continental slope that marks the western edge of the shelf. This boundary stopped short at its southern end, at the north of France, to avoid spurious reflections from the nearby French coast. Similarly, the northern section stopped immediately after the Norwegian trench, to avoid spurious reflections from the nearby Norwegian coast.

The remainder of the domain was defined by the coastlines of the UK, France, Germany, Norway, and other nearby European countries.

The Baltic Sea was omitted from the domain as it has a comparatively minimal affect on the tides within the shelf. It was accounted for by a tidal–forced boundary across the entrance of the Baltic sea, placed approximately between the western Pomerania Lagoon Area National Park (Germany) and the town of Höllviken (Sweden).

3.4.4 Bathymetry

The model bathymetry was created using the latest release of the GEBCO One Minute Grid, published in November 2008 GEBCO. This dataset is an update to that originally published in 2003, and includes version 2.23 of the International Bathymetric Chart of the Arctic Ocean (IBCAO) and improved bathymetry in some shallow water areas. The GEBCO One Minute Grid is a global bathymetric grid with one arc-minute spacing that was originally based on the bathymetric contours contained within the Centenary Edition of the GEBCO Digital Atlas. Additional control contours and sounding point data were used in many regions, particularly shallow water areas and semi-enclosed seas, to constrain the gridding process. It is a continuous digital terrain model for ocean and land, with land elevations derived from the Global Land One-km Base Elevation database GLOBE. An image of the model domain, showing the bathymetry is shown in Figure 3.8.

The model includes a 10 m minimum depth limitation. This limitation overrides the input bathymetry data in shallow water, to ensure that each node the bottom depth is at least 20 m. This is an alternative to

using wetting & drying techniques for handling coastline interaction.

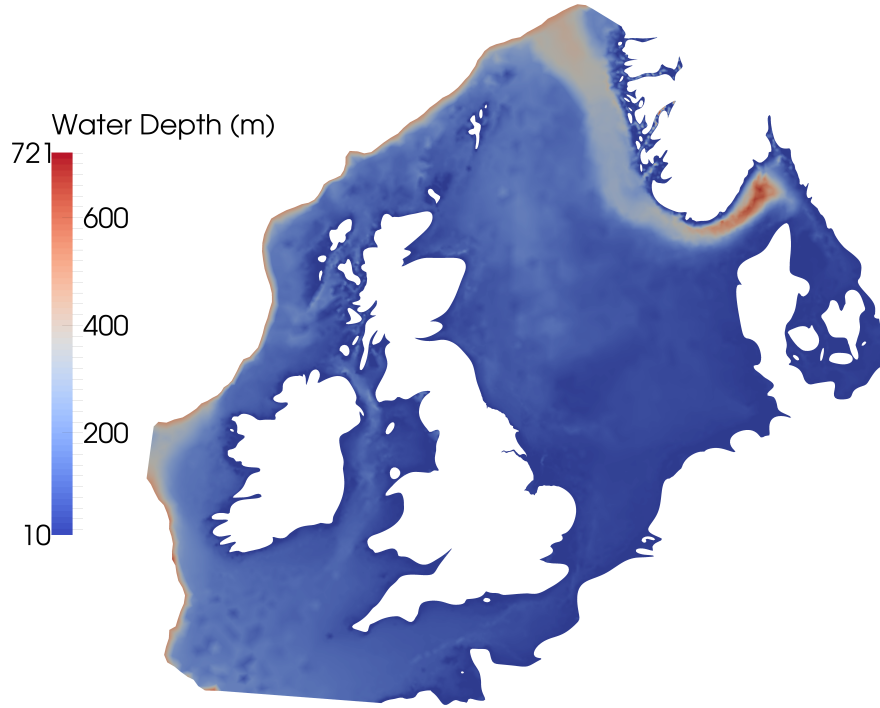


Figure 3.8: Bathymetry for the European Continental Shelf tidal model

3.4.5 Coastline

The model coastline was created using methods described within Avdis et al. [2015b]. Underlying coastline data was taken from the Global Self-consistent, Hierarchical, High-resolution Geography Database (GSHHG, Wessel and Smith [1996]). This coastline data was simplified using Principal Component Analysis (PCA); The coastline was partitioned into segments, a smoothed best-fit description of each segment was generated, and then the coastline was reconstructed from these smoothed best-fit lines. This method allows the user to control the variation of coastline resolution throughout the model, and so avoid unnecessary resolution in areas of the domain that have less influence on the accuracy of the required result. To control resolution, the user can choose the size of the partitions and the number of modes to be used in the best-fit reconstruction.

For this model, the coastline resolution was staggered in three stages:

- the coastline nearest the hypothetical site used the “full resolution” data from GSHHS, with no PCA simplification (the black line in Figure 3.9),
- at intermediate distances from the site, the coastline was defined using a five-mode reconstruction of the PCA based simplification with 100 point segments (the green lines in Figure 3.9),
- and at distances far from the site, the coastline was defined using one-mode reconstruction using 500 point segments (the purple lines in Figure 3.9).

Figures 3.9 and 3.10 shows the final generated coastline, describing the spatial variation of coastline resolution.

3.4.6 Tidal forcing

Tidal forcing was generated using tidal constituent data from Finite Element Solution (FES) tide model, FES2004 (Lyard et al. [2006]). FES2004 is based on the resolution of the tidal barotropic equations on a global finite element grid (~ 1 million nodes) which leads to solutions independent of in situ and remote-sensing data (no open boundary conditions and no data assimilation). Tidal constituents are distributed on $1/8^\circ$ grids (amplitude and phase).

An effluent dispersion model within the North Sea would typically use the nine principal tide constituents that have significant amplitude within the region (see Table 3.1 for their relative period and amplitude of these constituents). To determine the amplitude of these constituents at a given site using a tidal model, the tidal model would be run once for each constituent.

The European Continental Shelf model was forced by the M_2 and S_2 tide constituents. These are the two dominant tide constituents within the region and so confirmation of their accurate prediction was imperative for model validation.

Tidal-forcing was applied to open ocean domain boundaries through setting a Dirichlet condition for the non-hydrostatic component of the pressure. Co-oscillating tides are forced as cosine waves of specified phase and amplitude along designated boundaries:

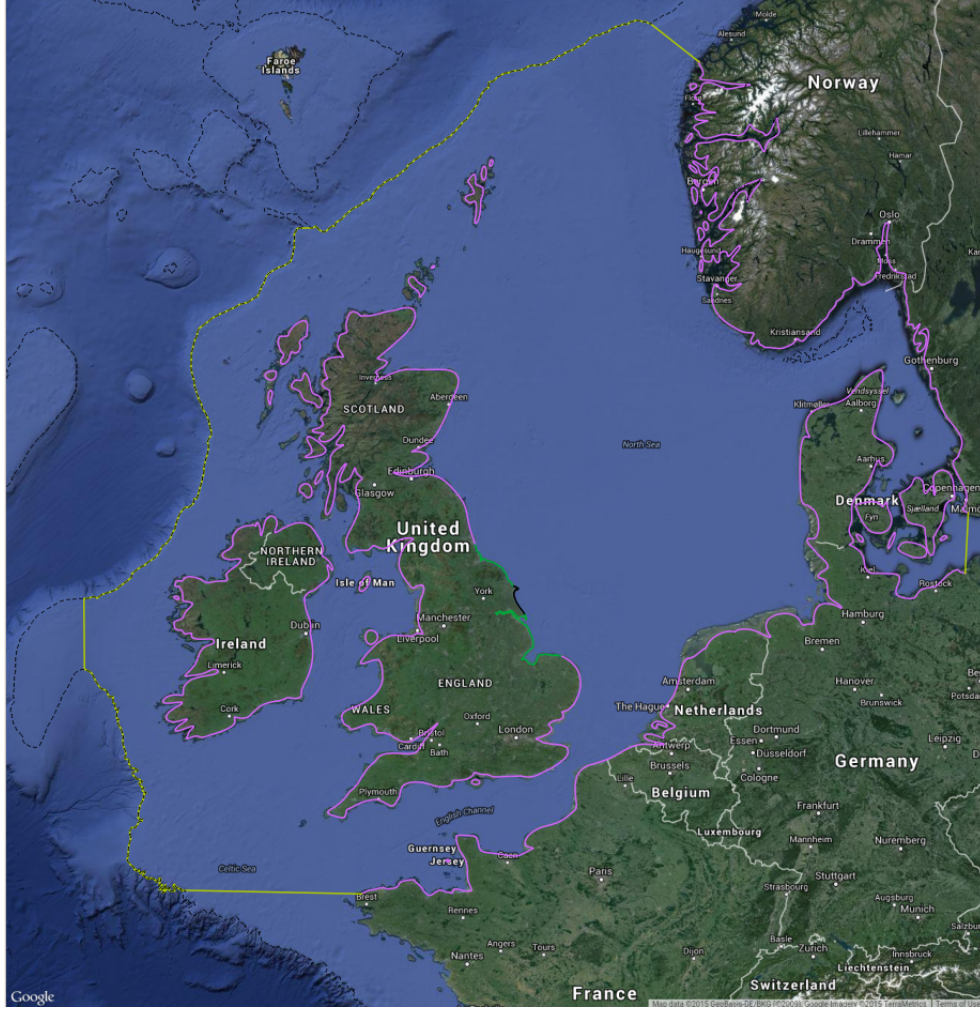


Figure 3.9: The model domain, showing the three levels of coastline resolution. Purple boundaries are the coarsest resolution, green are medium resolution, and black are the finest. Yellow lines show ocean boundaries.

$$\eta = \sum_i A_i \cos(\sigma_i t - \theta_i) + \sum_j A_j \cos(\sigma_j t - \theta_j) \quad (3.20)$$

where A is the amplitude of the tidal constituent (m), and θ is the phase of the tidal constituent (radians), Wells [2008].

The gravitational forces of the Sun and Moon cause a flexing of the crust of the Earth, so-called “body tides”. This resulting variation in bathymetry is relatively small (± 0.2 m) and as such this effect is not included in this tidal model.

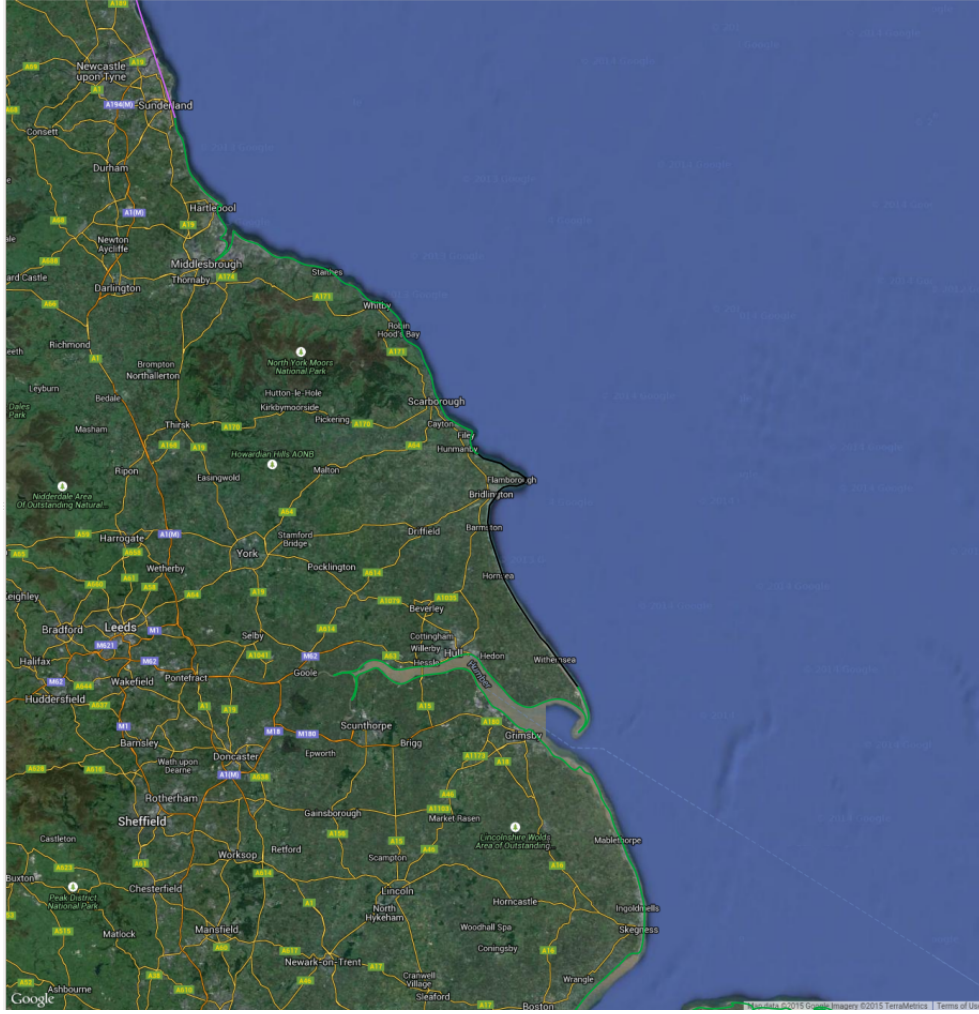


Figure 3.10: A zoom in on the domain boundary around the hypothetical outfall site, showing details of the medium and fine resolution coastline in that area.

3.4.7 Coriolis effect

The rotation of the Earth creates the Coriolis Effect, which is accounted for in this tidal model using the “ β -plane” approximation (Cushman-Roisin [1994]). A Coriolis Parameter, f , can be expressed as

$$f = 2\Omega \sin\theta, \quad (3.21)$$

where Ω is the angular velocity of the Earth, taken as $86\,164\text{ s}$ (a sidereal day) and θ is the latitude. This can be approximated for a given

point on Earth, with a reference latitude, ϑ_0 , and local coordinate in the northwards direction, y , as:

$$f = f_0 + \beta y, \quad (3.22)$$

$$\vartheta = \vartheta_0 + \frac{y}{R_E}, \quad \text{and} \quad (3.23)$$

$$\beta = \frac{2\Omega}{R_E} \cos \vartheta_0. \quad (3.24)$$

where R_E is the radius of the Earth, taken as 6378 km. Using the first two terms of the Taylor expansion, this can then be expressed as:

$$f = f_0 + 2\Omega \sin \vartheta_0 \frac{y}{R_E}. \quad (3.25)$$

For this model, the Coriolis parameter at the lowest latitude within the domain, $f_0 = 4.019 \times 10^{-5}$, and the constant used to calculate f at other points within the domain, $\beta = 1.586 \times 10^{-11}$

3.4.8 Mesh generation

Coastline data was translated on to Universal Transverse Mercator (UTM) coordination system to generate the domain boundary. The UTM zone 30N was chosen for this projection, as this aligns most closely with the position of the hypothetical site.

The simulation mesh was generated using the QMESH software (Jones [1974]). QMESH can be used to produce unstructured meshes over realistic ocean domains, in a variety of coordinate reference systems. The QMESH design, software and user interfaces are described in Avdis et al. [2015a]. Broadly, the QMESH design centers around the coupling of QGIS and a mesh generator GMSH, Geuzaine and Remacle. In this way the mesh is fully described in terms of domain boundaries and mesh edge length, both encoded in data-structures native to QGIS inside a user-friendly environment. In addition the QMESH output can be directly read into fluidity, creating a robust tool-chain.

Figure 3.11 shows the element edge length distribution throughout the simulation domain. As shown the element edge gradates to finer sizes towards the shorelines. A coarser mesh, with edge lengths of 5 km, is

prescribed in the open ocean (shown as blue areas in figure 3.11). In areas with an intermediate shoreline approximation, an intermediate mesh resolution of 5 km is prescribed (green areas in figure 3.11). In the vicinity of the hypothetical outfall (shown in orange) the edge lengths are prescribed to be 400 m.

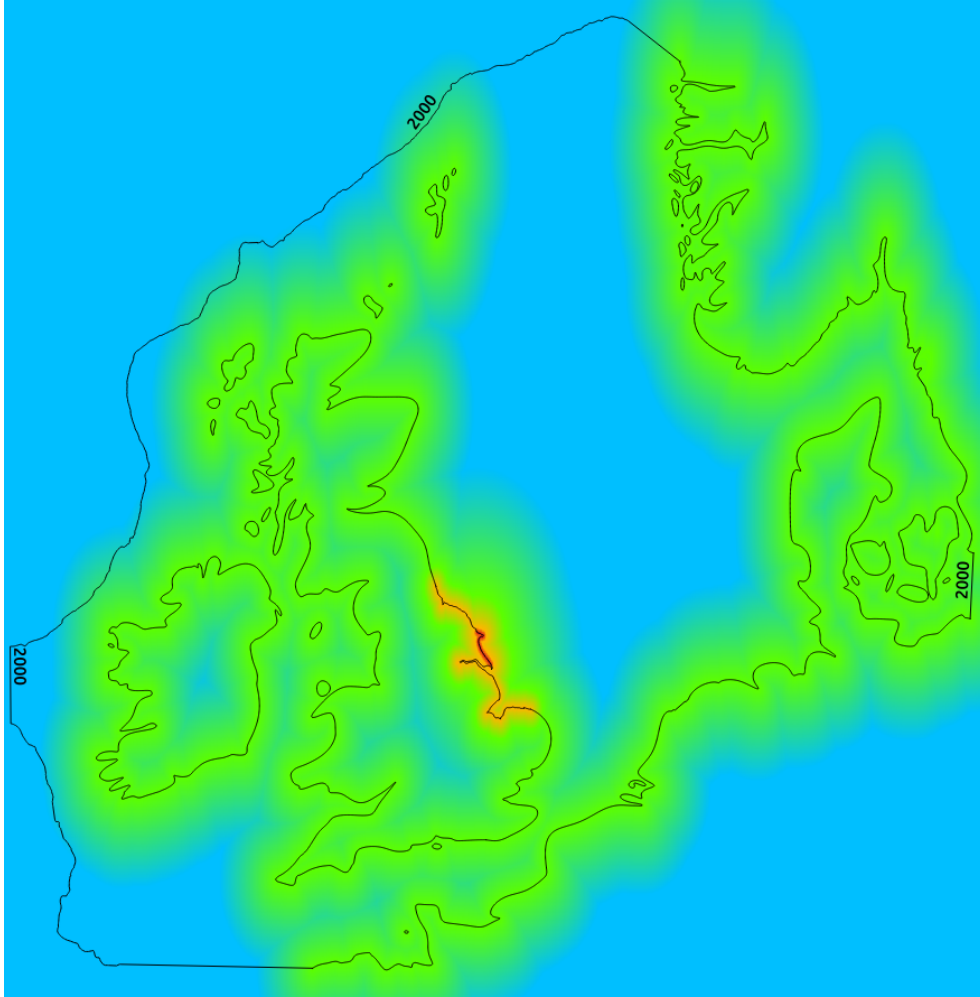


Figure 3.11: Edge length distribution within the model domain. Blue areas correspond to a coarser mesh resolution, with edge lengths of 5 km; Green areas have an intermediate mesh resolution, with edge lengths of 5 km, areas in the vicinity of the hypothetical outfall (shown in orange), have edge lengths of 400 m. The label “2000” marks the tidally forced boundaries.



Figure 3.12: The mesh for the European continental shelf tidal model

3.5 Comparison tide gauge data

3.5.1 Introduction to tide measurement

Tides are measured using “tide gauges”, a catch-all term for a range of instrument types that measure sea-level variation. Sometimes stand-alone tide gauges are deployed and maintained by the owner of a port, harbour, etc. and sometimes a network of gauges will be managed by larger organisations. There are many (usually government-led) organisations that collate, process and publish data from tide gauges across the world. International examples include the Global Sea Level Observing System (GLOSS), International Association for the Physical Sciences of the Oceans (IAPSO [2015]) the International Center for Earth Tides (ICET), whereas in the USA there is the National Oceanic and Atmospheric Administration, (NOAA), and in the UK we have National



Figure 3.13: A zoom-in of the mesh for the European continental shelf tidal model, showing details of the finer mesh around the hypothetical outfall site.

Oceanography Centre (NOC), British Oceanographic Data Centre (BODC) and the United Kingdom Hydrographic Office (UKHO).

Historically, sea-level measurements were made using tide poles or staffs, but technology has progressed substantially and now automatic, electronic measurement is the norm.

Bubble gauges are the most common type of gauge deployed in the UK. These are a form of differential pressure gauge that measure the difference between atmospheric pressure and the water pressure at some point safely below the expected minimum water-level. An advantage of bubble gauges is that the sensitive instrumentation can be housed onshore, which protects it from storm damage. Unfortunately bubble gauges suffer from lower accuracy during large wave events (NOC).

Underwater pressure transducers are a further type of pressure gauge, this time placed someway underwater. A sealed quartz crystal measures the variation in a cyclic current and compares against readings taken onshore. This type of tide gauge also loses accuracy during large wave event, but is often preferred in places with harsh weather conditions (such as the Antarctic) where the ocean can act as protection against the environment (NOC).

Acoustic gauges are the most common type of gauge deployed in the USA and Australia. They use the doppler effect to measure the distance to the free-surface from the mounted position above. A tube is placed around the device to ensure that reflected sound waves return to the receiver. Unfortunately the speed of sound varies significantly with air temperature which can introduce errors in measurement (NOC).

Radar gauges are a relatively new form of tide gauge that again use the doppler effect, but this time with microwaves. The speed of microwaves is not effected by air temperature, and allows for far greater recording frequency (NOC). Recent studies have shown that their performance is comparable to that of bubbler gauges (Woodworth and Smith [2003]).

3.5.2 Details of comparison tide gauge data

Comparison tide gauge data was used from 714 sets of recordings, supplied and post-processed by the NOC. The data are an assortment of measurements, gathered by a mix of different people and organisations, some taken using the best up-to-date equipment, whilst most were taken using traditional bubble gauges. This data was taken from a total of 487 sites, with a further 227 recordings being taken either from the same place as another recording, but at a different time, or using a supplementary gauge at a site very close by (within ~ 100 m). A map of the domain showing the positions of the tide gauges is shown in Figure 3.14.

The time period over which measurements were taken, and the frequency of measurements, varied between recordings. Some assumptions about the accuracy of readings were made in order to make use of this comparison data.

Finally, tidal models are notoriously inaccurate within shallow water areas, where non-linear effects start to dominate. As such, the comparison data was arbitrarily segregated into shallow and deep water gauges, to make a relative assessment of model accuracy within the shallow water

regions. Gauges in water less than 25 m deep were considered shallow water gauges, which accounted for about 80% of the recordings within the comparison data.

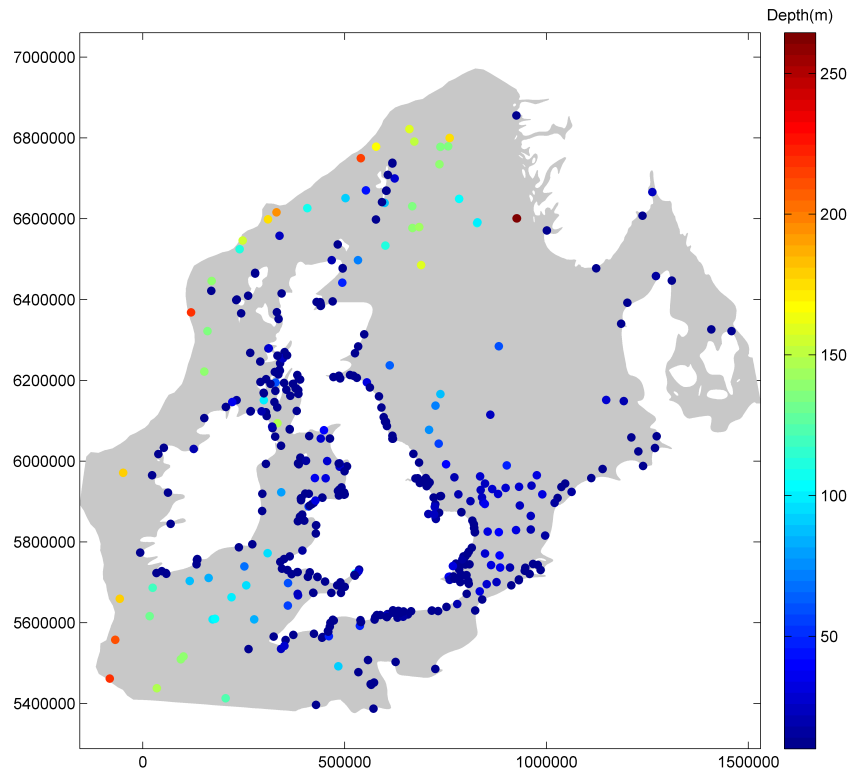


Figure 3.14: Positions of the comparison tide gauges within the domain, coloured by the relative depth of their surrounding water.

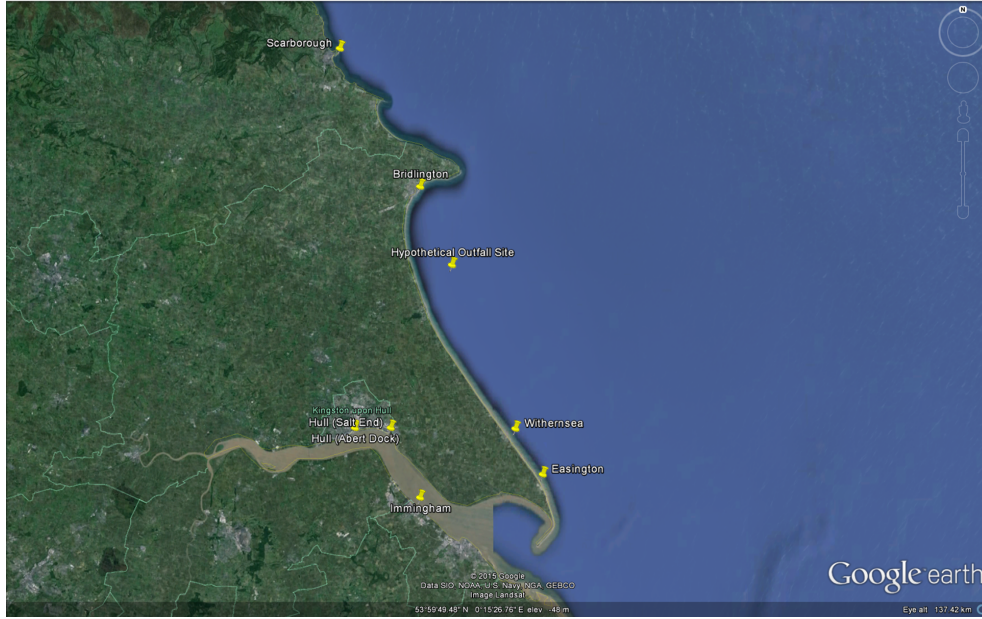


Figure 3.15: Positions of tide gauges within the vicinity of the hypothetical outfall site.

3.6 Results

The tidal model was run to simulate 888 hours (37 days), with a 24 hour spin-up period assumed for the tides to stabilise. Free surface predictions were recorded every timestep at “detectors” placed at the location of the comparison tide gauges.

Python package uptide (Kramer) was used to analyse the data and produce constituent predictions (using an assumed spin-up time of 48 hours).

M_2 and S_2 tide amplitudes as predicted by the tidal model compared to the physical data are shown in Figures 3.16. and 3.17, respectively.

The predictions (and comparison) for the hypothetical site within the North Sea and nearby gauges are shown in Tables 3.2 and 3.3. These sites correspond to regions of shallow water, and so are more likely to be inaccurate, but they have been given relatively high mesh resolution within the model in the hope of improving accuracy.

Summary tables of the results for predictions of M_2 and S_2 tides are shown in Tables 3.4 and 3.5, respectively. These tables also show results separated into those predicted in shallower water (< 11 m) and those

predicted in deeper water (> 50 m). These categorisations are arbitrary, but assist in assessing the model's ability to predict tidal constituents near the shoreline.

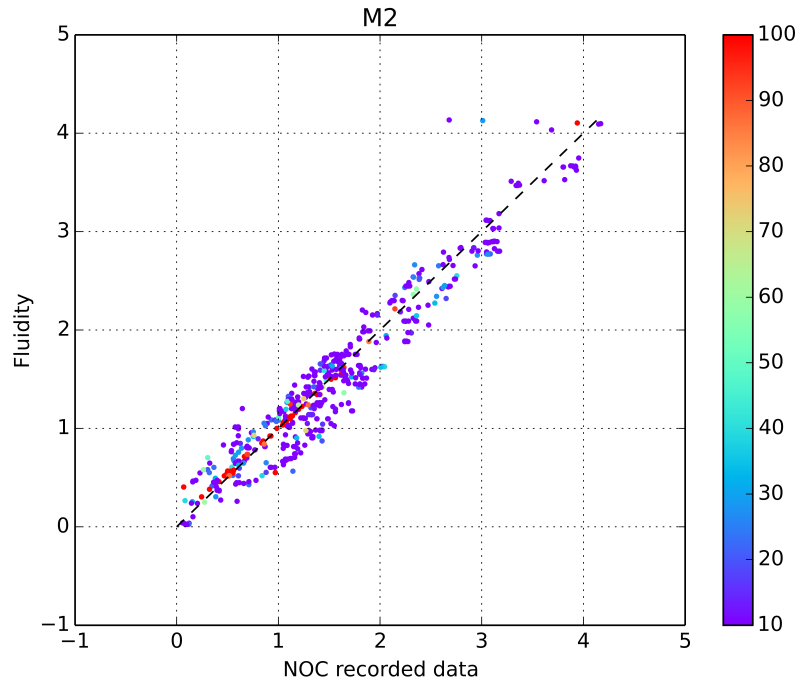


Figure 3.16: Comparison between measurements and model predictions for M_2 tidal constituent amplitude. Data point colour indicates the site water depth.

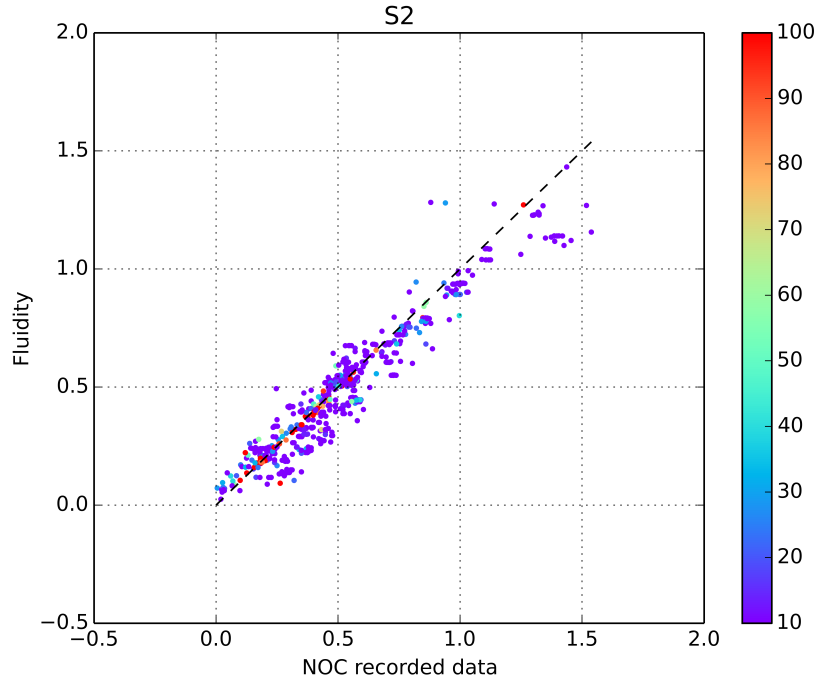


Figure 3.17: Comparison between measurements and model predictions for S_2 tidal constituent amplitude. Data point colour indicates the site water depth.

Table 3.2: Predictions of the M_2 tidal constituent amplitude, at tide gauge sites near to the hypothetical North Sea outfall

Tide gauge site	Distance from outfall (km)	Physical (m)	Model (m)	Error (m)
Bridlington	13.7	1.84	1.98	0.14
Easington	36.7	1.83	2.20	0.37
Hull (Albert Dock)	30.5	2.41	2.61	0.20
Hull (Salt End)	28.0	2.38	2.57	0.19
Immingham	37.8	2.27	2.45	0.18
Scarborough	39.4	1.71	1.83	0.12
Withernsea	28.2	1.93	2.15	0.22

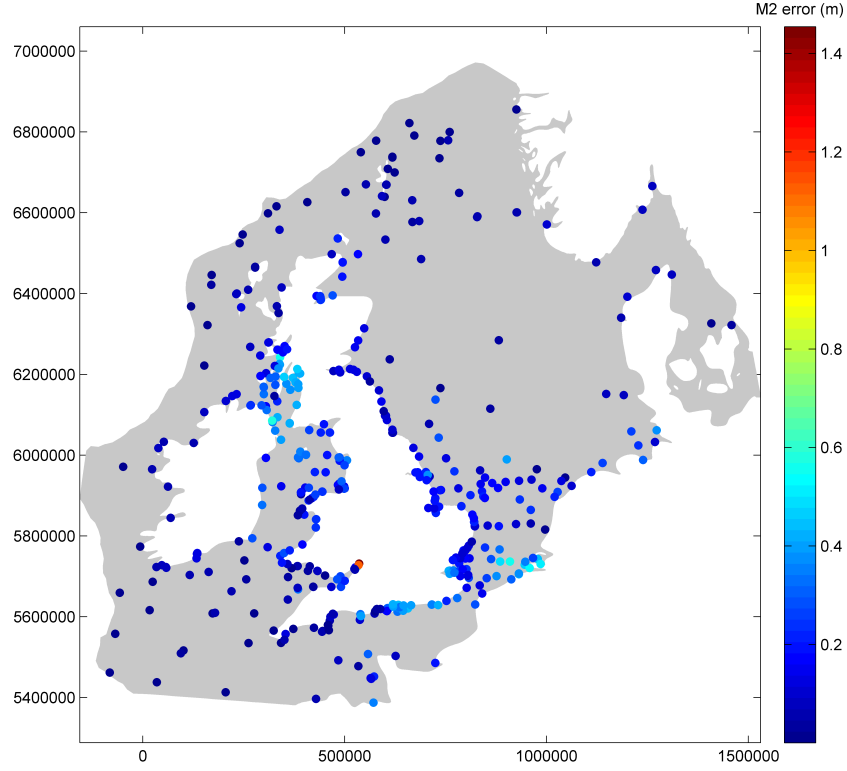


Figure 3.18: A map of difference between measurements and model predictions for M_2 tidal constituent amplitude. Data point colour indicates the magnitude of difference.

Table 3.3: Predictions of the S_2 tidal constituent amplitude, at tide gauge sites near to the hypothetical North Sea outfall

Tide gauge site	Distance from outfall (km)	Physical (m)	Model (m)	Error (m)
Bridlington	13.7	0.63	0.63	0.00
Easington	36.7	0.61	0.69	0.07
Hull (Albert Dock)	30.5	0.79	0.77	0.02
Hull (Salt End)	28.0	0.77	0.76	0.01
Immingham	37.8	0.75	0.72	0.03
Scarborough	39.4	0.58	0.59	0.01
Withernsea	28.2	0.66	0.68	0.02

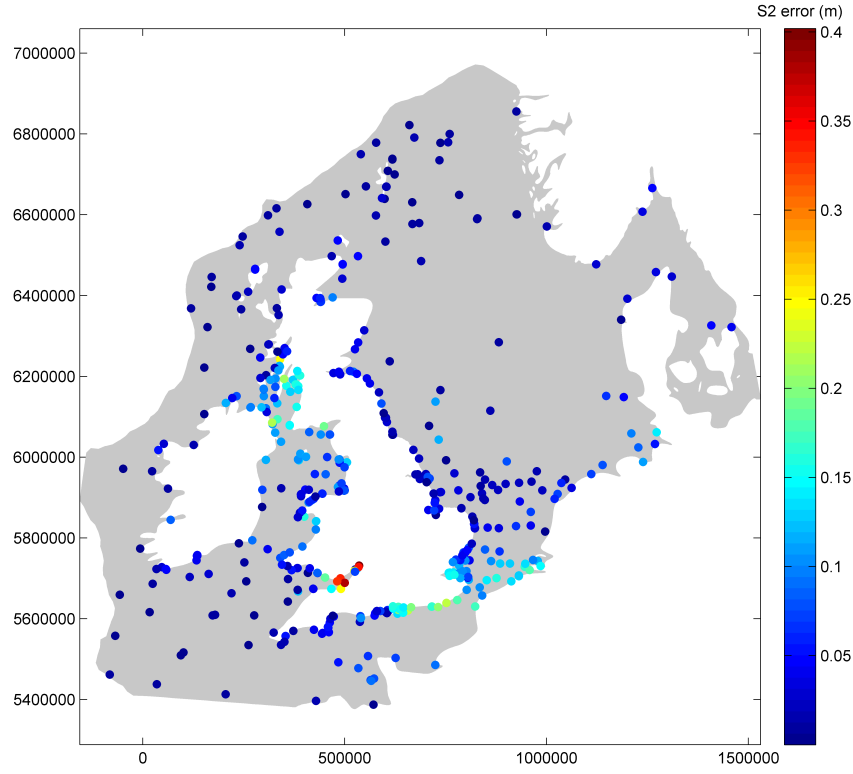


Figure 3.19: A map of difference between measurements and model predictions for S_2 tidal constituent amplitude. Data point colour indicates the magnitude of difference.

Table 3.4: Predictions of the M_2 tidal constituent

	Number	Mean value (m)	RMS error (m)
Total gauges	714	1.59	0.23
Shallow gauges	503	1.68	0.24
Deep gauges	74	0.99	0.12

Table 3.5: Predictions of the S_2 tide constituent

	Number	Mean value (m)	RMS error (m)
Total gauges	714	0.53	0.09
Shallow gauges	503	0.56	0.10
Deep gauges	74	0.35	0.05

3.7 Discussion

The prediction of M_2 tide amplitude in the vicinity of the site had an average error of 10.1% compared with tide gauge measurements. The prediction of S_2 tide amplitude in the vicinity of the site were even closer to tide gauge measurements, with an average error of 3.7%. In comparison, Wells [2008] achieved “<15%”.

As expected, model predictions in deeper water showed closer agreement than gauges in shallower water. The average percentage RMS error in M_2 predictions for gauges in deeper water was 12.1%, in comparison with an average error of 14.3% for model predictions in shallower water. For S_2 predictions, average percentage RMS error for gauges in shallower water was 14.3%, in comparison with an average error of 17.9% for model predictions in shallower water.

The greatest disagreement between model results and the tide gauge data was seen in the Severn Estuary, at the contraction of the English Channel, and the north of the Irish Sea. These gauges were in regions of shallow water within narrow channels, where non-linear effects have their greatest influence.

The tide amplitude predictions are notably more accurate for the locations near to the hypothetical site, with the S_2 predictions especially showing a significant increase in accuracy. The mesh resolution at these locations was much higher than in the rest of the domain, which may have improved accuracy in these regions, but it should also be noted that there are relatively few locations categorised as “within the vicinity of the site” and so some of this improvement may be due to location-specific influences.

At the site, there appears to be a systematic over-prediction of the tidal constituent amplitude. In contrast, throughout the remainder of the model there appears to be a slight under-prediction. It is conjectured that the under-prediction of constituent amplitude in the bulk of the domain is due to numerical diffusion caused by low resolution. In areas of higher resolution, such as near the site, this numerical diffusion is much lower and the diffusion observed is dominated by the bed shear stress. In this model, a constant bed shear stress is assumed, which is likely to be a low estimation for bed shear in shallow regions, such as near the site. To confirm both of these conjectures it would be necessary to check for mesh convergence test and use a more complex bed shear model, such as the Manning equation.

The speed of the model solve was a vast improvement over that described by Wells [2008]. Using 12 processors in parallel (approximately 16,000 degree of freedom per processor), 37 days of tidal motion was simulated in 15.2 hours (i.e. 182.4 processor hours). A simple check of the parallel scaling showed that scaling was close to linear and so further decomposition would be possible if necessary. The equivalent simulation published by Wells [2008] (with a 150,000 node mesh) with a similar level of accuracy, would have required approximately 444 processor hours to solve 37 days of simulation length.

3.8 Conclusions

This modelling showed that Fluidity is capable of efficiently modelling tidal model motion within the European continental shelf, with an accuracy suitable for determining tidal forcing constituents for a far-field effluent dispersion model.

4 Advection–diffusion solvers and their validation

4.1 Introduction

Each chapter of this thesis isolates and investigates an important aspect of coastal effluent dispersion modelling. This chapter concentrates on the most fundamental aspect of this modelling: how the discretisation and solver methods effects the accuracy and efficiency of equation solving.

For both ocean and local-scale models, the advection–diffusion equation is solved to model the transport of scalar fields. This can include the transportation of turbulent kinetic energy, turbulent dissipation, salinity and temperature, as well as the mesh adaptivity metric. As such, all of the ocean or local models described throughout this thesis are at least partially dependent on the accurate and efficient solving of the advection–diffusion equation. This is especially true for models that include Coriolis and / or buoyancy effects, where the discretisation method is influential on the accuracy and stability of the pressure field.

In this chapter, a series of simplified test cases were run to assess the performance of a common advection–diffusion solution method (taken from the library of those available within Fluidity). This work is intended to give general confidence that the numerical methods available within Fluidity are suitable for modelling coastal processes and so give confidence in later multi-scale results.

The two-dimensional advection–diffusion equation is given by,

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_i}(u_i c) = \frac{\partial}{\partial x_i} \left\{ D \frac{\partial c}{\partial x_i} \right\}. \quad (4.1)$$

It is very difficult if not impossible to exactly solve a non-linear equation like the advection–diffusion equation in all but the most idealised scenarios. Both the finite-element and finite-volume methods allow an approximation to the exact solution by utilising a “weakened” form of the equation. The equation is multiplied by a test function, ϕ , and then

integrated over the domain. Assuming a closed boundary, and integrating by parts the diffusion term, the weak form of the advection–diffusion is then given by,

$$\int_{\Omega} \frac{\partial c}{\partial t} + \nabla \phi \cdot \mathbf{u}c + \nabla \phi \cdot D \cdot \nabla c + \int_{\partial\Omega} \phi \{ \mathbf{n} \cdot \mathbf{u}c - \mathbf{n} \cdot D \cdot \nabla c \} = 0. \quad (4.2)$$

This form of the equation is called “weak” because it only contains first derivatives. The constraints on the possible solutions have been weakened so that they do not require a second derivative. This will not produce a sufficiently smooth solution to be a “classical” solution, but will allow discretisation on to a finite element / volume mesh using a range of basis functions that make an approximation to the solution a practical possibility.

The choice of finite–element or finite–volume method for solving the weak form of the advection–diffusion equation is a compromise between varying degrees of:

- Accuracy: The degree to which the discretised equation agrees with the exact solution to the equation,
- Boundedness: local un–physical over– and under–shoots in the solution,
- Numerical diffusion: un–physical diffusion, usually caused by up–winding advection schemes,
- Conservation: the degree to which the total amount of the quantity being transported is conserved within the model,
- Stability: the degree to which the solving is numerically stable, Lesser stability will either require higher spatial and temporal resolution to gain a solution, or the use of limiters, upwinding or other stabilisation that can add to numerical diffusion, and
- Cost: the time and computational resources required to gain a solution.

These properties of the solving methodology are affected by:

- The spatial discretisation: the “shape” of the basis functions used to describe the field between nodes,

- The temporal discretisation: the method used to step the solution forward in time,
- The advection scheme: the method for calculating the scalar flux across element faces, and
- The diffusion scheme: the discretisation of the diffusion term.

For further reading on the finite–element and finite–volume methods, the author found the textbooks of Elman et al. [2005] and Pepper and Heinrich [2006] to be very useful introductions.

The test cases used within this chapter were taken from the published validation document for open–source free surface flow solver Open TELEMAC (EDF–R&D [2011a,b]). Open TELEMAC is a world–leading free surface modelling code managed by a consortium of core organisations: Artelia (formerly Sogreah, France), BundesAnstalt für Wasserbau (BAW, Germany), Centre d’Etudes Techniques Maritimes et Fluviales (CETMEF, France), Daresbury Laboratory (United Kingdom), Electricité de France R&D (EDF, France), and HR Wallingford (United Kingdom).

The test cases chosen were relevant to coastal dispersion, including those testing tracer advection, diffusion, point sources and stratification. An assessment was made of numerical diffusion, conservation, and boundedness, and model results were compared to those results published using Open TELEMAC.

4.2 Numerical methods

4.2.1 Spatial discretisation

All simulations within this chapter used a control volume discretisation for the tracer field. It was shown by Hiester [2011] that the control volume (and discontinuous Galerkin method) provide a generally good performance in terms of the levels of numerical diffusion and the overshoots and undershoots and the conservation properties are much improved over the continuous Galerkin method.

Control volume discretisation is in a sense equivalent to a lowest–order discontinuous Galerkin method. A dual mesh is created by connecting element centroids to edge midpoints. Field values are calculated at

element centres, with fluxes conserved across lines (or planes in 3-d) between centres.

The test function for control volume discretisation is unity, and the gradient (across an element) is zero. Simplifying Equation 4.2, the advection–diffusion equation is then,

$$\int_v \frac{\partial c}{\partial t} + \int_{\partial v} \widehat{\mathbf{n} \cdot \mathbf{u} c} - \widehat{\mathbf{n} \cdot \mathbf{D} \cdot \nabla c} = 0. \quad (4.3)$$

4.2.2 Advection scheme

Due to the discontinuous nature of the fields, there is no unique value for the fluxes between volumes. However the requirement that tracer be a conserved quantity does demand that adjacent volumes make a consistent choice for the flux between them. The choice of flux schemes therefore forms a critical component of the control volume method.

This study used the finite–element interpolation method to calculate face fluxes. The value of the field at each quadrature point is interpolated using the finite element basis functions on the parent mesh. This is possible as the nodes of both the dual and parent meshes are co–located. This method is less diffusive than the more common first–order upwinding but it is usually unstable. As such, a Sweby limiter (Sweby [1984]) was applied to limit spatial derivatives to realistic values and remove spurious oscillations.

4.2.3 Diffusion scheme

Diffusion was discretised using the Bassi–Rebay method, Bassi and Rebay [1997]. This method introduces an additional variable and equation for the tracer gradient which is directly solved and re–inserted into the control volume equation. This is a second–order accurate discontinuous method (and so also suitable for control volumes).

4.2.4 Temporal discretisation

The spatially discretised advection–diffusion equation produces a semi–discrete matrix equation of the following form:

$$M \frac{dc}{dt} + A(\mathbf{u})c + Dc = r \quad (4.4)$$

Where M is the mass matrix, $A(\mathbf{u})$ is the advection operator, D is the diffusion operator, and r contains the boundary, source and sink terms.

When using control volume spatial discretisation it is required that the face values are “tested” against an (estimated) upwind value. To avoid instability, an extra advection iteration loop is introduced and the face value is replaced by a first-order implicit pivot face value estimated using first-order upwinding.

4.2.5 TELEMAC simulations

The majority of the comparison TELEMAC simulations described within this chapter were published within EDF-R&D [2011a,b], and performed by the Electricité de France Research and Development department. Where supplementary simulations were necessary (for instance, the point-source simulations using unstructured meshes), these were performed and provided by HR Wallingford (i.e. not by the author).

The TELEMAC simulations used:

- For velocity: a centred semi-implicit advection scheme with an Streamline-Upwind / Petrov-Galerkin method,
- For tracer: the method of characteristics.

For further information on these methods and the general model set-ups, please see EDF-R&D [2011a,b].

4.3 Point source with zero explicit diffusion

4.3.1 Problem outline

This test case models a point source of passive tracer in a two-dimensional rectangular channel under constant flow conditions, with the diffusion term in the tracer advection-diffusion equation neglected.

Neglecting the diffusion term, from the advection–diffusion equation:

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_i}(u_i c) = \frac{\partial}{\partial x_i} \left\{ \overset{0}{\cancel{D}} \frac{\partial c}{\partial x_i} \right\}, \quad (4.5)$$

gives

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_i}(u_i c) = 0. \quad (4.6)$$

This allows a simple assessment of numerical diffusion present in the advection scheme. Any numerical diffusion can be isolated and quantified.

An analytical solution exists for the dispersion of a point source of diffusive tracer in a constant current. Assuming a steady–state solution, the 2–d advection–diffusion equation described in Equation 4.1 can be reduced to,

$$u \frac{\partial c}{\partial x} = D_{\text{eff}} \left\{ \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right\} + \frac{Q}{h}. \quad (4.7)$$

For uniform diffusivity, this equation has an exact solution (EDF–R&D [2011b]),

$$c(x, y) = \frac{Q}{2\pi D_{\text{eff}} h} \exp\left\{ \frac{ux}{2D_{\text{eff}}} \right\} K_0 \left\{ \frac{ur}{2D_{\text{eff}}} \right\}. \quad (4.8)$$

Where Q is the flowrate of tracer into the domain, K_0 is the modified Bessel function, of the second kind and order zero, and $r = (x^2 + y^2)^{1/2}$. By fitting this equation to the measured tracer profile within the simulation, the numerical (effective) diffusion, D_{eff} , can be estimated.

For these simulations, to maintain similarity when investigating different mesh resolutions, the input source term was normalised by the area of the elements surrounding the source node. A few elements away from the source node, the effect of this approximation is negligible, and comparisons can be made with theory.

4.3.2 Model details

The model domain was a channel 10 m wide and 50 m long. The depth was assumed to 5 m. The mass and momentum equations were not solved

in this simulation. Instead a prescribed velocity field of 1 m/s was used throughout the domain. A point source was created at a node near to the centre of the channel, 5 m downstream of the inlet boundary. A schematic of the model domain is shown in Figure 4.1.

The model mesh used in the comparison TELEMAC simulation had a structured mesh with a node spacing of 0.5 m (shown in Figure 4.2). The use of a structured mesh for this simulation likely gave a misrepresentation of advection scheme diffusion as the mesh is aligned with the flow direction, something that rarely happens in practice. To make comparison more useful, a further TELEMAC simulation was run with an unstructured mesh of the same node spacing (shown in Figure 4.3). Simulations using Fluidity were then set-up using the same mesh and two further meshes with halved and quartered node spacing.

The simulation was run for 500 s with a timestep that gave a Courant number $= 0.2$ (i.e. 0.1 s for the coarsest simulation and 0.025 s for the coarsest simulation).

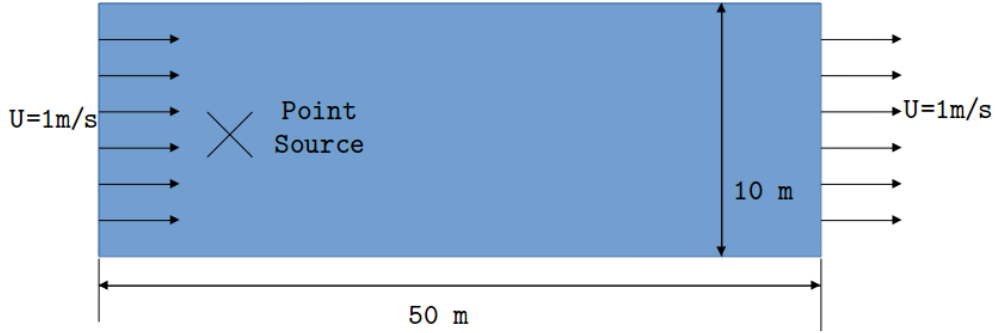


Figure 4.1: Schematic of the point source without diffusion test case.

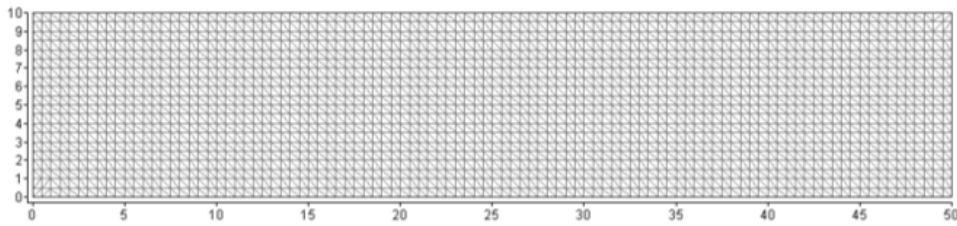


Figure 4.2: Structured mesh used for the Telemac point source test cases. This mesh had 2121 nodes with a node spacing of 0.5 m

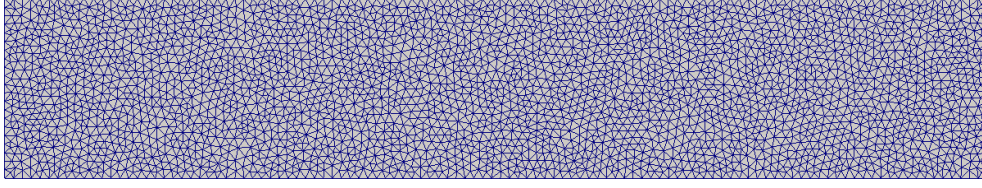


Figure 4.3: Unstructured mesh with a coarse resolution. This mesh had 3057 nodes with a node spacing of 0.5 m

4.3.3 Results

Fluidity predictions of tracer concentration simulations using 0.5 m, 0.25 m and 0.125 m node spacing are shown in Figures 4.4 – 4.6. Comparison TELEMAC results are shown in Figure 4.7 - 4.9. Fluidity predictions of tracer concentration decay in the streamwise and cross-stream direction are shown in Figures 4.10 and 4.11, respectively. Comparison TELEMAC results are shown in Figures 4.12 and 4.13, respectively. For both Fluidity and TELEMAC results, tracer concentrations were least-squares fitted to Equation 4.8. The calculated numerical diffusion and tracer conservation for the Fluidity and TELEMAC simulations are shown in Table 4.1. The conservation of tracer is shown in Table 4.2.

Table 4.1: Diffusion calculated during the point source without explicit diffusion test case.

Node spacing (m)	Fluidity	Fluidity	TELEMAC	TELEMAC
	Streamwise diffusion (m^2/s)	Crossstream diffusion (m^2/s)	Streamwise diffusion (m^2/s)	Crossstream diffusion (m^2/s)
0.5	0.051	0.061	0.025	0.015
0.25	0.021	0.026	0.017	0.011
0.125	0.008	0.010	0.008	0.006

Table 4.2: Fluidity tracer conservation during the point source without explicit diffusion test case.

Node spacing (m)	source tracer flow rate (g/l/s)	outlet tracer flow rate (g/l/s)
0.5	10.000	10.000
0.25	10.000	10.000
0.125	10.000	10.000

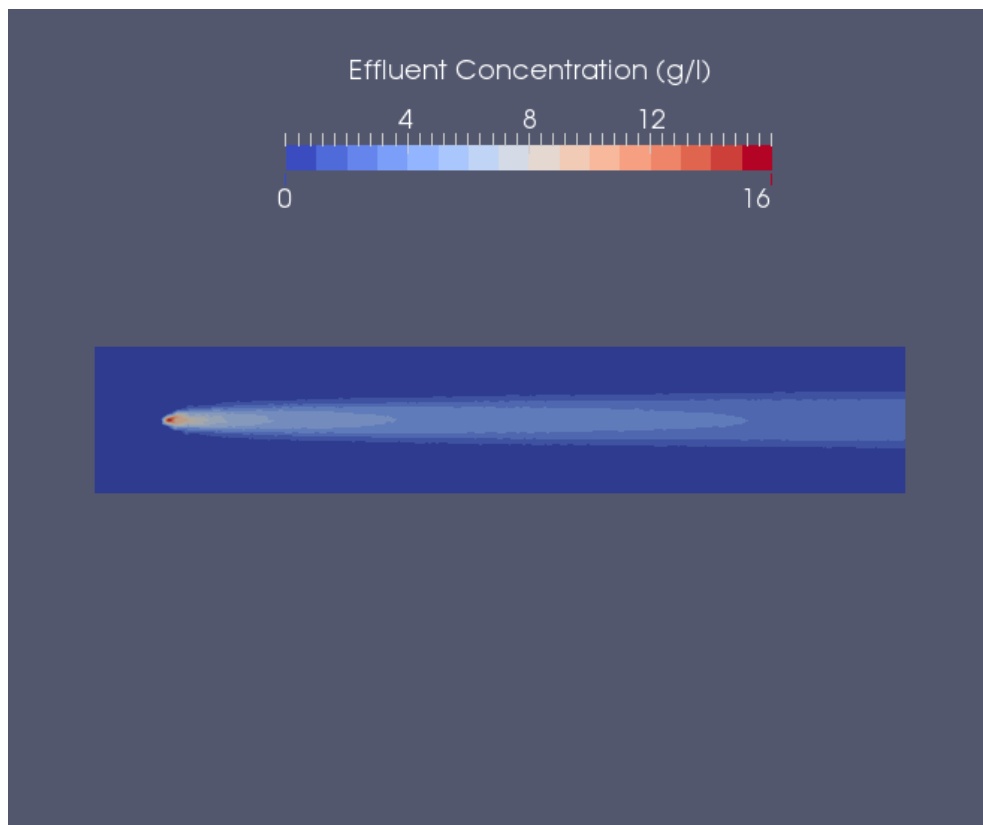


Figure 4.4: Fluidity prediction of tracer concentration for the point source without explicit diffusion simulations, with a node spacing of 0.5 m.

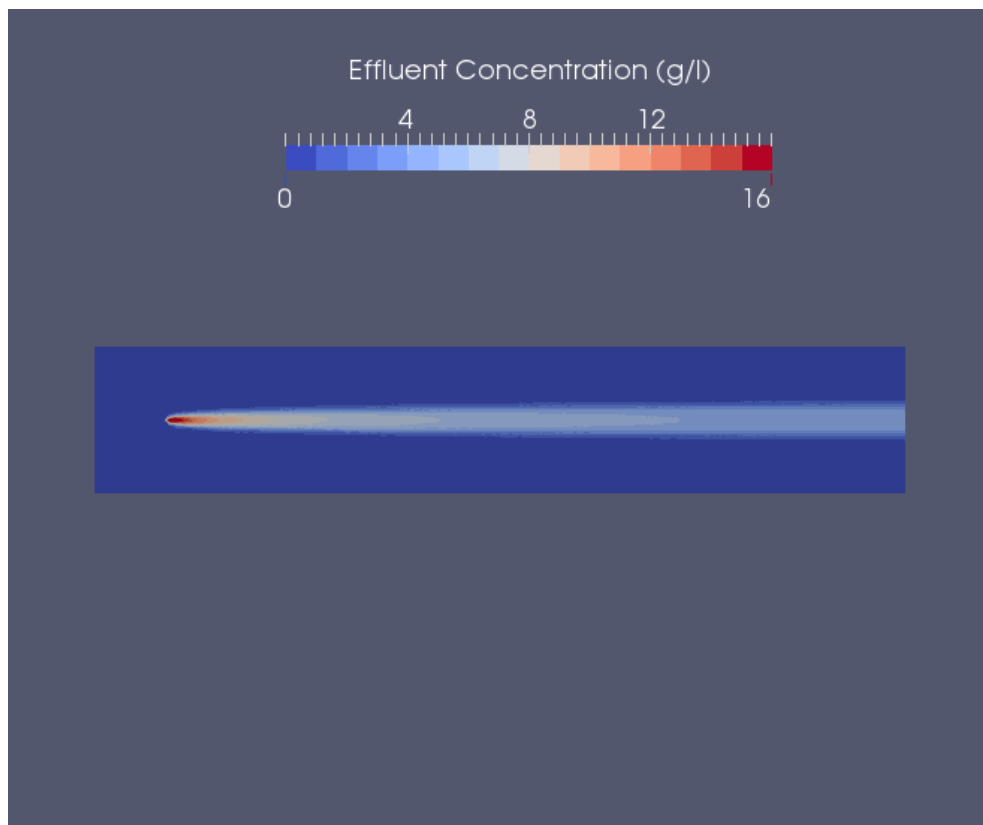


Figure 4.5: Fluidity prediction of tracer concentration for the point source without explicit diffusion simulations, with a node spacing of 0.25 m.

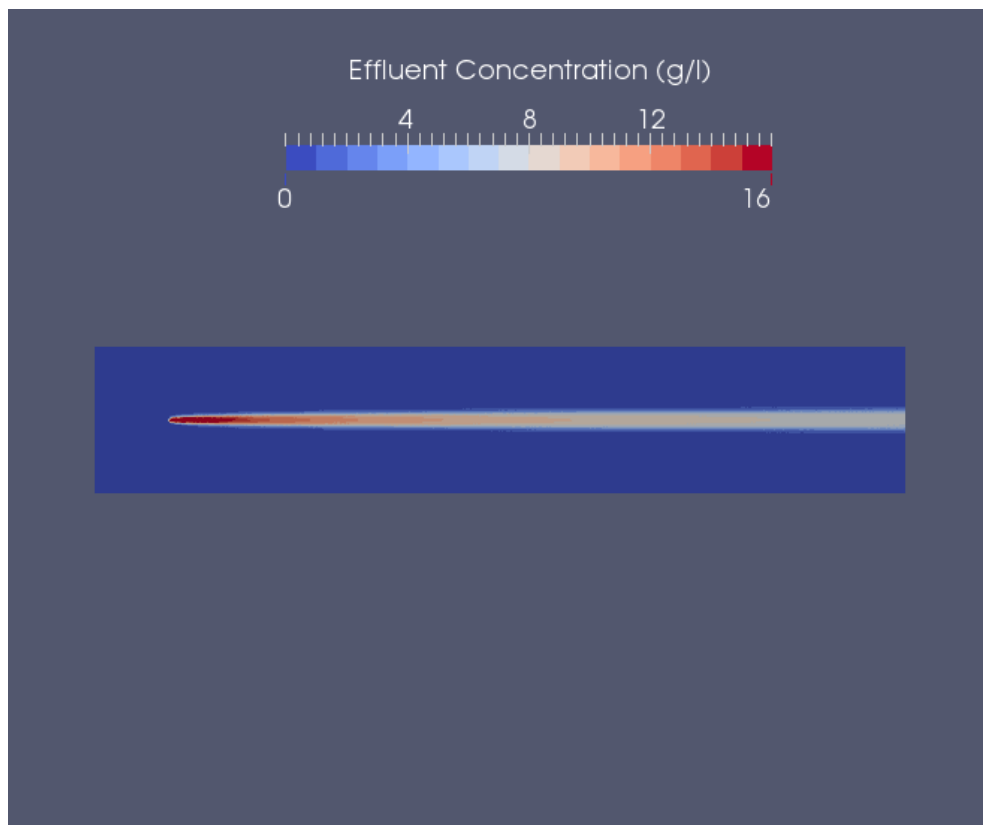


Figure 4.6: Fluidity prediction of tracer concentration for the point source without explicit diffusion simulations, with a node spacing of 0.125 m.

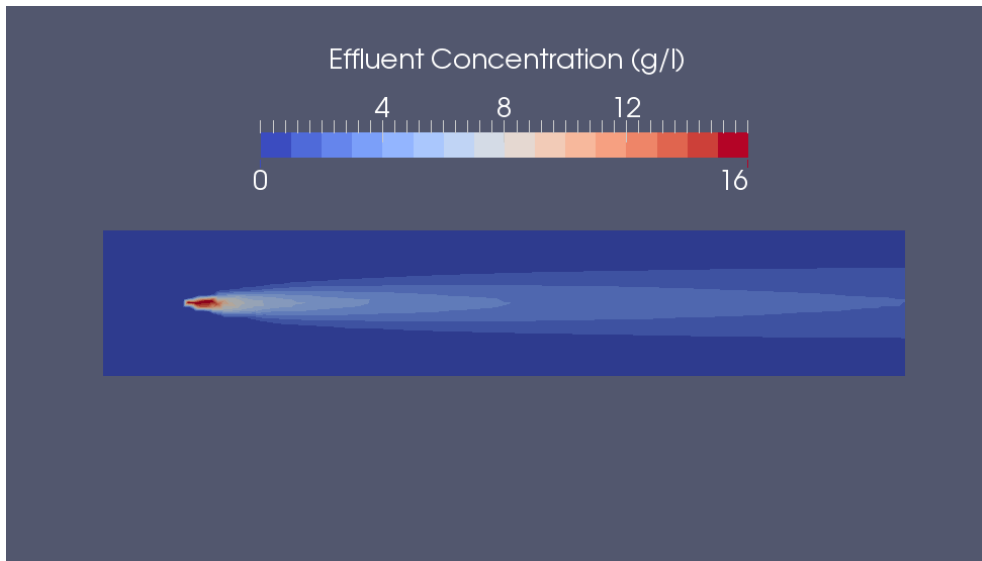


Figure 4.7: TELEMAC prediction of tracer concentration for the comparison TELEMAC simulation for point source without explicit diffusion simulations, with a node spacing of 0.5 m.

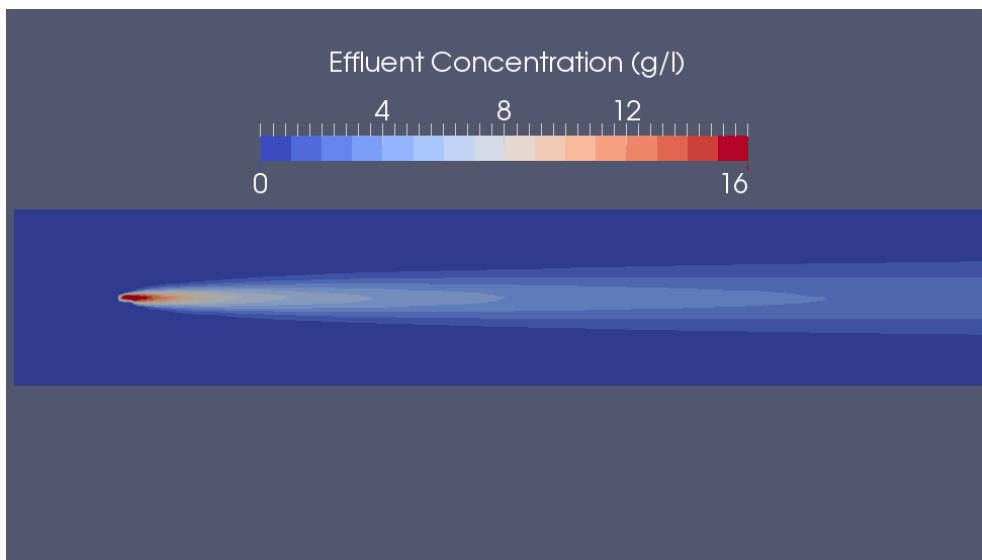


Figure 4.8: TELEMAC prediction of tracer concentration for the comparison TELEMAC simulation for point source without explicit diffusion simulations, with a node spacing of 0.25 m.

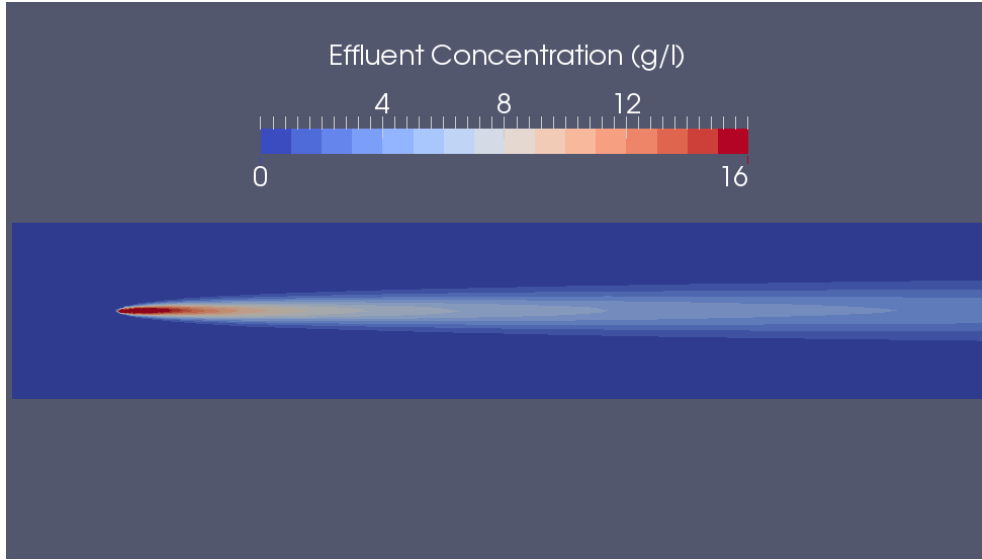


Figure 4.9: TELEMAC prediction of tracer concentration for the comparison TELEMAC simulation for point source without explicit diffusion simulations, with a node spacing of 0.125 m.

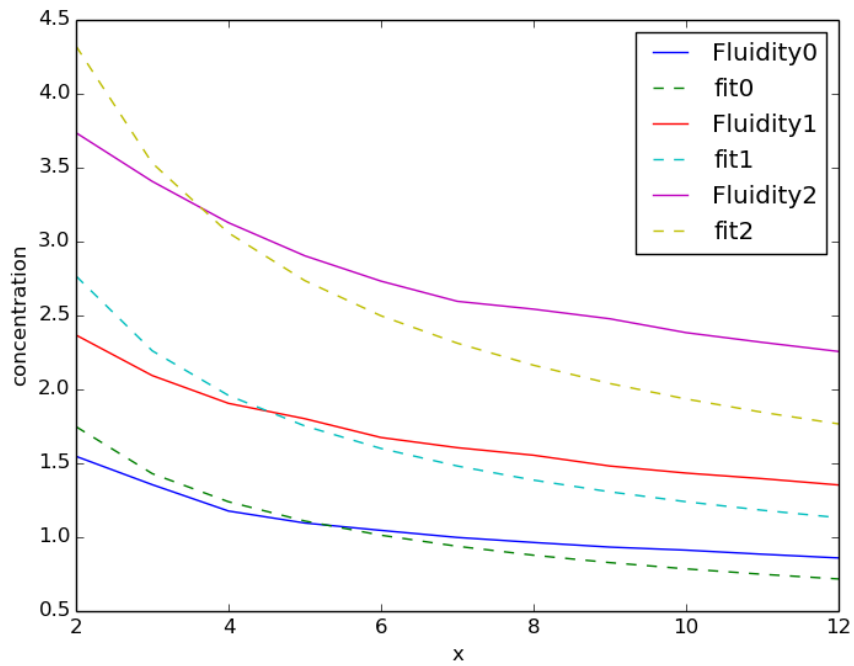


Figure 4.10: Fluidity prediction of stream-wise tracer concentration for the point source without explicit diffusion simulations. Fluidity0 is for the finest mesh and Fluidity2 is the coarsest.

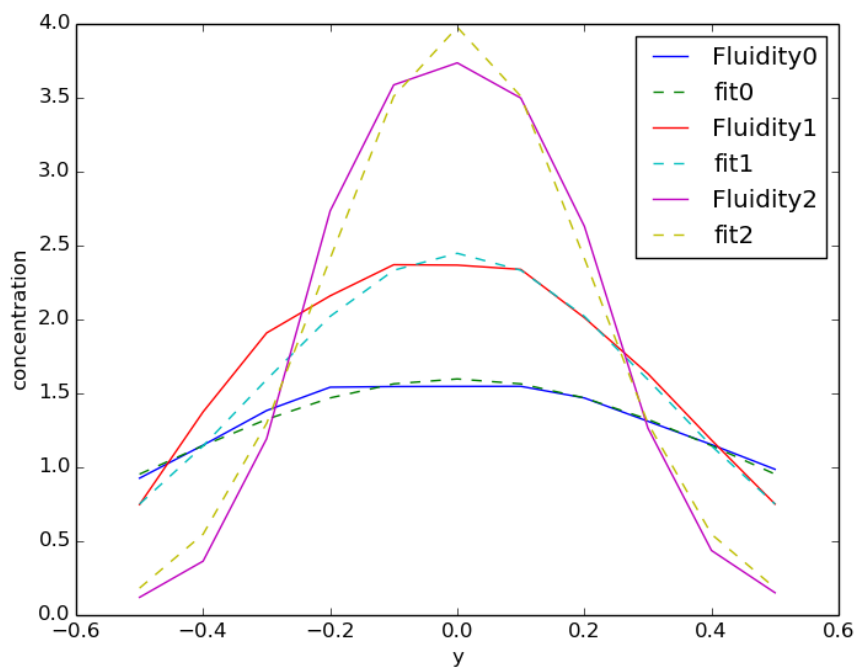


Figure 4.11: Fluidity prediction of cross-stream tracer concentration for the point source without explicit diffusion simulations, 2 m downstream of the point source. Fluidity0 is for the finest mesh and Fluidity2 is the coarsest.

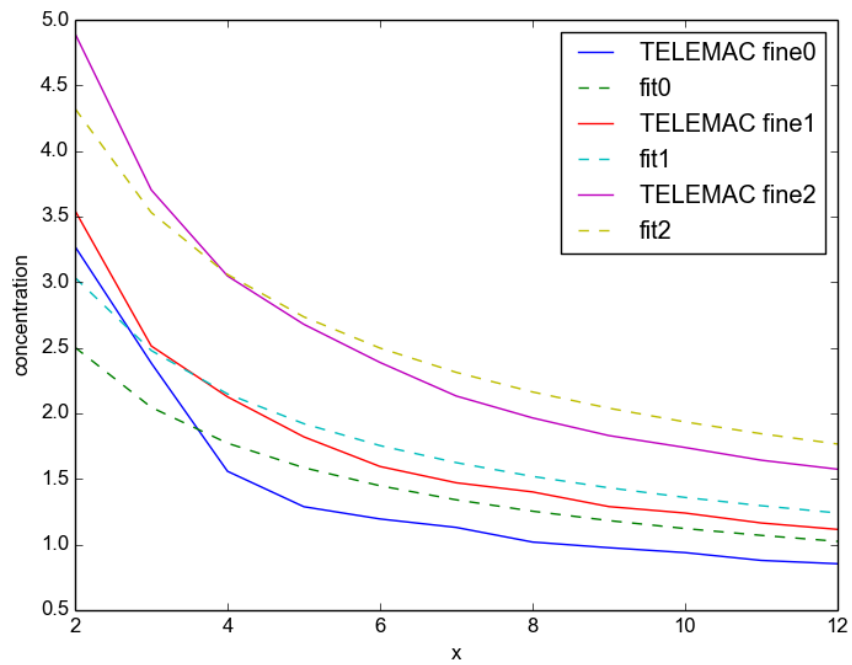


Figure 4.12: TELEMAC prediction of stream-wise tracer concentration for the point source without explicit diffusion simulations.

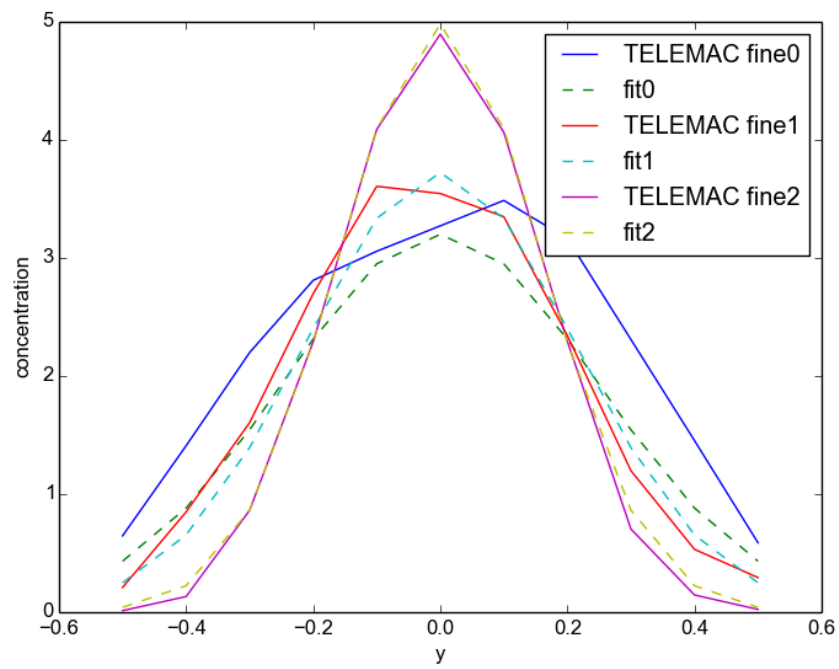


Figure 4.13: TELEMAC prediction of cross-stream tracer concentration for the point source without explicit diffusion simulations, 2 m downstream of the point source

4.3.4 Discussion

The Fluidity simulations had decreasing levels of numerical diffusion with increased resolution, with the finest simulations showing minimal numerical diffusion ($0.008 \text{ m}^2/\text{s}$ in the stream-wise direction and $0.010 \text{ m}^2/\text{s}$ in the cross-wise direction). The simulations were shown to conserve the tracer field.

The fit of the analytical Equation 4.8 was sufficient to give an approximation of numerical diffusion within the models, but not good. Especially for the TELEMAC simulations, there were significant differences between the model data and the calculated fit. This suggests that the numerical diffusivity was not completely uniform throughout the domain.

4.4 Point source with explicit diffusion

4.4.1 Problem outline

This test case models a point source in a two-dimensional rectangular channel under steady state flow conditions. The model domain, mesh, equations and discretisation was the same as that used for the previous point source test case, (see Sub-section 4.3), but for the inclusion of a diffusion term in the tracer advection-diffusion equation (set to $0.1 \text{ m}^2/\text{s}$). The channel 10 m wide and 50 m long, the depth was assumed to 5 m, and a prescribed velocity field of 1 m/s was used throughout the domain.

The streamwise and cross-stream tracer concentration profile can be compared to the analytical solution for the problem (4.8) to assess the accuracy of the numerical scheme.

4.4.2 Results

Fluidity predictions of tracer concentration simulations using 0.5 m, 0.25 m and 0.125 m node spacing are shown in Figures 4.14 – 4.16. Comparison TELEMAC results are shown in Figure 4.17 - 4.19. Fluidity predictions of tracer concentration decay in the streamwise and cross-stream direction are shown in Figures 4.20 and 4.21, respectively. For both Fluidity and TELEMAC results, tracer concentrations were least-squares fitted to Equation 4.8. Comparison TELEMAC results are shown in Figures 4.22 and 4.23, respectively. The calculated diffusion and tracer conser-

vation for the Fluidity and TELEMAC simulations are shown in Table 4.3. The conservation of tracer is shown in Table 4.4.

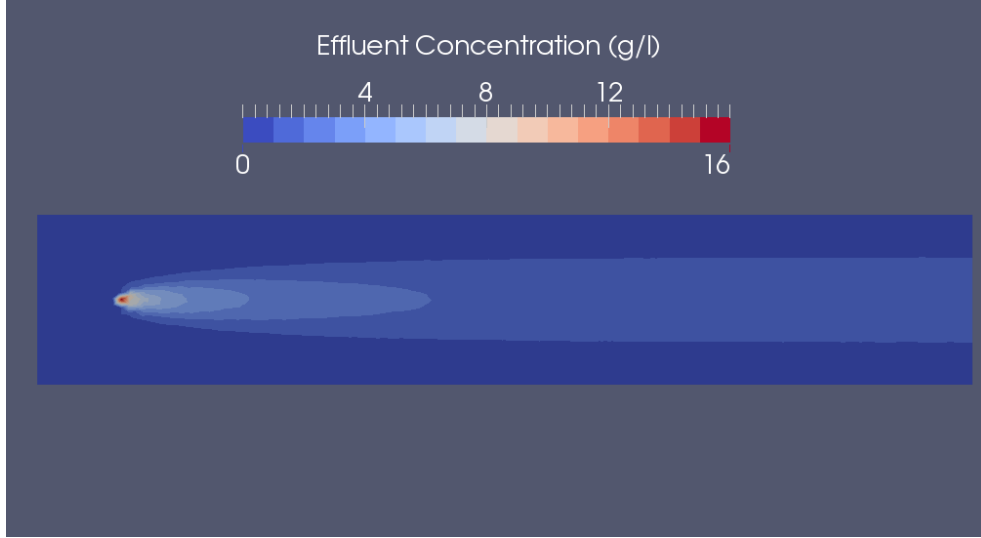


Figure 4.14: Fluidity prediction of tracer concentration for the point source with explicit diffusion simulations, with a node spacing of 0.5 m.

Table 4.3: Diffusion calculated during the point source with explicit diffusion test case.

Node spacing (m)	Fluidity	Fluidity	TELEMAC	TELEMAC
	Stream-wise diffusion (m^2/s)	Cross-stream diffusion (m^2/s)	Stream-wise diffusion (m^2/s)	Cross-stream diffusion (m^2/s)
0.5	0.126	0.134	0.124	0.103
0.25	0.107	0.110	0.089	0.066
0.125	0.100	0.100	0.081	0.061

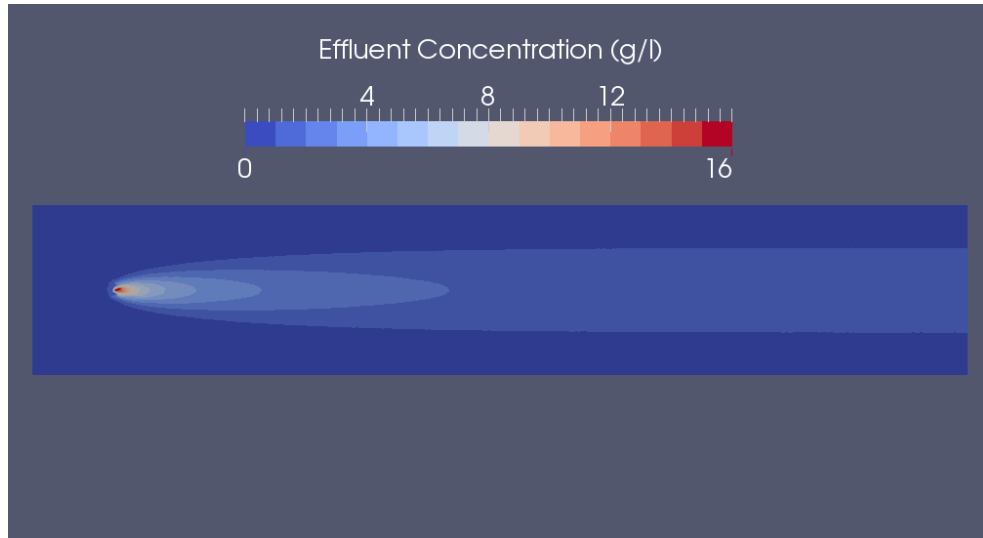


Figure 4.15: Fluidity prediction of tracer concentration for the point source with explicit diffusion simulations, with a node spacing of 0.25 m.

Table 4.4: Fluidity tracer conservation during the point source with explicit diffusion test case.

Node spacing (m)	source tracer flow rate (g/l/s)	outlet tracer flow rate (g/l/s)
0.5	10.000	10.000
0.25	10.000	10.000
0.125	10.000	10.000

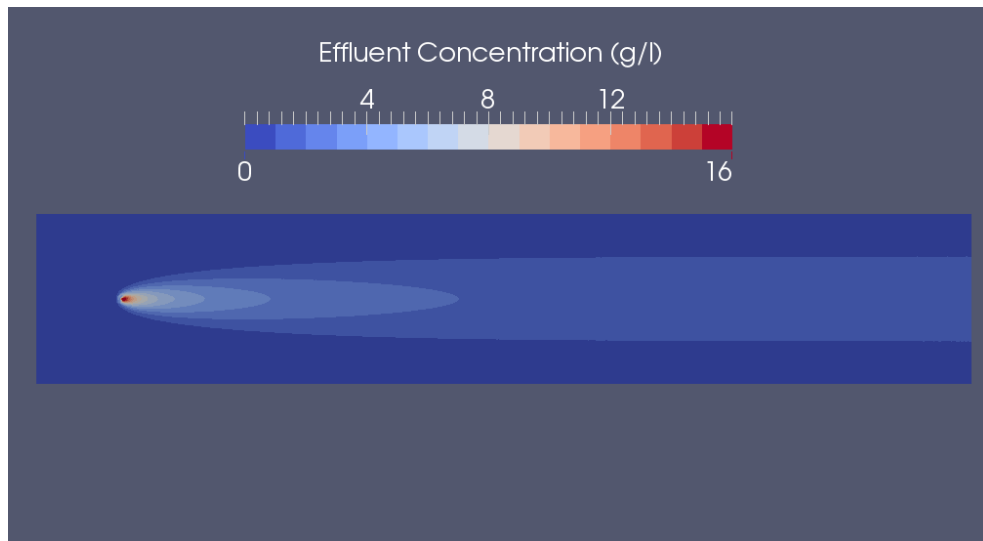


Figure 4.16: Fluidity prediction of tracer concentration for the point source with explicit diffusion simulations, with a node spacing of 0.125 m.

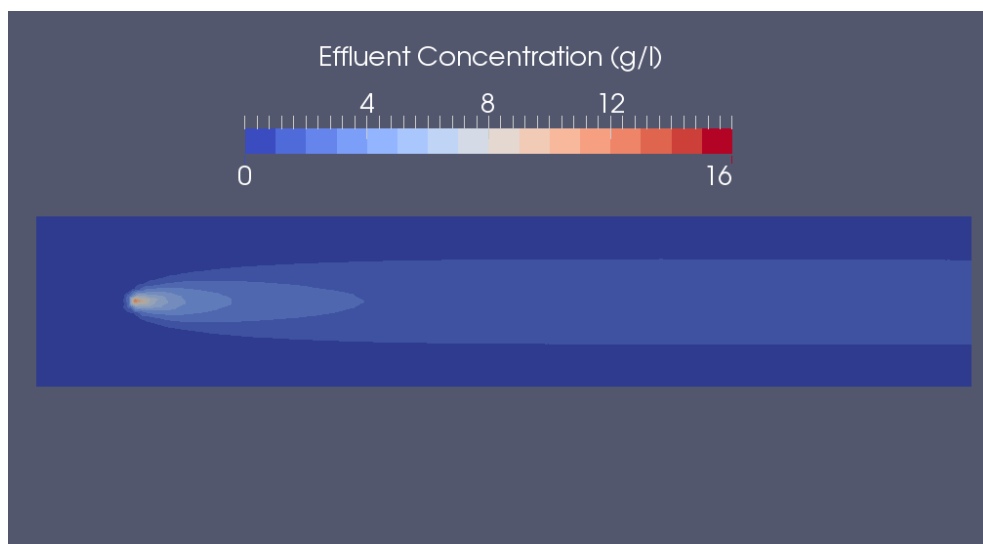


Figure 4.17: TELEMAC prediction of tracer concentration for the comparison TELEMAC simulation for point source with explicit diffusion simulations, with a node spacing of 0.5 m.

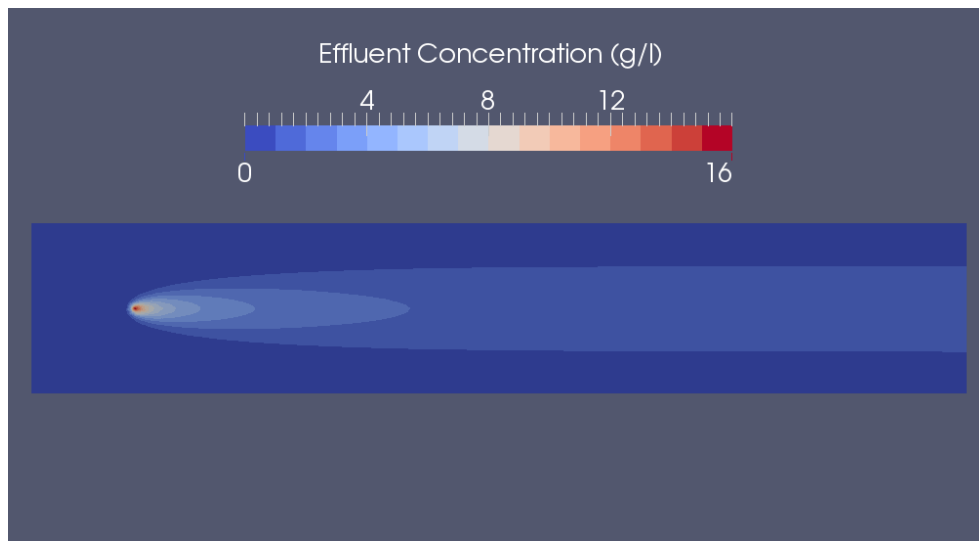


Figure 4.18: TELEMAC prediction of tracer concentration for the comparison TELEMAC simulation for point source with explicit diffusion simulations, with a node spacing of 0.25 m.

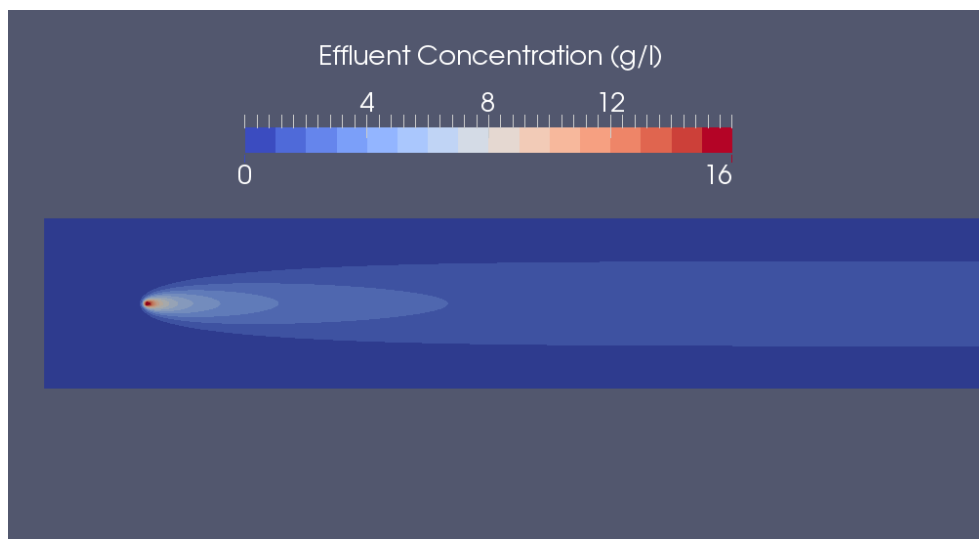


Figure 4.19: TELEMAC prediction of tracer concentration for the comparison TELEMAC simulation for point source with explicit diffusion simulations, with a node spacing of 0.125 m.

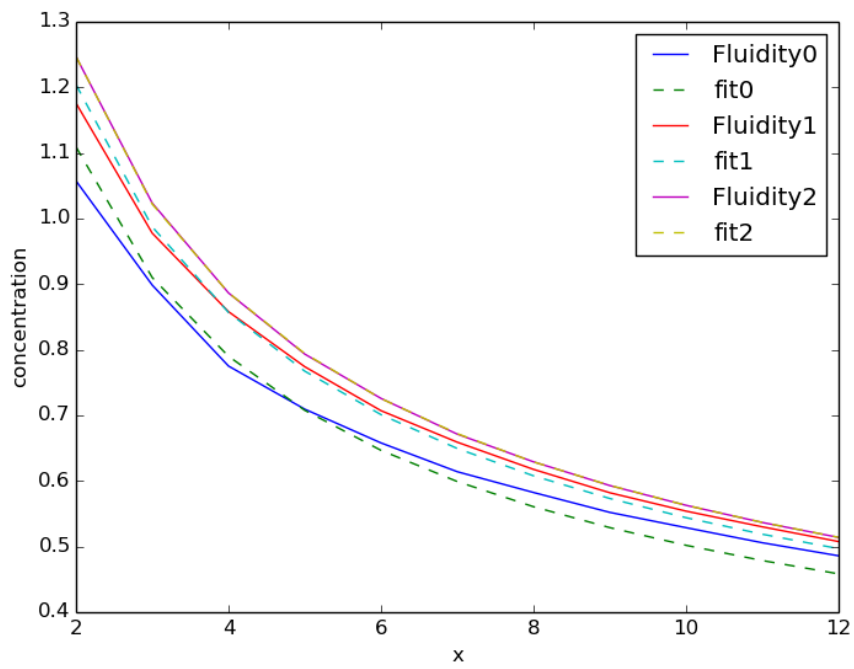


Figure 4.20: Fluidity prediction of stream-wise tracer concentration for the point source with explicit diffusion simulations. Fluidity0 is for the finest mesh and Fluidity2 is the coarsest.

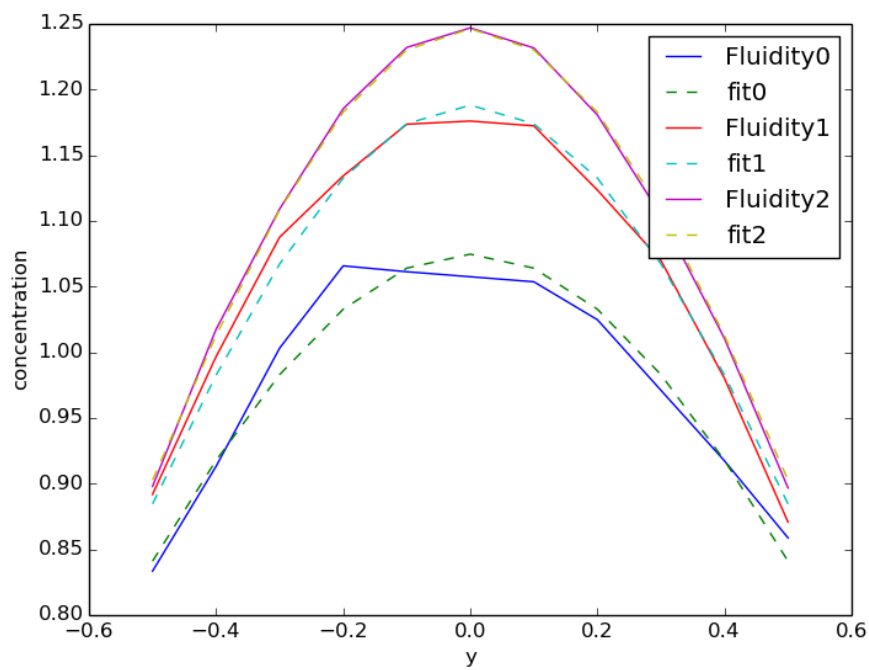


Figure 4.21: Fluidity prediction of cross-stream tracer concentration for the point source with explicit diffusion simulations, 2 m downstream of the point source. Fluidity0 is for the finest mesh and Fluidity2 is the coarsest.

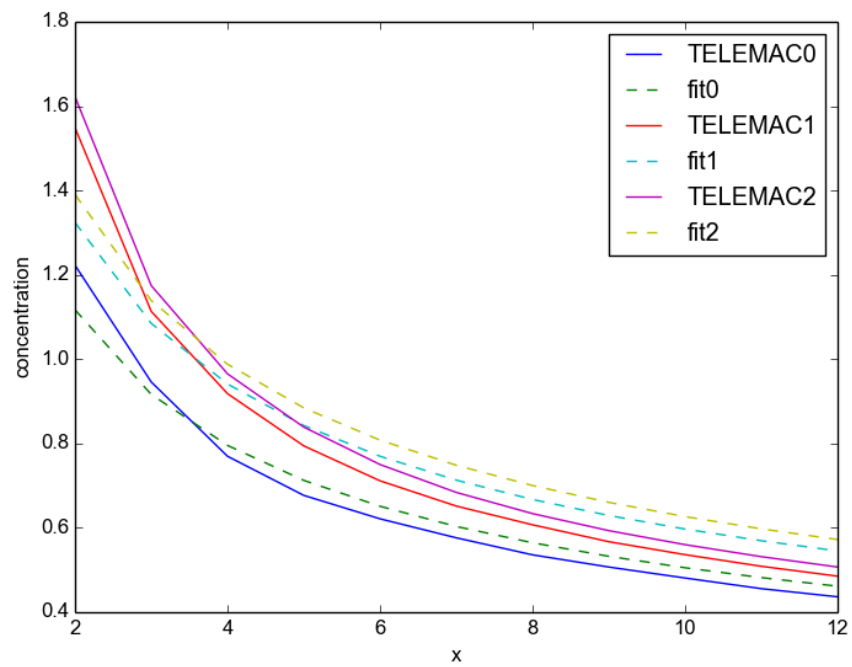


Figure 4.22: TELEMAC prediction of stream-wise tracer concentration for the point source with explicit diffusion simulations.

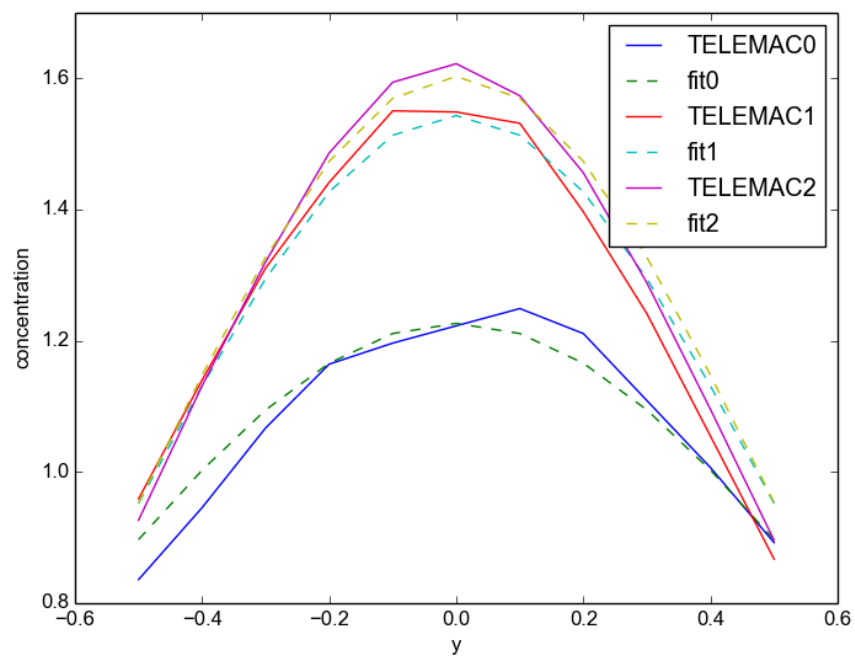


Figure 4.23: TELEMAC prediction of cross-stream tracer concentration for the point source with explicit diffusion simulations, 2 m downstream of the point source

4.4.3 Discussion

The Fluidity simulation diffusivity calculated using a fit to Equation 4.8 was shown to converge on the prescribed diffusivity of $0.1 \text{ m}^2/\text{s}$ and conserve the tracer field.

The analytical fit to the model data was better than was seen in the test case with zero explicit diffusivity. This is likely due to the explicit diffusivity drowning-out any anisotropy in the numerical diffusion.

4.5 Source of tracers

4.5.1 Problem outline

Three point sources of passive tracer are defined within a short channel with constant flow. The channel was 100 m wide and 40 m long, the depth was assumed to 1 m, and a prescribed velocity field of 1 m/s was used throughout the domain. A spurious result occasionally seen in models that have sources of more than one passive tracer is that tracer fields can interact and / or aggregate. This test case demonstrates the ability to compute the transport of multiple passive tracers with no influence on the flow patterns.

The simulation was three-dimensional. An unstructured two-dimensional mesh with node spacing of 4 m was used, was extruded vertically with 5 layers in the mesh through the depth of water (giving a total of 1805 nodes). The simulation was run for 1100 s with a timestep of 1.1 s (giving a Courant number of 0.275).

Point 1 was at coordinates $[-21, 5.3, -0.5]$ and Point 2 was at coordinates $[-0.8, -10.0, -0.5]$. Tracer 1 (“green”) was released from Point 1. Tracer 2 (“yellow”) was released from both Point 1 and Point 2. Tracer 3 (“red”) was released from Point 2. In the comparison TELEMAC simulation, Tracer 3 was released with an initial velocity, but that functionality is not available with Fluidity and so this was released with a stationary initial velocity. The source flow rate for all Tracers from all source points was 10 kg/s . A schematic of the model domain is shown in Figure 4.24.

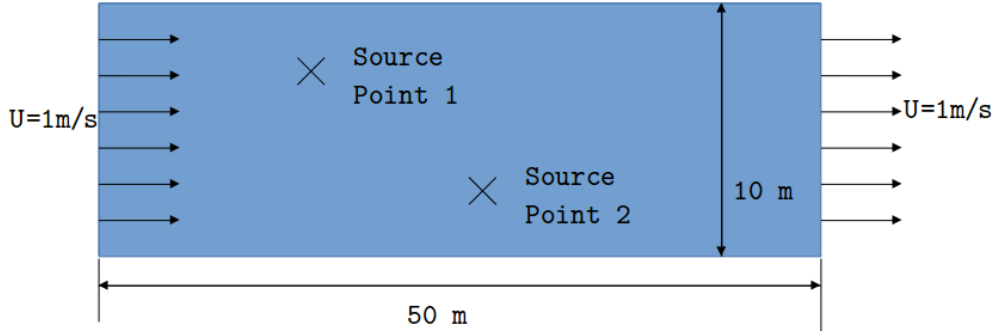


Figure 4.24: Schematic of the source of tracer test case.

4.5.2 Results

The profile of red tracer concentration from the TELEMAC and Fluidity model are shown in Figure 4.25 and 4.26, respectively. The profile of green tracer concentration from the TELEMAC and Fluidity model are shown in Figure 4.27 and 4.28, respectively. The profile of yellow tracer concentration from the TELEMAC and Fluidity model are shown in Figure 4.29 and 4.30, respectively.

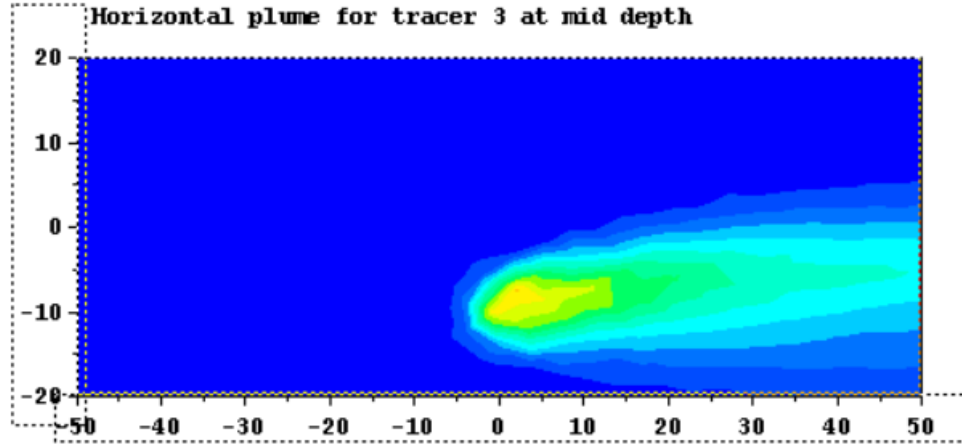


Figure 4.25: Concentration of the red tracer published in the TELEMAC validation report, for the 'source of tracer' test case.

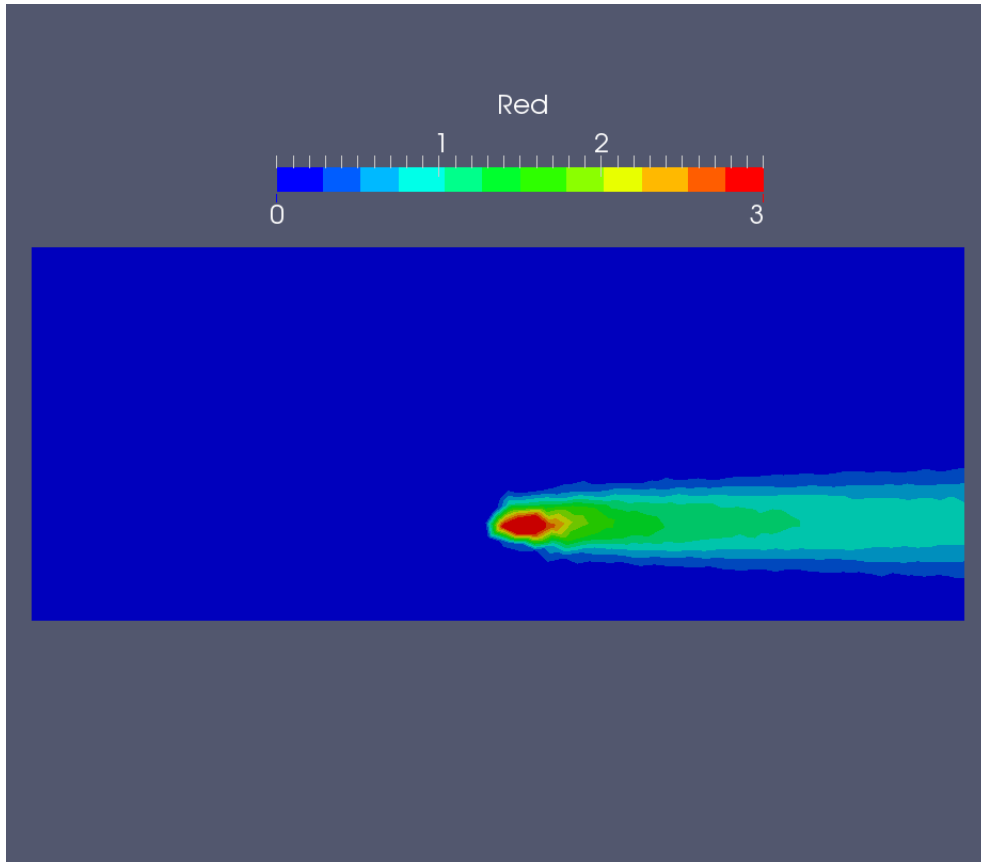


Figure 4.26: Concentration of the red tracer for the 'source of tracer' test case, as modelled by Fluidity.

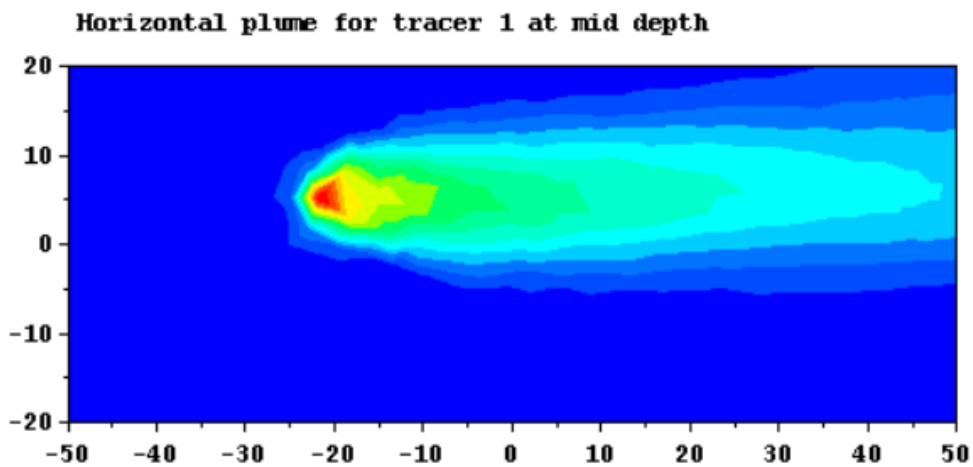


Figure 4.27: Concentration of the green tracer published in the TELEMAC validation report, for the 'source of tracer' test case.

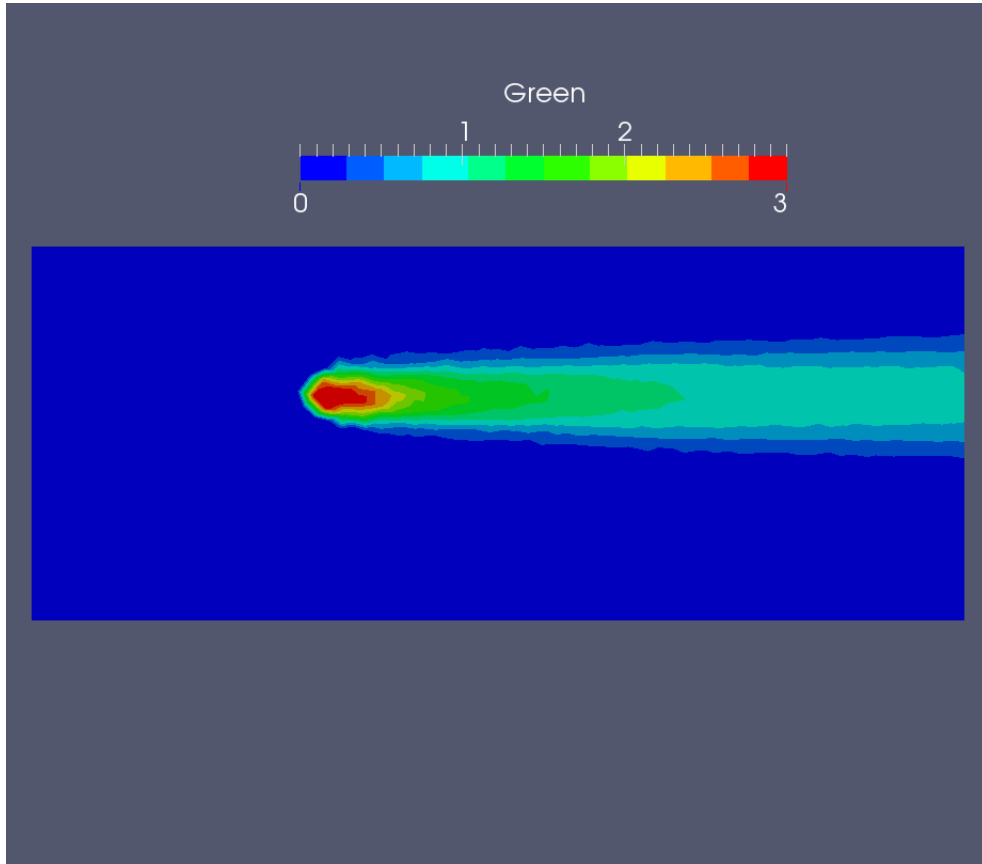


Figure 4.28: Concentration of the green tracer for the 'source of tracer' test case, as modelled by Fluidity.

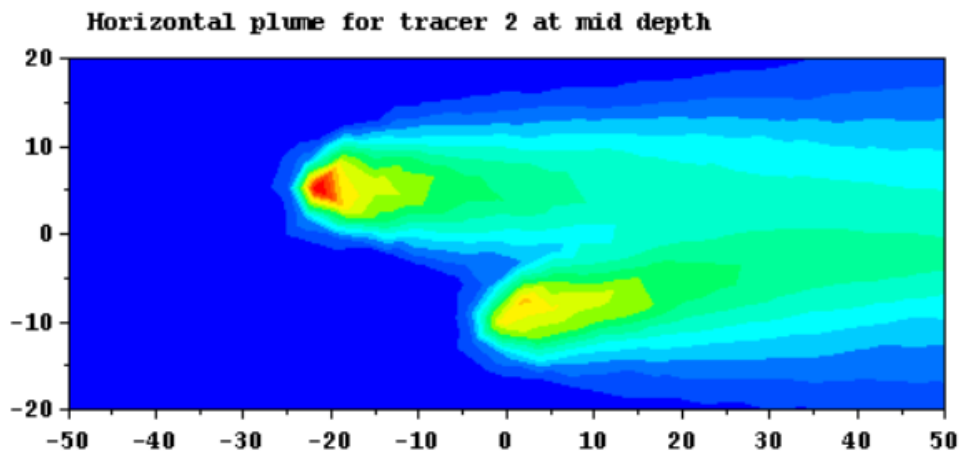


Figure 4.29: Concentration of the yellow tracer published in the TELEMAC validation report, for the 'source of tracer' test case.

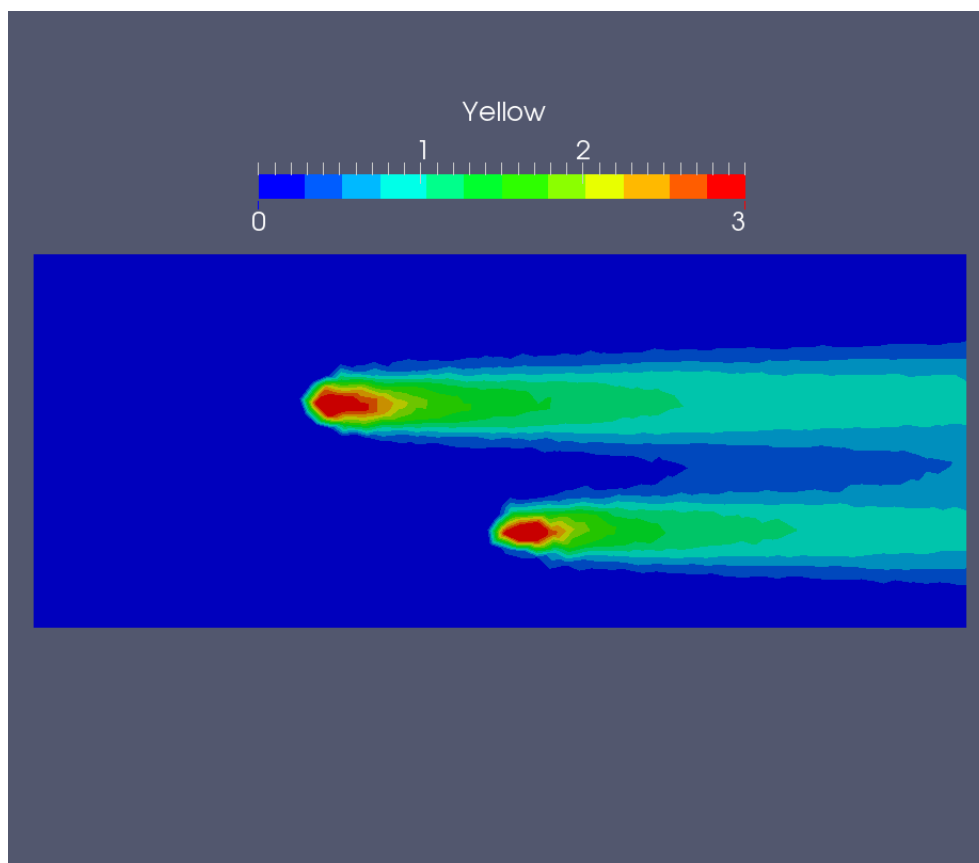


Figure 4.30: Concentration of the yellow tracer for the 'source of tracer' test case, as modelled by Fluidity.

4.5.3 Discussion

It is difficult to analytically assess whether any interaction was occurred between the tracer sources, but it can be seen from the model images that the tracer fields have not aggregated or distorted.

There are differences between the diffusion patterns predicted by the Fluidity and TELEMAC model that are likely due to the numerical diffusion caused by the relatively low mesh resolution.

4.6 Flat channel with saline stratification

4.6.1 Problem outline

This test case concerns the modelling of active tracer, salinity. For the previous point-source test cases all tracer fields were passive, i.e. the tracer had no influence on the flow. There was no need to solve the continuity or momentum equations as these equations would not have contained any tracer concentration term and the velocity and pressure field could be simply described. These two assumptions could not be made for this test case.

Salinity is an active tracer because its variation effects the fluid buoyancy, and so has an influence on the momentum equation. When modelling stratified flow within ocean models, the so-called geostrophic balance between Coriolis forces, buoyancy and the pressure gradient is very important. This test demonstrates the ability to model stratified flow with a particular focus on the stability of the stratification.

Current is modelled running through a domain with saline stratification. The results should show that the stratification remains stable, but a very mild slope in the domain is designed to trigger any vulnerability to geostrophic balance instability.

4.6.2 Model details

The domain is a channel 2000 m long and 100 m wide. The bottom of this channel has a very mild downwards slope of 1:10526. The general water depth is 10 m and the velocity along the channel is constant and equal to 1 m/s.

The contained a uniform horizontal resolution with edge lengths of 15.5 m and a vertical resolution with 21 sigma layers.

The Boussinesq form of the momentum equation was solved with the $k - \varepsilon$ turbulence model (see Equations 2.17, 2.18 and 2.18).

To maintain geostrophic stability, the $P_{1\text{DG}} - P_2$ finite element pair was used (piecewise-linear discontinuous representation of velocity and piecewise-quadratic continuous pressure).

A linear equation of state used to calculate the density, ρ ,

$$\rho = \rho_{\text{ref}}(1 - \beta(S - S_{\text{ref}})), \quad (4.9)$$

with saline contraction coefficient of $7 \times 10^{-6} \text{ l/g}$.

4.6.3 Results

An image of the salinity field at the final timestep of the TELEMAC and Fluidity models are shown in Figures 4.31 and 4.32. The vertical scale has been increased by 40 times to aid visualisation. A plot of salinity through the depth of water for the TELEMAC and Fluidity models is shown in Figures 4.33 and 4.34.

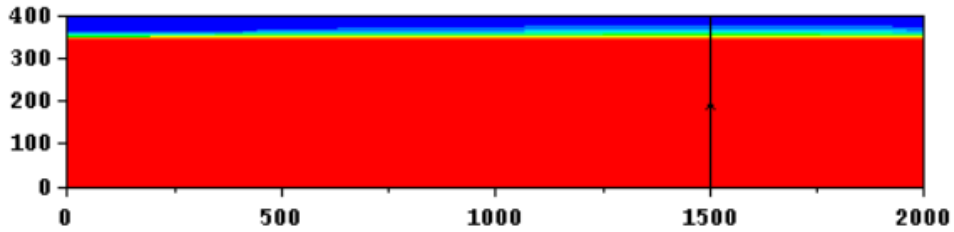


Figure 4.31: The salinity field from the TELEMAC model. The vertical scale has been increased by 40 times.

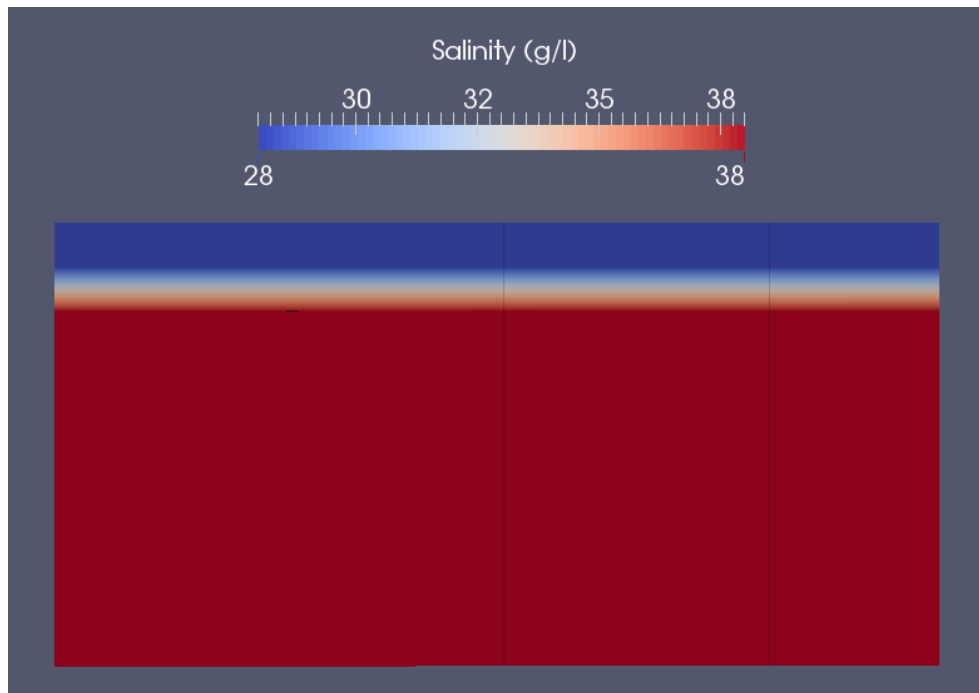


Figure 4.32: The salinity field from the Fluidity model. The vertical scale has been increased by 40 times.

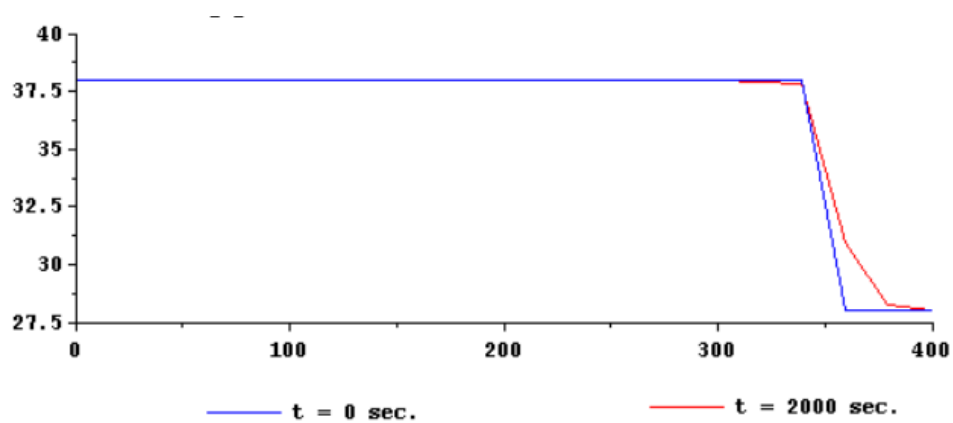


Figure 4.33: A plot of salinity variation on a vertical line through the centre of the TELEMAC model. The vertical scale has been increased by 40 times.

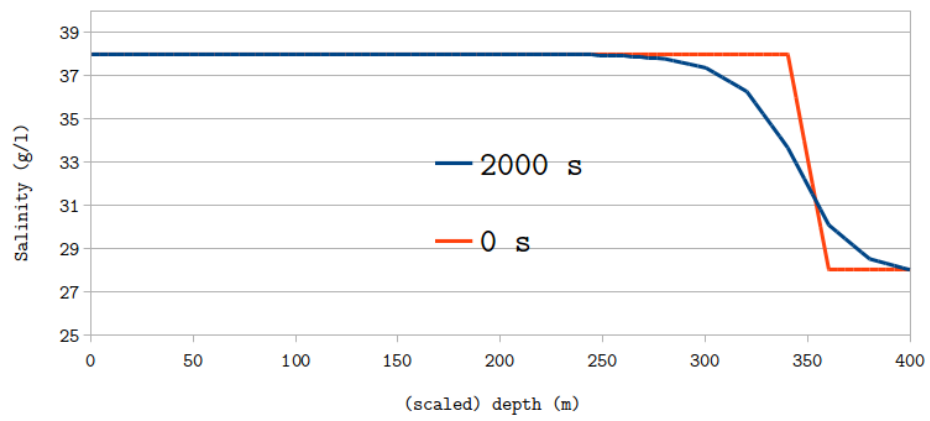


Figure 4.34: A plot of salinity variation on a vertical line through the centre of the Fluidity model. The vertical scale has been increased by 40 times.

4.6.4 Discussion

The salinity field within the Fluidity model did not maintain the step function prescribed in the initial conditions, but there was a similar level of tracer mixing as was seen in the TELEMAC model (even if the Fluidity model showed mixing both above and below the position of the initial step), which suggests a similar level of accuracy between the two models.

4.7 Variable vertical density in a V-shaped channel

4.7.1 Problem outline

A particularly difficult test of geostrophic stability comes in situations of slow moving flow over steep bathymetry. Haney [1991] was the first to describe how increasing vertical resolution in a 3-d ocean model could lead to error in computing the pressure gradient near steep bathymetry (known as “hydrostatic inconsistency”).

For this test case, a closed rectangular channel is initialised without motion, but with a vertical tracer distribution. This stratification should be stable and the distribution of the tracer should not evolve in time neither generate any flow. The purpose of this test is to verify the validity of the diffusion step and the proper treatment of the buoyancy terms. Moreover, this test demonstrates the ability to model a vertical stratification induced by an active tracer distribution on a non-horizontal topography.

4.7.2 Model details

The domain was horizontal V-shaped channel with a width of 100 m and a length of 500 m. The centre of the channel had a depth of 13 m and the domain sloped linearly up to a depth of 1 m at the side boundaries.

The model used a structured uniform-resolution horizontal mesh, with edge lengths of 12.5 m and 11 sigma layers in the vertical. To maintain geostrophic stability, the $P_{1DG} - P_2$ finite element pair was used (piecewise-linear discontinuous representation of velocity and piecewise-quadratic continuous pressure). The pressure field was split into hydrostatic and non-hydrostatic components, and solved separately, as was shown by Ford et al. [2004] to avoid additional instabilities often present in convectively dominated problems.

The Boussinesq form of the momentum equation was solved with an eddy viscosity of $1.0 \text{ m}^2/\text{s}$. It should be noted here that the TELEMAC simulations assumed a hydrostatic pressure for this test case where the Fluidity simulations did not.

4.7.3 Results

A plot of the vertical component of the velocity field on a slice through domain for the TELEMAC and Fluidity models is shown in Figures 4.35 and ???. The vertical scale has been increased by 12.5 times to aid visualisation.

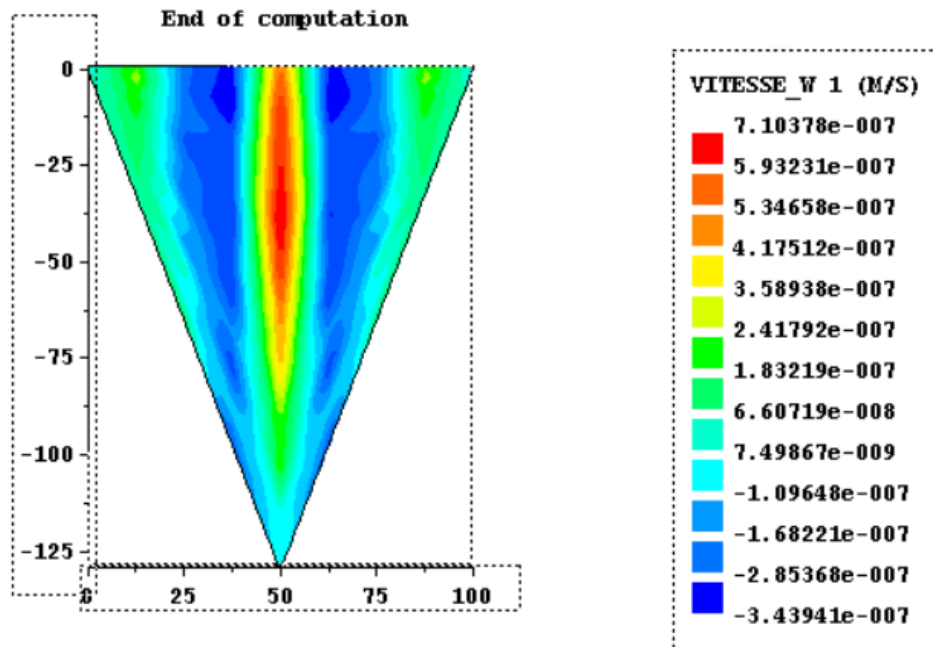


Figure 4.35: A plot of the vertical component of the velocity field on a slice through domain for the TELEMAC model. The vertical scale has been increased by 12.5 times.

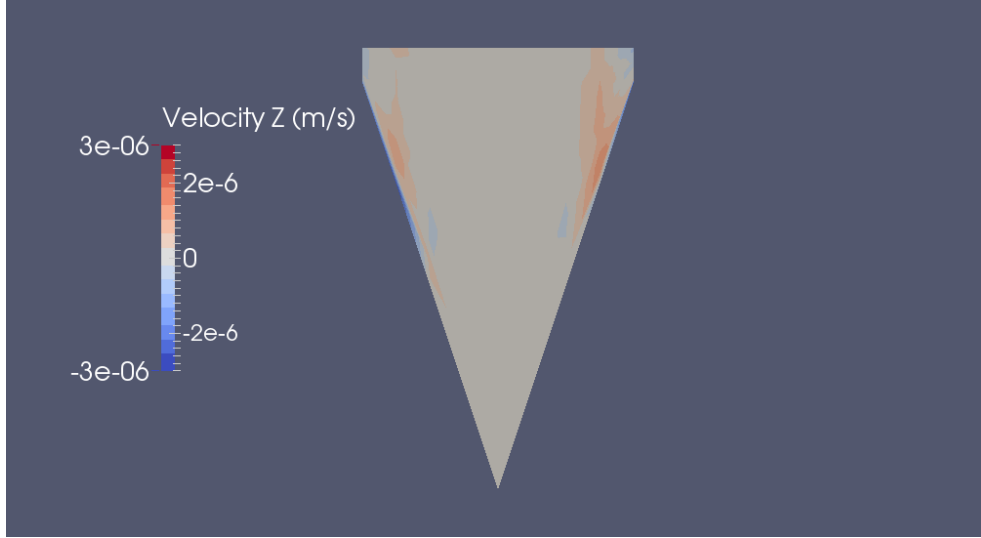


Figure 4.36: A plot of the vertical component of the velocity field on a slice through domain for the Fluidity model. The vertical scale has been increased by 12.5 times.

4.7.4 Discussion

The Fluidity model showed very gentle recirculations in flow at the sea-bed, likely due to some small inaccuracies in the calculation of the geostrophic pressure. Despite this, the model maintained stability, and the vertical velocities seen within the domain were minimal.

The much smaller vertical velocities seen within the TELEMAC simulations (and the different recirculation paths) were likely due to the hydrostatic assumption made within the TELEMAC model.

4.8 Conclusion

A series of test cases were run to assess the performance of a standard advection–diffusion solver method available within the Fluidity CFD model. The method compared well to world-leading free surface modelling software, Open TELEMAC. Numerical diffusion was shown to be relatively low, and the modelling of active tracers was shown to have good geostrophic balance.

The positive outcome of these tests give confidence in the discretisation and solver methods available within Fluidity. This allows the investiga-

tion and application of some of the numerical methods that aren't readily available in commercial CFD codes, such as mesh adaptivity.

5 Barotropic modelling of pollutant dispersion within the North Sea using 2-d mesh adaptivity

5.1 Introduction

This chapter describes the modelling of the dispersion of neutrally-buoyant dissolved pollutant from a hypothetical outfall off the east coast of the UK, using open-source CFD code Fluidity. The assumed effluent is typical of that released from a manufacturing plant. The aim of this modelling was to validate the use of Fluidity for modelling effluent dispersion within the coastal zone, and investigate the benefit of using 2-d horizontal mesh adaptivity to optimise model mesh resolution during the course of the simulation.

The UK is a developed country with a densely populated coastline. There are numerous power stations, industries, and wastewater treatment plants along the coastline, many of which discharge effluent of some sort to the surrounding waters through offshore outfalls. These outfalls can be near public beaches and / or areas of sensitive ecology, and their impact on the environment needs to be tightly regulated. A comprehensive review of water quality standards in the UK, Europe and beyond was carried out by Turnpenny and Liney [2007]. This review gave proposed limits to a range of pollutant concentration (including temperature and salinity limits) in order to meet Water Framework Directive (WFD) requirements (European Union [2010]). These proposals were suggested as interim action levels for coastal water by the UK Technical Advisory Group for the WFD (UKTAG) until more specific thresholds could be produced. These limits apply to effluent outside of the mixing zone, the definition of which is reviewed by Bleninger and Jirka [2011] (specifically concerning EU waters). They suggest that mixing zone should be defined by a perimeter drawn a radial distance from the diffuser opening(s). This radial distance should be a multiple, N , of the average water depth, somewhere between 1 and 10, depending on the sensitivity of the environment.

“Common values for most coastal water might be $N = 2$ to 3.”

This study will model the dispersal of a generic hypothetical neutrally-buoyant pollutant, and so no specific piece of legislation is relevant, but far-field concentrations will be predicted and compared, with a typical mixing zone marked to aid interpretation.

The position of the hypothetical outfall was assumed to be 53.97°N latitude, -0.10° E longitude, which is approximately 3 km from the UK coast-line, within the North Sea, at a water depth of approximately 10 m. A map of the United Kingdom showing the position of hypothetical outfall is shown in Figure 3.1.

The North Sea has a large tidal range (~ 5.6 m), with a dominant M_2 tide (see Table 3.1). This produces strong tidal currents of up to ~ 0.5 m/s, alternating from northwards to southwards with a period of roughly 12 h (semi-diurnal). The outfall is south of a headland that extends out into the sea about 12 km north. This headland affects the current patterns at the site and may be important for mixing.

During the warmer months of summer, the northern part of the North Sea becomes thermally stratified. In this period, the water column is divided into two layers, which can move independently, and will require a depth-resolving model to simulate accurately. In autumn, heat is lost to the atmosphere and the resultant mixing breaks-down stratification. van Leeuwen et al. [2015] identified regions of the North Sea that are stratified, non-stratified (mixed), regions of freshwater influence (ROFI), and intermittently (seasonally) stratified (see Figure 5.1). The location of the hypothetical outfall near the boundary between regions categorised “permanently mixed” and “intermittently mixed”. For the purposes of this study it has been assumed that the water is mixed, meaning that a 2-d model of flow is sufficient. If one were concerned about mixing further offshore then it would be necessary to perform a depth-resolving (3-d) model study.

It should be noted that these simulations also did not account for the effects of surface temperature flux, rainfall, wind or evaporation. These physical phenomena can all have an influence on stratification and mixing, especially for buoyant effluent released into deep water, but for neutrally-buoyant pollution released into well mixed receiving water, the effects will be negligible.

This study used 2-d horizontal mesh adaptivity in order to optimise the model mesh resolution during the course of the simulation. As was dis-

cussed in Section 2.6.2, mesh adaptivity offers a benefit when important flow features that require higher resolution are unsteady and move significantly within the domain during the course of the simulation. The flow within the vicinity of the site is dominated by the tidal currents, which oscillate between flowing northwards and southwards during a tidal cycle. This means that both the direction of effluent transport and flow around the headland vary considerably during the course of a tidal cycle.

To adequately model this motion using a static mesh (without mesh adaptivity) requires a fine mesh resolution over the entire footprint of effluent transport, and around both sides of the headland.

To assess the benefit of mesh adaptivity, results were compared between a simulation using a static mesh typical of that used within the consultancy, and a simulation using an adaptive mesh calibrated to contain a similar number of nodes (and so requiring a comparable computational resource).

5.2 State-of-the-art

As noted by Wood et al. [2014], hydrodynamic models are widely used to model effluent dispersion in the coastal zone.

The models used are largely 3-d finite element models that solve the shallow water form of the Navier-Stokes equations for transport and motion in multiple layers, using a Boussinesq assumption. Examples of widely used codes include Delft3D (Deltares), MIKE (DHI) and Open TELEMAC.

The model formulations usually include the effects of buoyant spreading and inhibition of vertical mixing associated with sharp density gradients, and can capture stratified layer structures. Variations through the water depth are usually resolved using a hybrid sigma approach, with a number of quasi-horizontal mesh planes that can either move up and down as the water depth changes (representing fixed proportions of the water depth), or can be set at fixed heights relative to a reference height (often the seabed or sea surface).

Further details of typical hydrodynamic models used for effluent dispersion assessments are given by Roberts et al. [2010].

Consultancy studies largely use static horizontal grids, with horizontal mesh refinement chosen on the basis of sensitivity tests and prior knowledge of the plume's likely location. HR Wallingford has also devel-

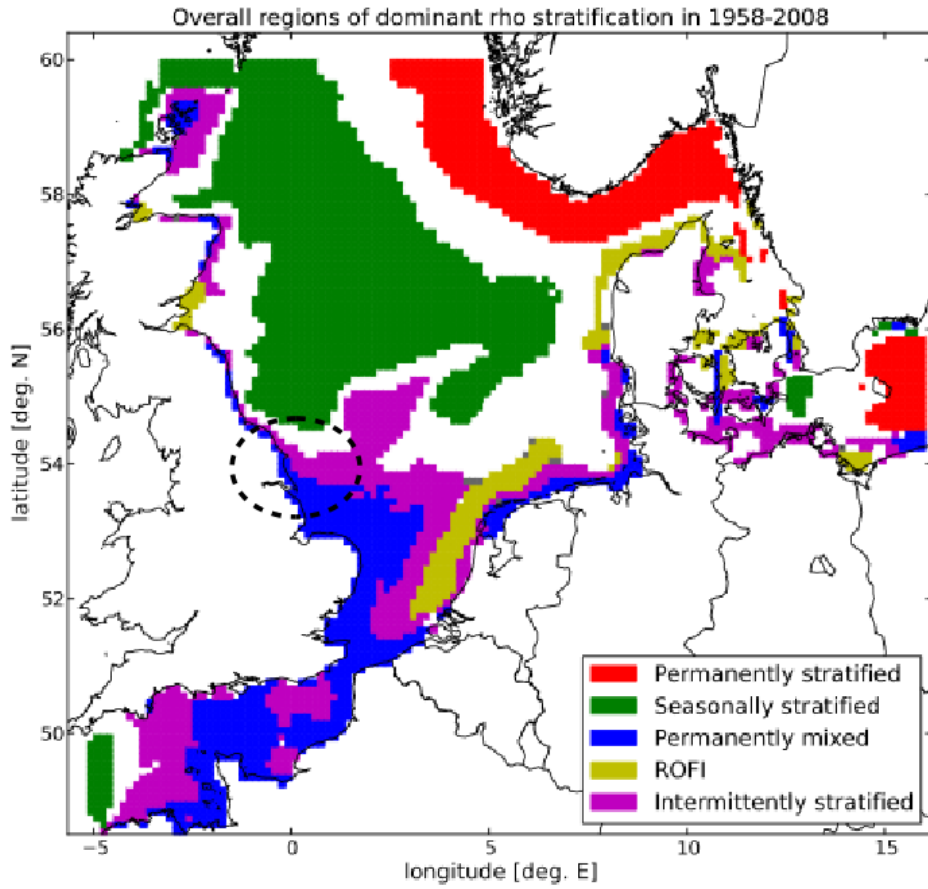


Figure 5.1: A map of the North Sea showing regions categorised stratified, non-stratified (mixed), regions of freshwater influence (ROFI), and seasonally stratified, van Leeuwen et al. [2015]. The dashed circle shows the region of the hypothetical outfall.

oped adaptive vertical mesh refinement techniques to capture the vertical structure of dense and buoyant plumes (e.g. Cawthorn et al. [2011], Mead et al. [2011]).

Publications investigating horizontal mesh refinement techniques have been rare and their application has largely been confined to structured grids with tree-based refinement (see Popinet and Rickard [2006]) that have limited application within complex domains. Recent studies investigating unstructured horizontal mesh refinement have been published by Wackers et al. [2012] and Santilli and Scotti [2015].

5.3 Model details

5.3.1 Model equations and their discretisation

Momentum and continuity were modelled using the Shallow-Water equations, discretised on a $P_{\text{IDG}} - P_2$ finite element (piecewise-linear discontinuous representation of velocity and piecewise-quadratic continuous free-surface height), to minimise the error in the pressure gradients resulting Coriolis accelerations, as described within Section 3.4.1.

Effluent concentration, c , was calculated using a discontinuous galerkin discretisation of the advection-diffusion equation (Equation ?).

Both the discontinuous Galerkin and control volume discretisation of the advection-diffusion equation were shown by Hiester [2011] to have low numerical diffusion for a given mesh resolution. Here the discontinuous Galerkin method was used because the calculation of advection using upwinding results in a natural “switching-off” of the advection-diffusion terms at inlet boundaries.

The viscosity and effluent diffusivity were both set to $0.1 \text{ m}^2/\text{s}$. The viscosity term acted as an eddy viscosity and kept the simulation stable. The diffusivity term gave a Peclet number (Lu/D , where L is the local edge length) of roughly unity in the regions of highest resolution. Ideally a suitable turbulence model would have been used to give a more accurate simulation, but a constant eddy viscosity and diffusivity are suitable for model inter-comparison.

5.3.2 Time discretisation, time step, and simulation length

All fields were solved using a fully implicit time discretisation. An adaptive timestep ensured a Courant number throughout the domain of less than 5.0. An upper limit of 200 seconds per timestep was applied to avoid model instability. To maintain stability, the advection term within the discontinuous Galerkin velocity field was sub-cycled with a reduced timestep to ensure a Courant number throughout the domain of less than 0.1.

The simulation was spun-up over three tidal cycles, and model results analysed and presented for the fourth tidal cycle. The total simulation time was 48 h).

5.3.3 Domain

The hypothetical outfall is South of the Flamborough headland. Approximately 30 km to the south is the Humbar estuary. The model domain stretches northwards sufficiently to include the headland, but stops short of the estuary to the south. The estuary was considered to have insignificant influence on the local tidal motion.

The domain extended approximately 35 km offshore, which was sufficient to avoid boundary effects to the effluent motion and flow around the headland.

The domain boundaries are defined by the coastline to the west, and tidally forced boundaries to the north, east and south. The forced boundaries within a coastal effluent dispersion model are typically aligned either perpendicular and parallel to the dominant currents within the site (to avoid angled inflow and outflow, which might be badly captured). The dominant currents within this site are tidal, and run roughly parallel to the coastline. As such, the domain boundaries are roughly perpendicular and parallel to the bathymetry contours.

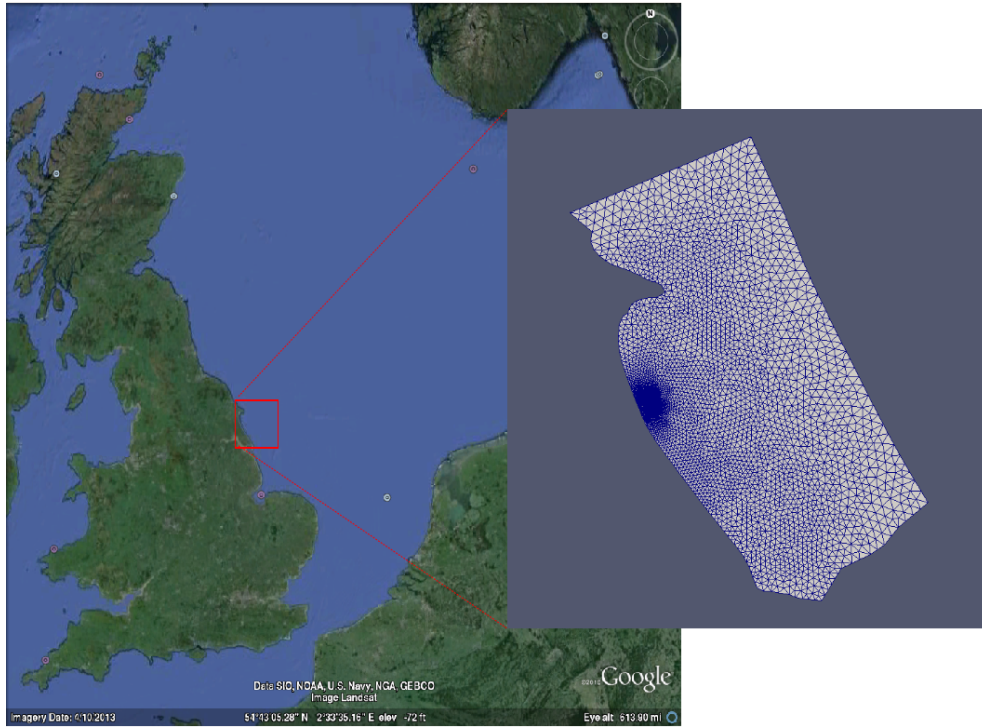


Figure 5.2: Site of hypothetical effluent outfall within the North Sea (off the UK coastline) and the model domain.

5.3.4 Bathymetry

The bathymetry in the vicinity of the hypothetical site is shown in Figure 5.3. On a regional scale, currents are influenced by variations in bathymetry. The bathymetry at the site is not flat, and so the assumption of a constant slope will result in some deviation of current predictions from reality. 2-d horizontal mesh adaptivity in a coastal model is currently only possible for a constantly sloping bathymetry as it is not possible to interpolate complex bathymetry between domain meshes without creating inconsistencies in the domain floor in areas where resolution has been added or removed. This study aims to act as a proof-of-concept that 2-d horizontal mesh adaptivity can offer a benefit if the assumption of a flat bathymetry is reasonable, but also act as a useful source of knowledge for the application of 2-d horizontal mesh adaptivity once a method for interpolating complex bathymetry between domain meshes becomes available.

The model bathymetry had a constant slope, going from roughly 5 m depth at the coastline to roughly 65 m depth at the offshore boundary (an image of the model bathymetry is shown in Figure 5.4). The model boundary at the coastline has a minimum depth within the model of 5 m. This is an alternative to using wetting and drying techniques for handling coastline interaction.

5.3.5 Coastline

Coastline data was taken from the Global Self-consistent, Hierarchical, High-resolution Geography Database (GSHHG, Wessel and Smith [1996]). This is a high-resolution geography data set amalgamated from three data bases in the public domain:

- World Vector Shorelines (WVS).
- CIA World Data Bank II (WDBII).
- Atlas of the Cryosphere (AC).

The GSHHG geography data come in five different resolutions: crude, low, intermediate, high, and full. The coastline of the model domain (shown in Figure 5.2) was created using the full resolution data.

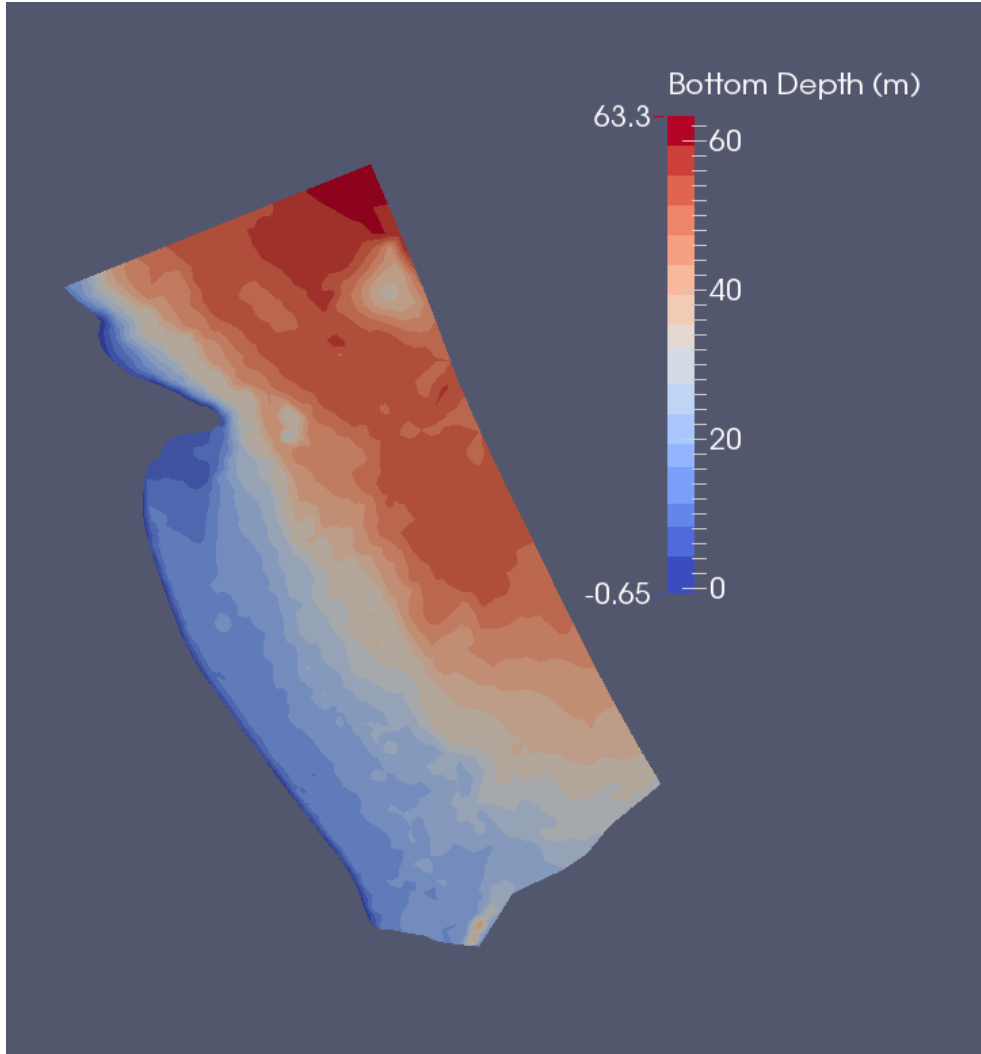


Figure 5.3: Bathymetry data taken at the site of the hypothetical outfall, provided by HR Wallingford.

5.3.6 Tides

Tidal forcing was generated using tide constituent data from Finite Element Solution (FES) tide model, FES2004 (Lyard et al. [2006]). FES2004 is based on the resolution of the tidal barotropic equations on a global finite element grid (~ 1 million nodes) which leads to solutions independent of in-situ and remote-sensing data (no open boundary conditions and no data assimilation). Tidal constituents are distributed on $1/8^\circ$ grids (amplitude and phase).

An effluent dispersion model would typically use all principal tide con-

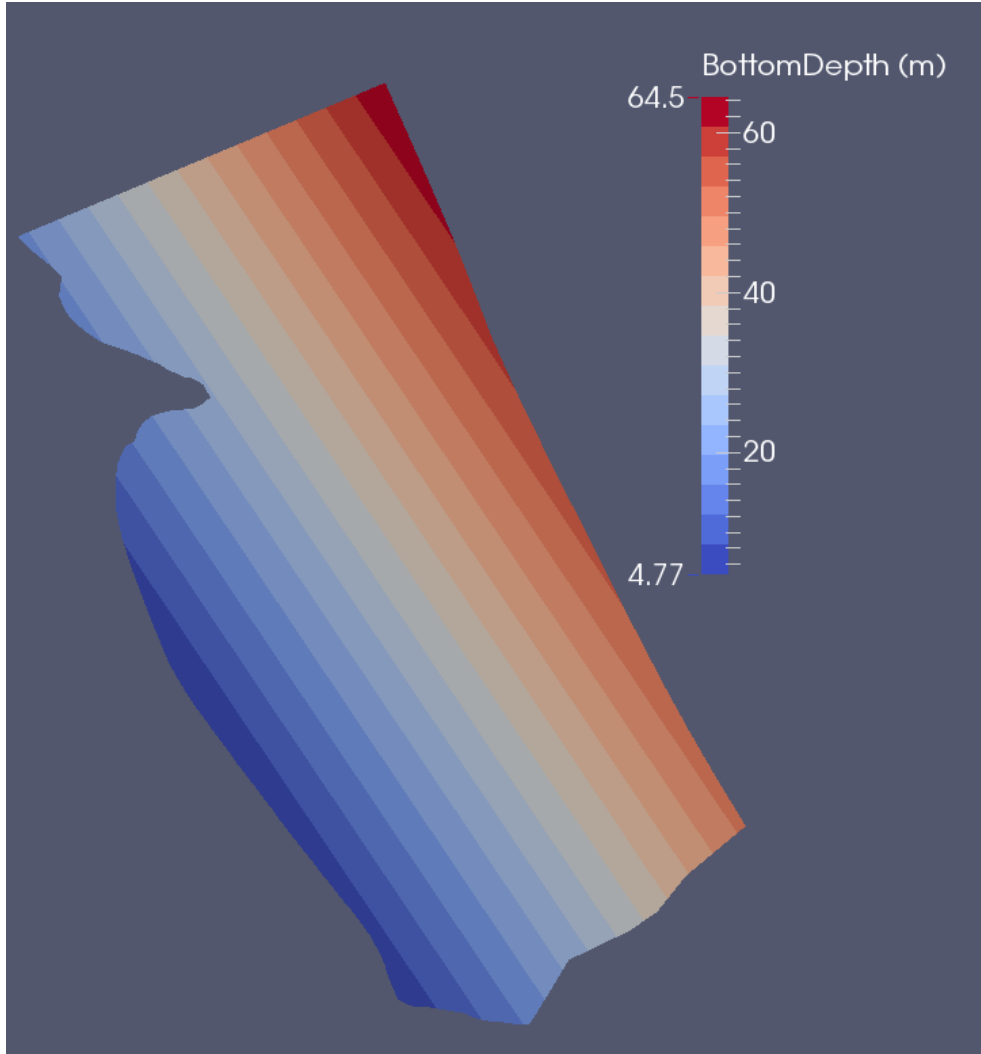


Figure 5.4: The model bathymetry for the North Sea effluent dispersion model.

stituents that have significant amplitude within the region. This model was forced by the M_2 , S_2 , N_2 , and K_2 semi-diurnal and the K_1 , O_1 , Q_1 , and P_1 diurnal tide constituents. Table 3.1 shows the relative period and magnitude of these constituents.

Tidal-forcing was applied to open ocean domain boundaries through setting a Dirichlet condition on the non-hydrostatic part of the pressure. Co-oscillating tides are forced as cosine waves of specified phase and amplitude along designated boundaries:

$$\eta = \sum_i A_i \cos(\sigma_i t - \theta_i) + \sum_j A_j \cos(\sigma_j t - \theta_j) \quad (5.1)$$

where A is the amplitude of the tidal constituent (m) and θ is the phase of the tidal constituent (radians), Wells [2008].

5.3.7 Coriolis effect

The rotation of the Earth creates the Coriolis effect, which is accounted for in this model using the “ β -plane” approximation (Cushman-Roisin [1994]), which was described in Section 3.4.7.

For this model, the Coriolis parameter at the lowest latitude within the domain, $f_0 = 3.709 \times 10^{-5}$, and the constant used to calculate f at other points within the domain, $\beta = 1.347 \times 10^{-11}$

5.3.8 Outfall model

The outfall was modelled as a 2-d Gaussian source of effluent,

$$g(x, y) = 1/100 \cdot \exp \left\{ \left(\frac{y - y_1}{15} \right)^2 - \left(\frac{x - x_1}{15} \right)^2 \right\}. \quad (5.2)$$

The width of 225 m and an amplitude of 0.01 g/l/s, giving a flow rate in the domain of 6.67 g/s. These parameters were chosen to approximate that expected at the near-field of an industrial plant outfall.

5.3.9 Mesh generation

Two simulations were created with different meshes:

- a static mesh typical of that used within consultancy for modelling effluent dispersion. This mesh was provided by HR Wallingford. This mesh had a smooth gradation from edge lengths of 10 m in the vicinity of the outfall, to edge lengths of 1500 m at the model boundaries. It contained 8656 nodes. An image of this mesh is shown in Figure 5.5,

- and an adaptive mesh, using Fluidity’s in-built mesh adaptivity algorithm, that was calibrated to produce a comparable number of nodes to the static mesh (varying by between approximately 8100 – 8700 nodes during the course of a tidal cycle).

A description of the methodology used for mesh adaptivity used within Fluidity was described in Section 2.4.6. For two-dimensional mesh adaptivity, the Hessian used to calculate the error metric is given by:

$$H = \begin{pmatrix} \frac{\partial^2 \eta}{\partial x^2} & \frac{\partial^2 \eta}{\partial x \partial y} \\ \frac{\partial^2 \eta}{\partial x \partial y} & \frac{\partial^2 \eta}{\partial y^2} \end{pmatrix}, \quad (5.3)$$

where η is the field being considered by the adaptivity algorithm. An error metric was calculated for both effluent concentration and velocity, and then combined to give a final error metric which defined a suitable mesh to adequately resolve both fields. For a given point within the domain, the final error metric is defined as the highest (i.e. finest) of the field error metrics. This means that different regions within the domain can have resolution determined by different fields, depending on the field’s relative curvature in that region. The absolute interpolation error prescribed for effluent concentration and velocity was 0.3 g/l and 20.0 m/s, respectively. This produced an optimised mesh that had a comparable number of nodes to the static mesh.

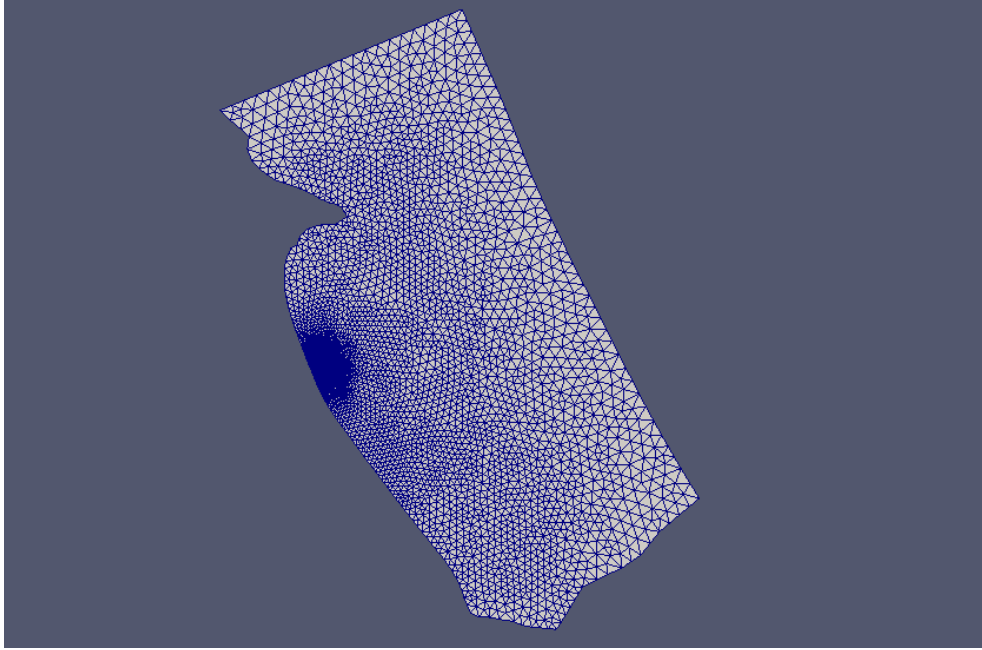


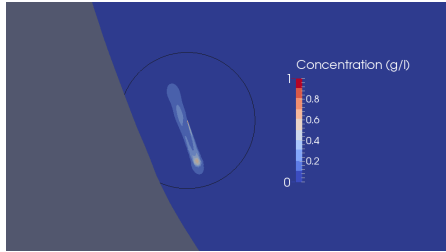
Figure 5.5: An image of the comparison static mesh typical of that used for modelling effluent dispersion. The region of high resolution is centred about the outfall.

5.4 Results

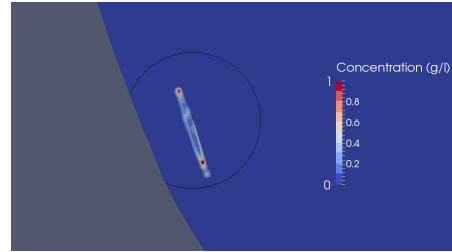
Effluent dispersion from a hypothetical outfall off the coast of the North-East of the UK was modelled for a 12 m tidal cycle (with a spin-up time of 36 h allowed for the velocity field to stabilise).

Model predictions of effluent dispersion at two hour intervals through a 12 hour tidal cycle were made using a static mesh, and using a mesh adaptivity algorithm to optimise resolution during the simulation. Plots of effluent concentration using a linear scale are shown in Figures 5.6 – 5.13. The linear scale allows an assessment of model agreement on the overall size and shape of the effluent plume. Plots of effluent concentration using a logarithmic scale are shown in Figures 5.14 – 5.21. The logarithmic scale allows an assessment of model agreement on the extent of the plume edges, where effluent concentrations are especially low. For easier visualisation and comparison of the concentration contours, a green contour marks the 0.1 g/l contour.

For scale, a black circle marks the 4 km distance from the outfall.

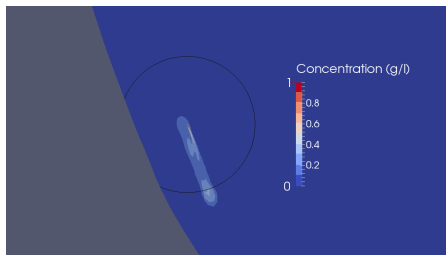


(a) Static mesh

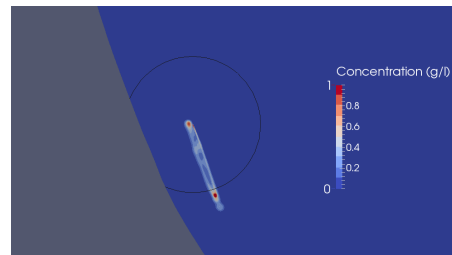


(b) Adaptive mesh

Figure 5.6: Linear-scale plot of effluent dispersion at the start of the 12 hour tidal cycle.

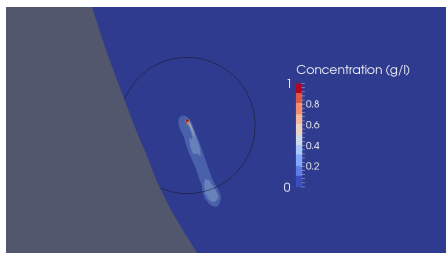


(a) Static mesh

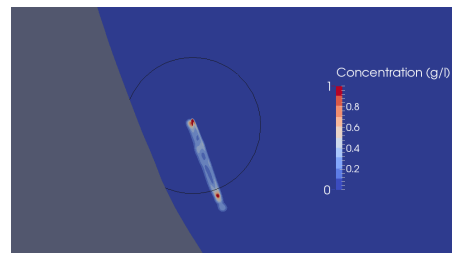


(b) Adaptive mesh

Figure 5.7: Linear-scale plot of effluent dispersion 2 hours into the 12 hour tidal cycle.

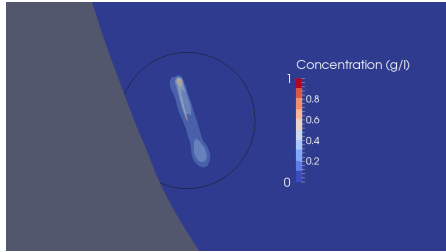


(a) Static mesh

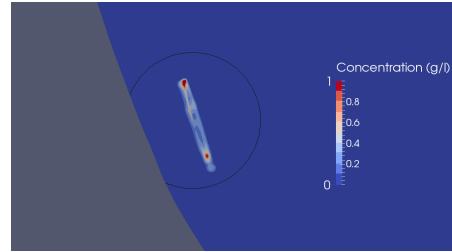


(b) Adaptive mesh

Figure 5.8: Linear-scale plot of effluent dispersion 4 hours into the 12 hour tidal cycle.

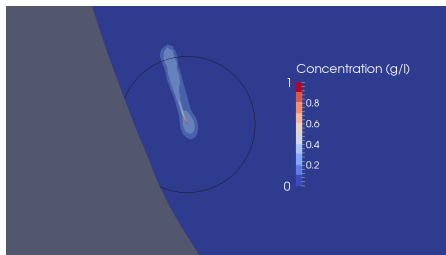


(a) Static mesh

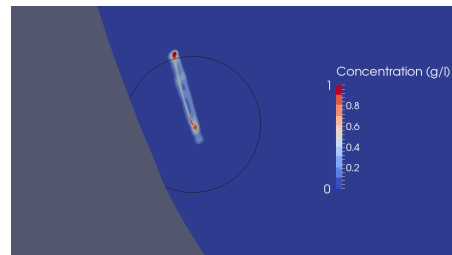


(b) Adaptive mesh

Figure 5.9: Linear-scale plot of effluent dispersion 6 hours into the 12 hour tidal cycle.

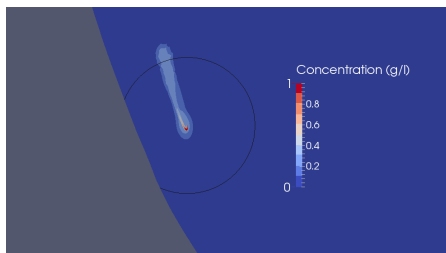


(a) Static mesh

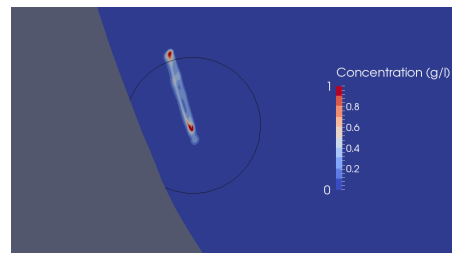


(b) Adaptive mesh

Figure 5.10: Linear-scale plot of effluent dispersion 8 hours into the 12 hour tidal cycle.



(a) Static mesh



(b) Adaptive mesh

Figure 5.11: Linear-scale plot of effluent dispersion 10 hours into the 12 hour tidal cycle.

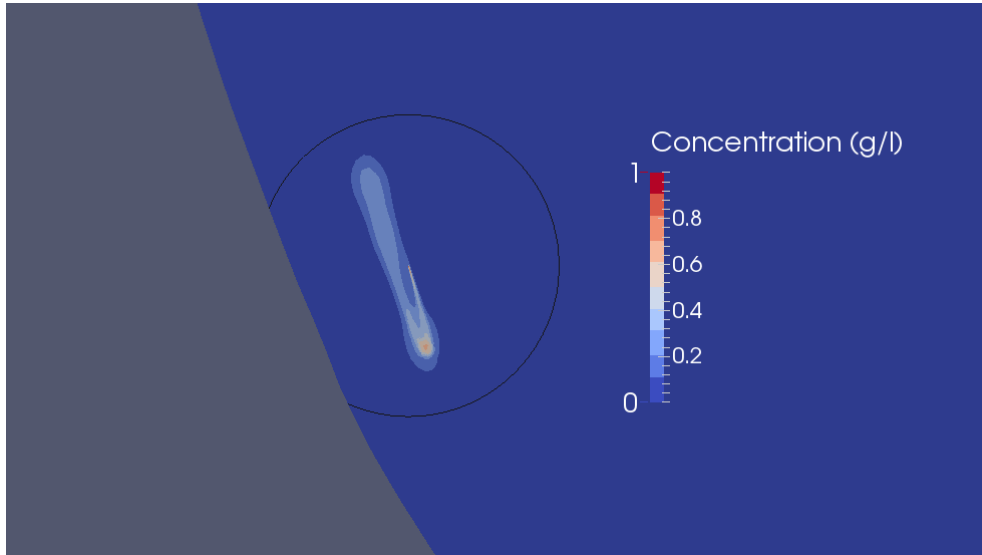


Figure 5.12: Linear-scale plot of effluent dispersion at the end of the 12 hour tidal cycle, using a static mesh.

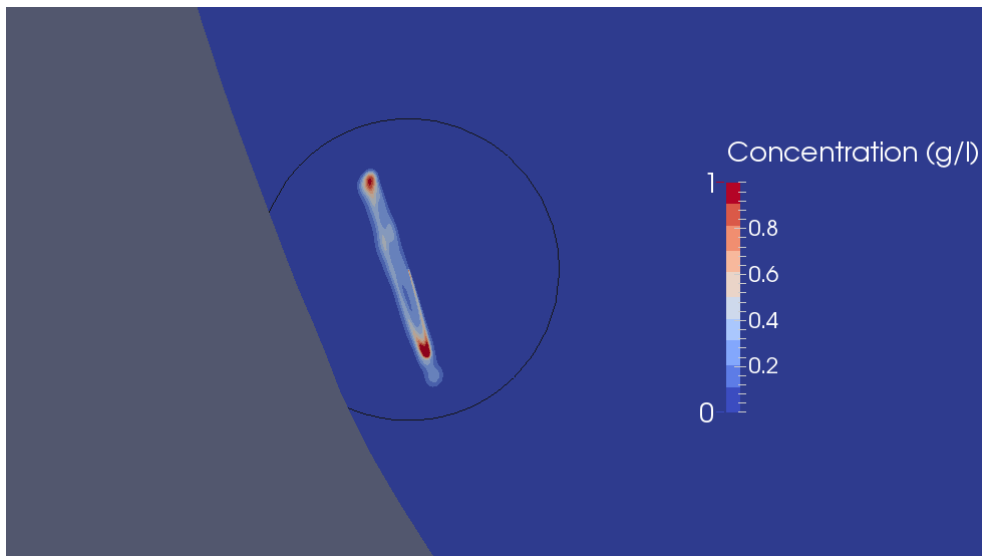
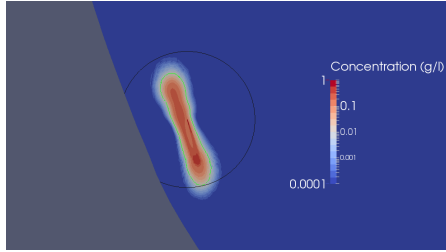
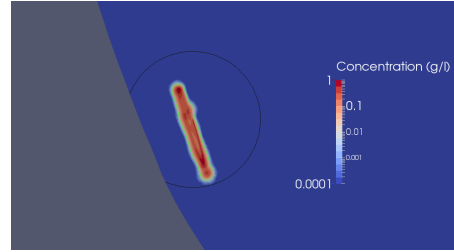


Figure 5.13: Linear-scale plot of effluent dispersion at the end of the 12 hour tidal cycle, using an adaptive mesh.

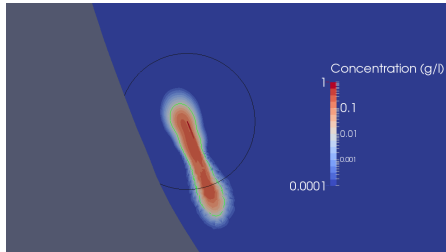


(a) Static mesh

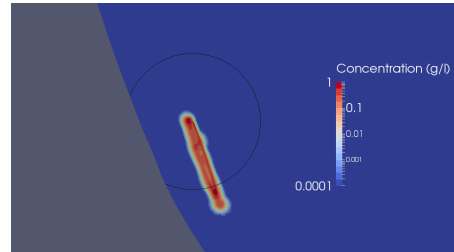


(b) Adaptive mesh

Figure 5.14: Logarithmic-scale plot of effluent dispersion at the start of the 12 hour tidal cycle.

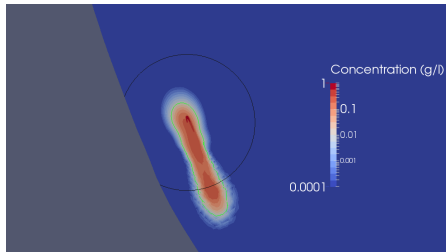


(a) Static mesh

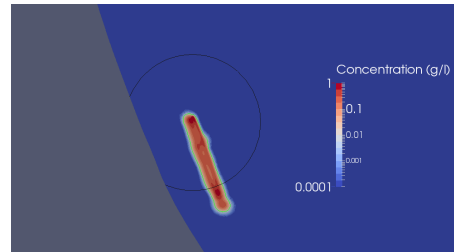


(b) Adaptive mesh

Figure 5.15: Logarithmic-scale plot of effluent dispersion 2 hours into the 12 hour tidal cycle.

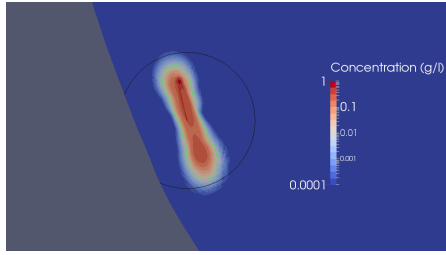


(a) Static mesh

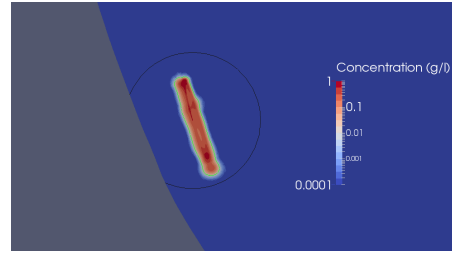


(b) Adaptive mesh

Figure 5.16: Logarithmic-scale plot of effluent dispersion 4 hours into the 12 hour tidal cycle.

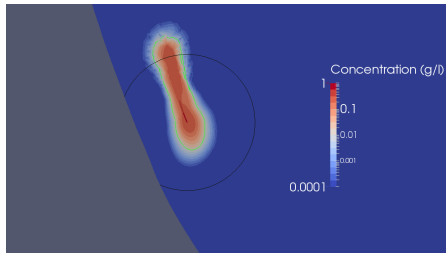


(a) Static mesh

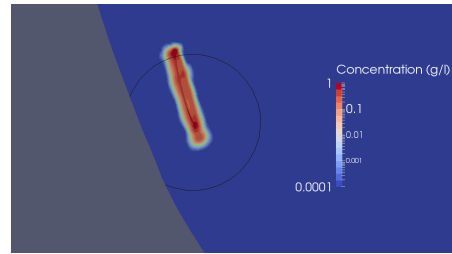


(b) Adaptive mesh

Figure 5.17: Logarithmic-scale plot of effluent dispersion 6 hours into the 12 hour tidal cycle.

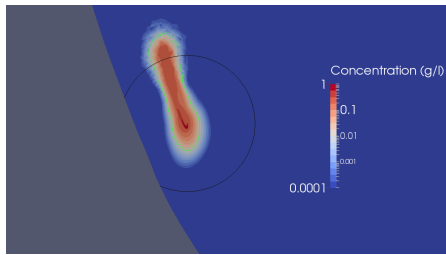


(a) Static mesh

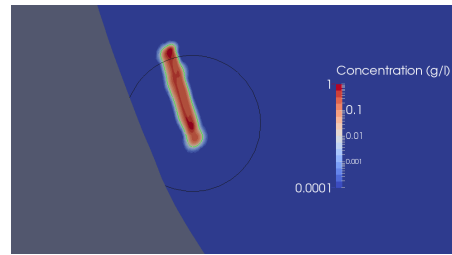


(b) Adaptive mesh

Figure 5.18: Logarithmic-scale plot of effluent dispersion 8 hours into the 12 hour tidal cycle.



(a) Static mesh



(b) Adaptive mesh

Figure 5.19: Logarithmic-scale plot of effluent dispersion 10 hours into the 12 hour tidal cycle.

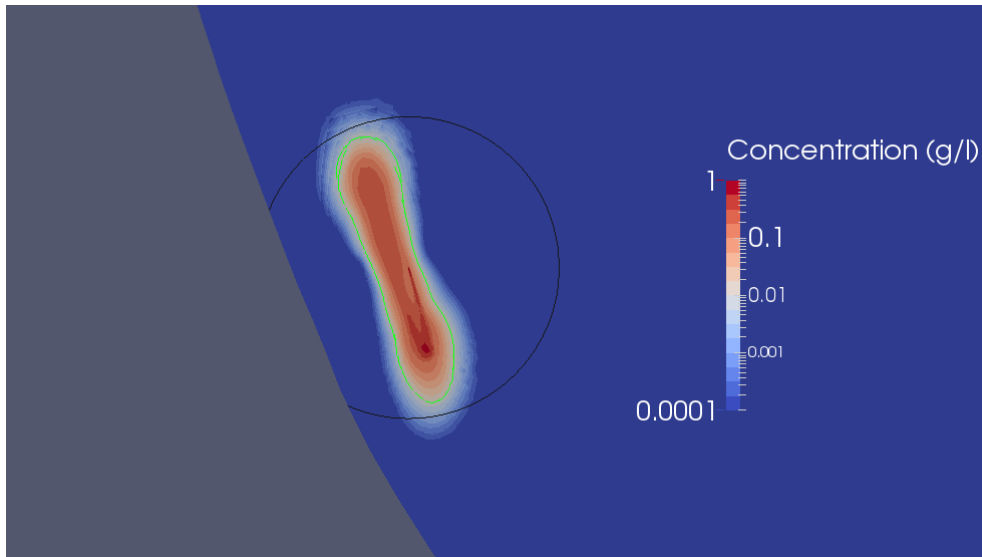


Figure 5.20: Logarithmic-scale plot of effluent dispersion at the end of the 12 hour tidal cycle, using a static mesh.

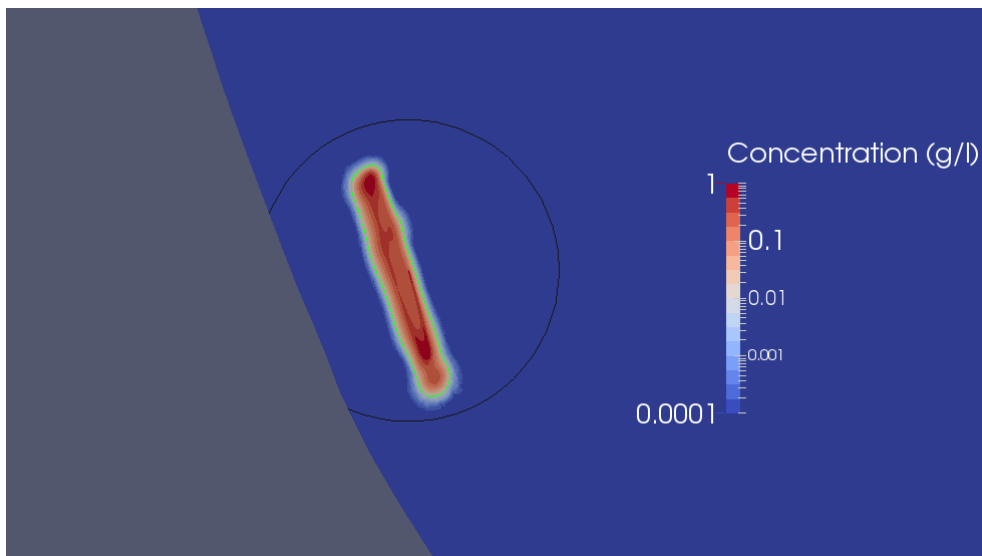


Figure 5.21: Logarithmic-scale plot of effluent dispersion at the end of the 12 hour tidal cycle, using an adaptive mesh.

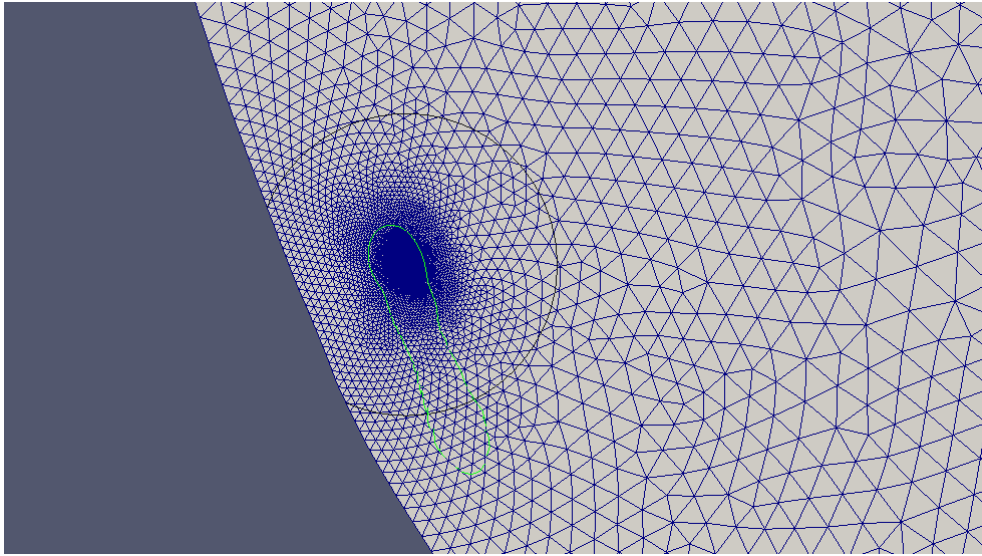


Figure 5.22: A close-up of the static mesh, in the region of the outfall

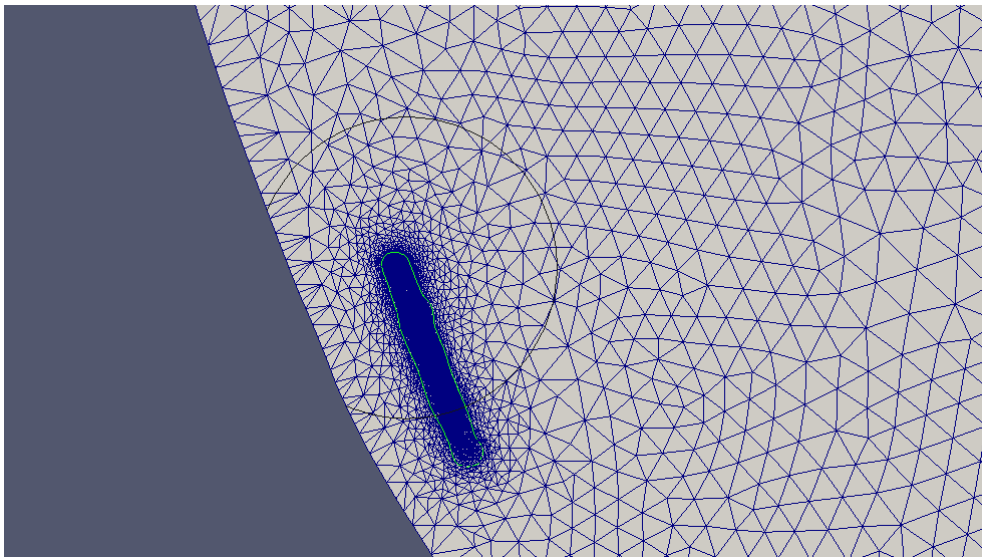


Figure 5.23: A close-up of the adaptive mesh, in the region of the outfall, two hours in the tidal cycle.

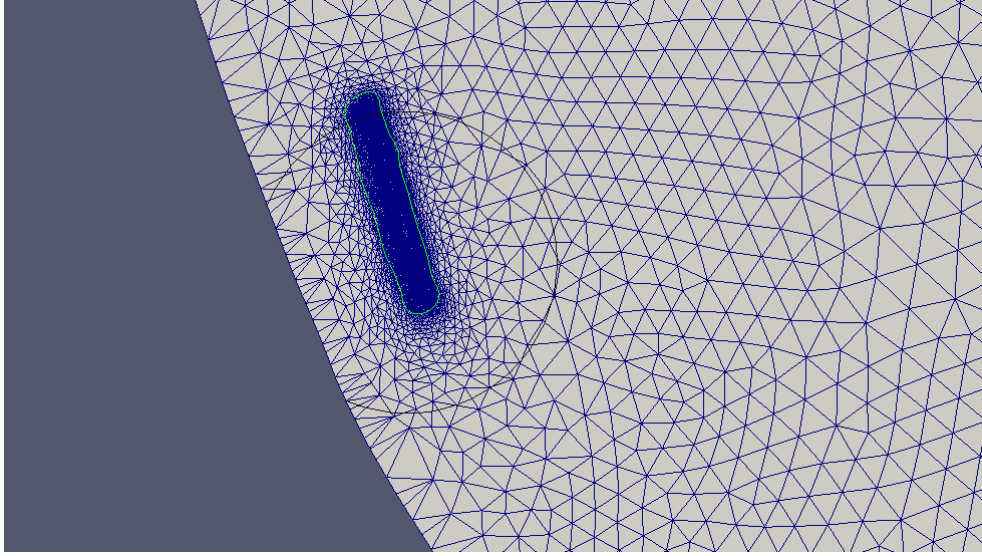
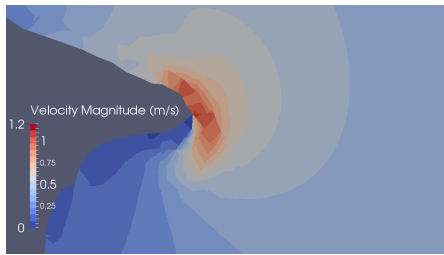
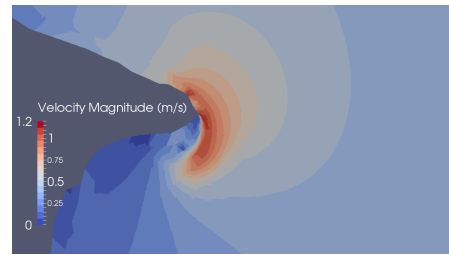


Figure 5.24: A close-up of the adaptive mesh, in the region of the outfall, eight hours in the tidal cycle.

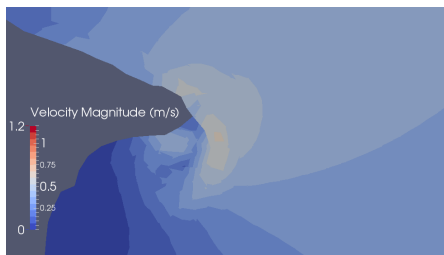


(a) Static mesh

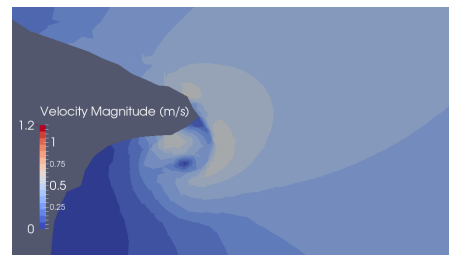


(b) Adaptive mesh

Figure 5.25: Velocity predictions at the start of the 12 hour tidal cycle.

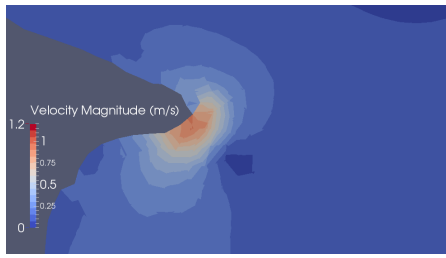


(a) Static mesh

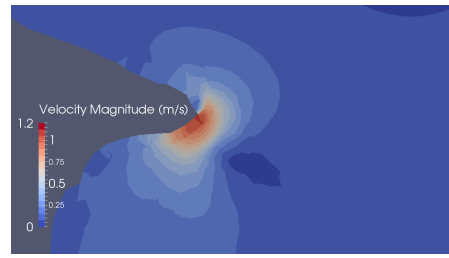


(b) Adaptive mesh

Figure 5.26: Velocity predictions 2 hours into the 12 hour tidal cycle.

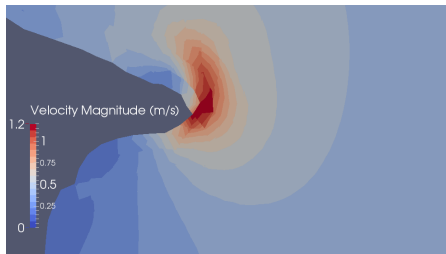


(a) Static mesh

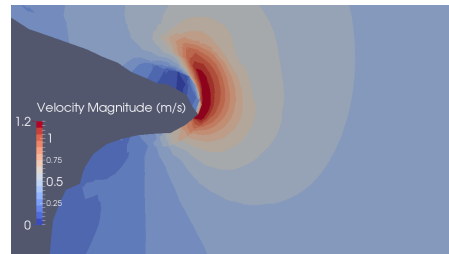


(b) Adaptive mesh

Figure 5.27: Velocity predictions 4 hours into the 12 hour tidal cycle.

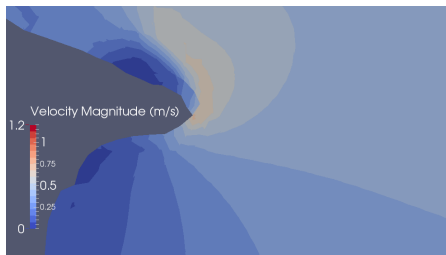


(a) Static mesh

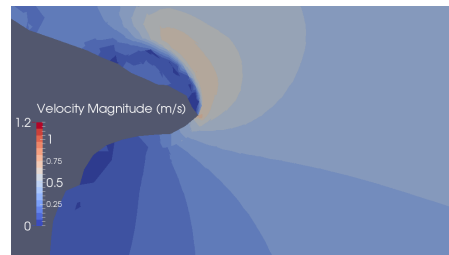


(b) Adaptive mesh

Figure 5.28: Velocity predictions 6 hours into the 12 hour tidal cycle.



(a) Static mesh



(b) Adaptive mesh

Figure 5.29: Velocity predictions 8 hours into the 12 hour tidal cycle.

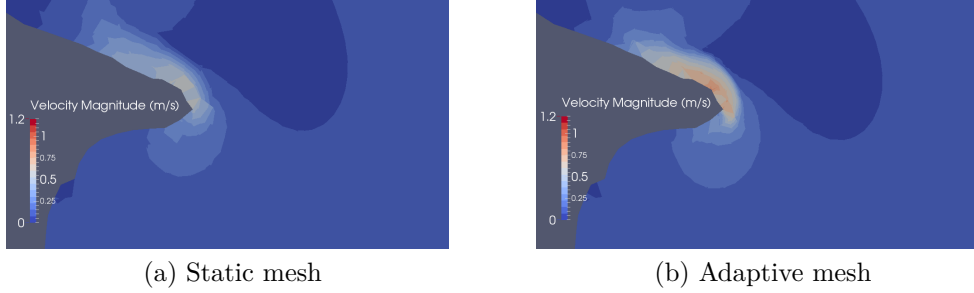


Figure 5.30: Velocity predictions 10 hours into the 12 hour tidal cycle.

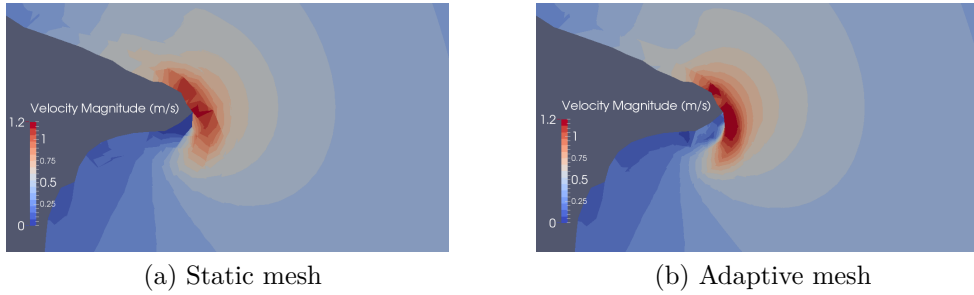


Figure 5.31: Velocity predictions at the end of the 12 hour tidal cycle.

5.5 Discussion

The linear-scale plots of effluent concentration, Figures 5.6 – 5.13, show that the shape and size of the higher concentration contours are approximately similar for the simulations using a static and adaptive mesh. The higher concentration contours predicted by the two models have approximately the same length and width, follow similar paths, and extend a similar distance from the outfall.

For the model using an adaptive mesh, the predictions show much higher peaks in concentration at either ends of the plume than is predicted with a static mesh. These peaks are maintained throughout the tidal cycle, for the model using an adaptive mesh, where the effluent concentration is predicted to be more dissipated in the model using a static mesh.

The logarithmic-scale plots of effluent concentration, Figures 5.14 – 5.21, show that the edges of the plume are far more diffused in the predictions from the model using a static mesh. The edges of the plume predicted using a static mesh are considerably wider at either end of the plume.

The sharp line of higher concentration extending southwards away from

the outfall, at the end of the tidal cycle, is seen in both model results, but the tail of this line has a higher concentration in the model using an adaptive mesh (see Figures 5.20 and 5.21).

It can be seen from the images of the model meshes in Figures 5.23 and 5.24 that the adaptive mesh algorithm has optimised the mesh such that the high resolution region follows the plume migration. The region of high resolution encapsulating the plume travels southwards as the plume moves southwards (see Figure 5.23) and travels northwards as the plume travels northwards (see Figure 5.23).

The static mesh is highly resolved in the near-vicinity of the outfall, but much less resolved at distances of the order 1000 m from the outfall. During the course of a tidal cycle, either ends of the plume travel some way outside of this region of high resolution, into areas of the domain where only 4–5 elements span the width of the plume.

As shown in Chapter 4, tracer advection–diffusion modelling with a low resolution mesh can lead to significant numerical diffusion. This phenomenon may explain why the low concentration contours predicted using a static mesh show considerable widening at either ends of the plume.

It is very likely that the simulation using a static mesh is mesh dependent (i.e. numerical diffusion is having a significant effect on model results). If this were a model study into the effluent dispersion at this hypothetical site, then the next step (if one wished to use a static mesh) would be to increase the mesh resolution further along the length of the plume path. This would require considerable extra computational resources, but would likely remove some of the effects of numerical diffusion.

Similarly, it has not been shown that the simulation using an adaptive mesh is mesh independent. This simulation is considerably more refined at the edges of the plume, and so likely effected considerably less by numerical diffusion, but that does not prove that it has been reduced to an insignificant level. The process of field interpolation between adapted meshes was performed using Galerkin projection, which is conservative but still possibly significantly diffusive if interpolating between coarse meshes.

The mesh adaptivity algorithm was configured to adapt to the curvature of both effluent concentration *and* velocity. Figures 5.25 to 5.31 show that the mesh adaptivity algorithm gave an increased resolution of the currents around the headland. This though did not result in any significant increase in the accuracy of the tidal currents predicted at the outfall

site by the effluent plume. It can be seen that the plume migration path was very similar for both models. It could therefore be argued that the increased resolution was superfluous, especially as it may have limited the adaptive timestep at several stages of the simulation. However, it is likely to be hard to know a-priori how velocity accuracy will propagate in the system, especially when the tidal current is moving from the headland towards the outfall. This further emphasises the advantages of individual calibration of the prescribed interpolation errors to gain the most efficient response from the mesh adaptivity algorithm. Further optimisation of the published simulation might be to spatially vary the velocity interpolation error to concentrate computational effort in the region of the plume.

The two simulations shown show that for model scenarios where the region of interest moves significantly about the domain during the course of a simulation, for a similar amount of computational effort (i.e. for a similar number of mesh degrees of freedom), the use of an adaptive mesh algorithm can yield a simulation with a considerably higher resolution in the regions of interest. The numerical diffusion created by mesh interpolation is considerably lower than that created by having a low resolution mesh.

The model using a static mesh solved 3.92 seconds of simulation time for every second of wall time. The model using an adaptive mesh solved 4.15 seconds of simulation time for every second of wall time. There will have been some solver time taken to perform the mesh adaptivity algorithm (that will have not been necessary when using a static mesh), but this may have been offset by a decrease in the number of solver iterations necessary for convergence at each timestep. The timestep for both simulations was roughly similar, with the adaptive timestep oscillating with twice the frequency of the tidal cycle, between 200 seconds (the prescribed upper limit) and 100 seconds.

The stability of the simulation using an adaptive mesh was dependent on the condition of the pressure matrix. As was seen when utilising mesh adaptivity for near-field jet modelling (see Section 2.6.3), the aspect ratio and edge-length gradation of elements needed to be constrained to limit the ill-condition of the pressure matrix. If left unconstrained, the pressure solver would either perform an impractically large number of iterations, or have a fatal divergence. For these simulations the aspect ratio was limited to 5.0 and the gradation was limited to 1.3. A further stability issue came from the resolution of the tidal forcing data. Inevitably, the tidal forcing data used to drive the model was of a lower

resolution than that of the domain. If the mesh adaptivity algorithm was left unconstrained near the tidally-forced boundaries this lack of resolution in the tidal data would cause instabilities to develop in the velocity field. This would either lead to excessive resolution in this region, or fatal instability. In order to maintain stability, it was necessary to increase the prescribed viscosity to $1000 \text{ m}^2/\text{s}$ within a 7 km margin of the model boundaries. As the tidal currents passed through the region of high viscosity, velocity instabilities were smoothed and the resulting simulation remained stable.

5.6 Conclusions

The use of mesh adaptivity improved the efficiency of the simulations described in this chapter. Adjusting the mesh resolution to follow the movement of the plume gave a more efficient use of the computational effort, significantly lowering the effect of numerical diffusion.

The main disadvantages of the methods described in this chapter are the limitations on its application. Currently 2-d horizontal mesh adaptivity for coastal dispersion modelling requires that the bed is assumed to be flat. It is possible to make this assumption at some sites, but not many. This method would be considerably more useful if a mathematical method were available to conserve mass and maintain stability whilst interpolating fields on complex bathymetry.

A further limitation of the methods described is that all efforts to create a depth resolving (3-d) model resulted in divergence of the pressure solver. The inevitably high aspect ratios required by depth resolution created a very ill-conditioned pressure matrix which caused a fatal pressure divergence. This could be solved by using extremely high resolution of the horizontal mesh, but this would then negate any advantages gained from mesh adaptivity. This currently limits the applicability of this method to neutrally buoyant effluent in mixed coastal areas.

6 Strategy for a two-way coupled model of effluent dispersion

6.1 Introduction

Two or more models are deemed to be “coupled” when they are solved separately but are inter-dependent, with a data exchange typically occurring at user-defined synchronisation intervals.

The coupling of models, as opposed to the merging of them into one model, allows the user to use separate software and hardware to solve each set of model equations on independent meshes, with different input parameters and time stepping.

It is a modelling technique widely used within a range of scientific disciplines to account for phenomena that are costly or difficult to represent accurately within the same model. For instance in sea-bed evolution modelling, separate models are often created of sediment transport, waves, and currents. These models then pass information to each other at set time periods.

A commonly used software for facilitating model coupling is the open-source Model Coupling Toolkit (MCT, Warner et al. [2008]), which allows single or multiple executable systems and sequential or concurrent execution, in serial or with parallel processing. MCT is coupling “middleware” that, independent of the scientific discipline being modelling, can handle the most common coupling operations for multi-physics and multi-scale models.

In the case of modelling effluent dispersion within the marine environment, model coupling is often used when the range of scales to be accounted for is too great to manage practically within a single model.

Effluent dispersion within the marine environment can be influenced by a wide ranging physical phenomena such as rain, evaporation, surges, tides, turbulent mixing, bathymetry variation, buoyancy forces, wave–

induced-mixing, thermal and saline stratification, molecular diffusion, particle half-life (in the case of biology or nuclear waste), etc.

When studying effluent dispersion at a given site, it is a complex decision to decide which physical processes need to be included and which ones are small or benign enough to be ignored. Many of these phenomena are highly non-linear, and so are too complex to be accounted for by simple analytical equations. If the range of processes to be included in a model is large, and the resulting range of scales is large, then often model coupling is the most suitable method available.

This short chapter contains out an outlined strategy for a prospective coupled-model using as a basis the techniques developed within this thesis.

6.2 State-of-the-art

For marine effluent dispersion, model coupling is typically performed between models of near- and far-field mixing. The coupling method to pass information between the near- and far-field models has been successfully performed in a number of different ways. Bleninger [2006] coupled the length-scale model CORMIX to the hydrodynamic model Delft3D to model wastewater dispersion from the Cartagena outfall in Colombia, using one-way coupling. The near-field results were projected onto a finely resolved region within the far-field model at regular time intervals. However, the method is less appropriate for cases in which the discharge produces an unstable near-field (that is, the discharge significantly influences the ambient dynamics) or if the far-field currents are significantly influenced by the outfall characteristics.

Choi and Lee [2007] developed the Distributed Entrainment Sink Approach (DESA) to coupling, representing the discharge within the far-field model as a series of entrainment sinks along the jet path, as predicted by the near-field model. An increased flow and diluted source concentration is then specified at the terminal level of the discharge. The inclusion of sink terms allows for conservation of water mass within the far-field model, as water entrained by the jet is removed from the domain. This is a suitable method of coupling, provided that the discharge does not significantly modify the ambient currents, and the near-field region is stable.

Several model coupling approaches have recently been validated against

field and laboratory data, for example Wood et al. [2014], and Morelissen et al. [2013].

In general, one-way coupling methods work well for small discharges with limited re-entrainment of the far-field plume back into the near-field over successive tidal cycles, and only small variations in the size of the near-field region during the simulation (if, say, variations in currents are relatively small).

In a one-way coupled approach, the key hydrodynamic inputs to the near-field model are based on ambient currents and water depths predicted by the far-field model. If the outfall imparts significant momentum on the ambient water, for example in cases with unstable mixing of the effluent over the full water depth, the ambient currents may be altered. Similarly, if the plume is re-entrained into the near-field (say, over successive tidal cycles), concentrations in this region will be underestimated. With one-way coupling, these changes in ambient conditions cannot be explicitly represented (Morelissen et al. [2013]).

6.3 Prospective method for model coupling

A proposed coupled model of effluent dispersion would include a near-field jet model two-way (i.e. “fully-coupled”) to a far-field plume model. Tidal forcing would be provided by a one-way coupled tidal model. Fluidity is capable of modelling all of these processes and so third party coupling software, such as MCT, would be unnecessary.

The tidal model would be run “offline” (hence one-way coupled). Just as was performed within Chapter 3, an ocean-scale model of tidal dynamics would be created using data from a publicly available global tidal model to define tidal forcing. Mesh concentration would be concentrated around the region of interest and predictions of tidal harmonic coefficients would be gathered to inform the tidal forcing of the far-field model.

The near-field model would provide an effluent source profile to the far-field model, and the far-field model would provide ambient current conditions to the near-field model. This information would be passed at pre-defined intervals in the tidal cycles (say, twelve times a cycle).

The near-field model would look much like those presented in Chapter 2, but with the addition of an ambient current to the initial and boundary conditions, and possibly a complex outfall design. The near-field model

would be run for a given current condition and then be characterised by fitting a 2-d Gaussian function to the effluent concentration at either the sea-bed or water surface (depending on the buoyancy of the effluent) and passing that information to the far-field model.

This suitable function would then be used to define the effluent source term within the far-field model (in the same way as was described within Chapter 5). The advantage of using a function to describe the effluent source profile, as opposed to directly projecting the effluent field onto the far-field mesh, is that it allows the use of mesh adaptivity within the far-field model. Field projection would require that the model mesh around the site remain static.

The interval at which information was passed (the coupling timestep) would need to be calibrated to ensure that it wasn't too long as to cause the model to lose accuracy, but also not too short as to be impractically slow to solve. It would also be necessary, if the effluent was buoyant, for the far-field model to be depth-resolving.

7 Conclusions

This research aimed to progress the state-of-the-art in various aspects of effluent dispersion modelling within the marine environment. There was also a longer-term ambition of working towards a coupled (or even single) model of effluent dispersion linking near- and far-field models to represent influencing factors from a wide range of scales (from tidal currents down to turbulent eddies) entirely using CFD techniques.

Studies were performed in a series of stages in which key aspects of effluent dispersion modelling were addressed. CFD models were created of near-field jet dispersion, tidal motion, and far-field plume dispersion. Idealised test cases were also performed to investigate the performance of advection-diffusion solver methods. At each stage the aim was to investigate the benefit of novel numerical modelling techniques and compare their accuracy and efficiency to existing methods.

All models showed a close agreement with comparison benchmark data, which shows that Fluidity is a suitable CFD code for modelling each of these aspects of effluent dispersion.

The assessment of a standard advection-diffusion solver method available within the Fluidity CFD model showed that the method compared well to world-leading free surface modelling software, Open TELEMAC. Numerical diffusion was shown to be relatively low, and the modelling of active tracers was shown to have good geostrophic balance.

Preliminary work investigating the use of mesh adaptivity in the modeling of jet dynamics showed that with modest parallel computing resources and expertise, high-resolution simulations of jet dynamics can be achieved with reasonable accuracy using CFD modelling. The experience of using mesh adaptivity during this research informed a detailed guide to when mesh adaptivity could offer a benefit to jet modelling, and also how to utilise the tool effectively.

The jet configurations investigated in this research had readily predictable and simply describeable mesh requirements. The benefits of the mesh adaptivity for these simulations were less than would possibly occur for jet simulations of more complex ambient conditions or outfall designs. It would be an interesting extension of this work to investigate

the benefits for more complex outfall configurations.

The use of mesh adaptivity improved the efficiency of 2-d coastal dispersion modelling. Adjusting the mesh resolution to follow the movement of the plume gave a more efficient use of the computational effort, significantly lowering the effect of numerical diffusion.

The main disadvantages of the use of mesh adaptivity for 2-d coastal dispersion modelling are the limitations on its application. Currently 2-d horizontal mesh adaptivity for coastal dispersion modelling requires that the bed is assumed to be flat. It is possible to make this assumption at some sites, but not many. This method would be considerably more useful if a mathematical method were available to conserve mass and maintain stability whilst interpolating fields on complex bathymetry.

A further limitation of use of mesh adaptivity for 2-d coastal dispersion modelling is that all efforts to create a depth resolving (3-d) model resulted in divergence of the pressure solver. The inevitably high aspect ratios required by depth resolution created a very ill-conditioned pressure matrix which caused a fatal pressure divergence. This could be solved by using extremely high resolution of the horizontal mesh, but this would then negate any advantages gained from mesh adaptivity. This currently limits the applicability of this method to neutrally buoyant effluent in mixed coastal areas.

A possible methodology for producing a two-way coupled model of effluent dispersion in the marine environment was outlined. The modelling results presented in the thesis show that Fluidity would be suitable for modelling all aspects of this proposed model. The interpolation of fields between models should be straight-forward but the coupling timestep and interface boundary would require investigation to optimise. This research has also indicated that the benefits of using mesh adaptivity for the various modelling components would need to be assessed on a case-by-case basis and would not currently be possible for non-neutral effluent.

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