

TUFLOW Classic/HPC

Advection Dispersion Module

User Manual



Release Build
2020-10-AF

www.tuflow.com

[TUFLOW Wiki](#)

[TUFLOW Tutorials](#)

support@tuflow.com

[How to Use This Manual](#)

[Chapters](#)

[Table of Contents](#)

[List of Figures](#)

[List of Tables](#)

[Appendices](#)

[.tcf Commands](#)

[.adcf Commands](#)

About This Manual

This is a user manual for the TUFLOW AD model, when it is called by TUFLOW.exe. TUFLOW AD relies on third party software to provide the interface between the user and the engine. These software packages are typically a text editor (e.g. UltraEdit), GIS platform (e.g. MapInfo), 3D surface modelling software (e.g. Vertical Mapper) and result viewing packages (e.g. SMS). Please refer to the user documentation or help of the third party software you have chosen to use in addition to this manual.

This manual focuses predominantly on the TUFLOW AD model, and the user is referred to the TUFLOW and ESTRY manual for guidance on these hydrodynamic engines. It is assumed that the user is familiar with TUFLOW and has read the TUFLOW manual.

How to Use This Manual

This manual is designed for both hardcopy and digital usage. It was created using Microsoft Word and has not been tested in its digital mode in other platforms.

Section, table and figure references are hyperlinked (hold down the Ctrl key and click on the Section, Table or Figure number in the text to move to the relevant page).

Similarly, text file commands are hyperlinked and are easily accessed through the lists at the end of the manual (e.g. see [.adcf File Commands](#)). To quickly go to the end of the manual press Ctrl End. There are also command hyperlinks in the text (normally blue and underlined). Command text can be copied and pasted into the text files to ensure correct spelling.

Some useful keys to navigate backwards and forwards are Alt Left / Right arrow to go backwards / forwards to the last locations. The Web Toolbar 'Back' and 'Forward' buttons can also be used to navigate. Ctrl Home returns to the front page.

Any constructive suggestions are welcome (<mailto:support@tufLOW.com>).

Chapters

1	Introduction	1-1
2	Overview	2-1
3	The Modelling Process	3-1
4	Data Input	4-1
5	Model Development	5-1
6	Data Output	6-1
7	References	7-1

Table of Contents

1	Introduction	1-1
1.1	Overview	1-2
1.2	Solution Method	1-2
1.3	Constituent Transformation	1-4
1.4	Dispersion Formulation	1-4
2	Overview	2-1
2.1	Software Structure	2-2
2.2	Data Input	2-2
2.2.1	Structure	2-2
2.2.2	Suggested Folder Structure	2-3
2.2.3	File Types and Naming Conventions	2-4
2.2.4	GIS Input File Types and Naming Conventions	2-6
2.3	Performing Simulations	2-6
2.4	Installing a Dongle	2-6
2.5	Data Output	2-6
2.6	Limitations and Recommendations	2-7
3	The Modelling Process	3-1
3.1	Data Input Requirements	3-2
3.2	Calibration and Sensitivity	3-2
3.3	Model Resolution	3-2
3.3.1	2D Cell Size	3-2
3.4	Computational Timestep	3-3
4	Data Input	4-1
4.1	Control Files – Rules and Notation	4-2
4.2	Simulation Control File	4-3
4.2.1	TUFLOW AD Control File (.adcf File)	4-3
4.2.2	Run Time and Output Controls	4-4
4.3	GIS Layers	4-4
4.4	2D Geometries	4-5
4.4.1	Multiple 2D Domains	4-5

Table of Contents

4.5	1D Geometries	4-5
4.6	Specification of Constituent Properties	4-5
4.7	Boundary Conditions	4-7
4.7.1	Boundary Condition (BC) Database	4-7
4.7.2	BC Database Example	4-9
4.8	Initial Conditions	4-9
4.9	Minimum Dispersion Coefficient (D_w)	4-10
4.10	UltraEdit	4-10
5	Model Development	5-1
5.1	Example Models	5-2
5.2	Setting up a New Model	5-2
6	Data Output	6-1
6.1	General	6-2
6.1.1	Console (DOS) Window Display	6-2
6.1.2	TUFLOW AD Log Files	6-2
6.1.2.1	<i>Simulation Log File</i>	6-3
6.1.2.2	<i>CFL Log File</i>	6-3
6.1.2.3	<i>Mass Log File</i>	6-4
6.2	2D Domains	6-5
6.2.1	SMS (Map) Output (.dat or .xmdf Files)	6-5
7	References	7-1

Appendices

Appendix A	.tcf File Commands	A-1
Appendix B	.adcf File Commands	B-1

List of Figures

Figure 2-1	TUFLOW and TUFLOW AD Relationship and Data Input / Output	2-3
------------	---	-----

List of Tables

Table 2.1	Recommended Sub-Folder Structure	2-4
Table 2.2	List of Most Commonly Used File Types	2-5
Table 2.3	GIS Input Data Layers and Recommended Prefixes	2-6
Table 4.1	Reserved Characters – Text Files	4-2
Table 4.2	Notation Used in Command Documentation – Text Files	4-3
Table 4.3	TUFLOW AD Interpretation of MIF Objects	4-4
Table 4.4	Global Database Keyword Descriptions	4-5
Table 4.5	BC Database Keyword Descriptions	4-8
Table 4.6	2D Initial Conditions (2d_ad_ic) Attribute Descriptions	4-9
Table 4.7	2D Minimum Dispersion Coefficient (2d_ad_md) Attribute Descriptions	4-10
Table 7.1	_ADcfl.csv File Columns	6-4
Table 7.2	_ADmass.csv File Columns	6-5

Glossary & Notation

AD	Advection dispersion.
attribute	Data attached to a GIS object. For example, a minimum dispersion coefficient is attached to a polygon using a column of Float type data.
Build	The TUFLOW Build number is in the format of year-month-xx where xx is two letters starting at AA then AB, AC, etc for each new build for that month. The Build number is written to the first line in the .elf and .tlf log files so that it is clear what version of the software was used to simulate the model.
cell	Square shaped computational element in a 2D domain.
centroid	The centroid of a region or polygon.
CFL	Courant–Friedrichs–Lewy condition. A stability criterion for explicit numerical schemes that sets the number of substeps TUFLOW AD executes within a single TUFLOW timestep.
command	Instruction in a file.
constituent	A water quality species to be simulated in TUFLOW AD.
control file	Text file containing a series of commands (instructions) that control how a simulation proceeds. The only control file in the AD module is the .adcf file.
dispersion coefficient	A coefficient applied to the diffusion terms of the conservation equation that increases or decreases the rate of spread of a constituent in response to ambient velocities and spatial gradients in constituent concentrations. It represents mixing that occurs in reality as a result of processes (e.g. sub-grid scale) that cannot be resolved in a numerical model.
GIS	Geographic Information System that can import/export files in MIF/MID format.
grid	The mesh of square cells that make up a TUFLOW model.
layer	A GIS data layer (referred to as a “table” in MapInfo).
mif/mid	MapInfo Industry standard GIS import/export format.
SMS	Surface Water Modelling Software distributed by Aquaveo (www.aquaveo.com) for viewing TUFLOW results.

1 Introduction

Section Contents

1.1	Overview	1-2
1.2	Solution Method	1-2
1.3	Constituent Transformation	1-4
1.4	Dispersion Formulation	1-4

1.1 Overview

The TUFLOW AD Module is an extension of the TUFLOW hydrodynamic engines. It is a computer program for simulating depth-averaged, two and one-dimensional constituent fate and transport. An example of such a constituent might include salinity. Both dissolved and particulate constituents can be simulated. TUFLOW AD takes depth and velocity fields computed by the TUFLOW Classic and HPC solvers and uses this information, together with initial and boundary conditions, to simulate the advection and dispersion of constituents. TUFLOW AD is specifically oriented towards such analyses in systems including coastal waters, estuaries, rivers, floodplains and urban areas. At present, it can handle 1D elements embedded into a single 2D domain within TUFLOW as SX connections.

TUFLOW AD has been compiled to support all precisions and platforms used by TUFLOW, with a tailored dll for each, specifically:

- Windows 64 bit operating system single precision (TUFLOW_AD_iSP_w64.dll);
- Windows 64 bit operating system double precision (TUFLOW_AD_iDP_w64.dll);

1.2 Solution Method

The TUFLOW AD 2D advection solution algorithm is based on the ULTIMATE QUICKEST method of Leonard (1991), Leonard & Niknafs (1991) and Leonard *et al.* (1993). It solves the full two-dimensional, depth averaged, constituent conservation equation, including sink terms such as settling (for particulate species) and decay. The continuity equation is used to ensure conservation of mass, as described in Wu & Falconer (2000). The scheme also includes representation of mixing due to sub-grid-scale turbulence and vertical shear via the dispersion formulation provided in Falconer *et al.* (2005).

The 2-D representation of the conservation equation is provided by the following partial differential equation for an in-plan Cartesian coordinate frame of reference:

$$\frac{\partial \phi}{\partial t} + \frac{\partial(u\phi)}{\partial x} + \frac{\partial(v\phi)}{\partial y} - \frac{\partial}{\partial x} \left(D_x \frac{\partial \phi}{\partial x} \right) - \frac{\partial}{\partial y} \left(D_y \frac{\partial \phi}{\partial y} \right) = S \quad (2D \text{ Conservation})$$

where

ϕ = Dissolved constituent concentration

u and v = Depth averaged velocity components in X and Y directions

x and y = Distance in X and Y directions

t = Time

D_x, D_y, D_z = Turbulent diffusion coefficients in the x, y and z directions

S = Source terms

The terms of the conservation equation can be attributed to different physical phenomena. These are (in order from left to right) the rate of change of concentration in time, the transport of constituent due to the presence of concentration and velocity gradients (the advective terms) and turbulent diffusion due to irreversible mixing processes. The source terms (S) include settling and decay.

Wu & Falconer (2000) demonstrated the need for an additional source term on the right hand side of the above equation to ensure mass conservation, this being S_a (with vertical velocities omitted):

$$S_a = \phi \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \quad (\text{Mass Conservation})$$

The meaning of the symbols is as per the above.

The TUFLOW AD computational procedure used is an explicit scheme based on Leonard (1991). This contrasts to the TUFLOW engine, which employs an implicit scheme. As such, TUFLOW AD is generally subject to stricter stability constraints than the hydrodynamic engine. As such, the TUFLOW AD calculation takes the form of three steps within each timestep.

The first step involves calculation of the Courant-Friedrichs-Lewy (CFL) condition at all wet cells, where the CFL in 1 dimension is:

$$CFL = \frac{u \cdot \Delta t}{\Delta x} \quad (\text{CFL Condition})$$

where u (or v) is fluid velocity and Δt and Δx are the timestep and grid scale, respectively. This condition is typically required to be less than 1.0 (additive for both X and Y directions) and has a broad physical interpretation requiring that the distance fluid is advected in one timestep ($u\Delta t$) is less than one grid cell (Δx).

The second step is the computation of a similar condition for the diffusive lengthscale (related to the Peclet number) that ensures that dispersion also does not cause instability at any grid cell. The CFL and dispersion dimensionless numbers are then added and the maximum sum at any given location within a timestep is used to compute the number of sub-stepping iterations required by TUFLOW AD to remain stable within one TUFLOW timestep.

The third step within each TUFLOW timestep is to execute the advection dispersion calculations for the required number of iterations, with a modified (smaller) Δt .

The original ULTIMATE QUICKEST solution method has been enhanced and improved as applied in TUFLOW AD. For example, TUFLOW AD also employs adaptive computational stencil expansion where it identifies sharp constituent concentration gradients (Leonard & Niknafs, 1991). Where possible (i.e. away from boundaries and dry cells) and required, the ULTIMATE QUICKEST stencil is expanded from the standard third order scheme to a ninth order scheme, only on principle computational axes. Cross terms greater than third order are not included. If insufficient wet cells exist to switch to ninth order, then seventh and fifth order schemes are progressively tested (with commensurately decreasing stencils) until all required wet cells are located.

Application of the ULTIMATE limiter (Leonard, 1991) has been found to induce steady flow anisotropy when extended to multi-dimensional problems and the numerical cross terms associated with additional dimensions are included in calculations. Wu & Falconer (2000) developed a modification to the ULTIMATE limiter that reduces this anisotropy, and this has been applied within the TUFLOW AD computational engine.

1.3 Constituent Transformation

In addition to pure advection and dispersion, constituents simulated within TUFLOW AD are modified by transient boundary conditions, and optional settling and decay processes (with the latter being specifically developed to accommodate simulation of particulate material such as total nutrients).

Boundary conditions can be set to vary in time for each constituent, and can be applied to all TUFLOW boundaries that set water levels and flows (either user-specified or computed), such as HT or QT. TUFLOW AD also supports SA inflow boundaries, where flows and concentrations are used to compute mass loads that are delivered to the model domain, mixed with ambient water and then resultant concentrations computed, prior to execution of the advection routines.

Settling of constituents to simulate removal of particulate matter from the water column has been included in the engine as a simple linear process. Once settled, constituents do not re-enter the computational domain. TUFLOW AD also supports the decay of individual species (if positive decay rates are specified) and employs first order rate equations to do so. These equations draw on user defined decay rates.

Up to twenty individual constituents can be simulated within TUFLOW AD.

1.4 Dispersion Formulation

TUFLOW AD applies the dispersion formulation described by Falconer *et al.* (2005). This formulation computes dispersion in the X and Y directions (D_{xx} and D_{yy} respectively, to suit the Cartesian computational grid) from user specification of longitudinal and transverse dispersion coefficients D_l and D_t , respectively. Specifically, D_{xx} and D_{yy} are computed dynamically at each grid cell and timestep as follows:

$$D_{xx} = \frac{(D_l U^2 + D_t V^2) H \sqrt{g}}{V C_s} + D_w \quad (\text{X Direction Dispersion})$$

$$D_{yy} = \frac{(D_l V^2 + D_t U^2) H \sqrt{g}}{V C_s} + D_w \quad (\text{Y Direction Dispersion})$$

where

D_l = User specified longitudinal dispersion coefficient

D_t = User specified transverse dispersion coefficient

U and V = Depth averaged velocity components in X and Y directions

H = Water depth

g = Gravitational acceleration

V_s = Velocity magnitude

C = Chezy coefficient

D_w = User specified lower bound dispersion coefficient

The value of D_w can be specified as constant or spatially variant as required.

2 Overview

Section Contents

2	Overview	2-1
2.1	Software Structure	2-2
2.2	Data Input	2-2
2.2.1	Structure	2-2
2.2.2	Suggested Folder Structure	2-3
2.2.3	File Types and Naming Conventions	2-4
2.2.4	GIS Input File Types and Naming Conventions	2-6
2.3	Performing Simulations	2-6
2.4	Installing a Dongle	2-6
2.5	Data Output	2-6
2.6	Limitations and Recommendations	2-7

2.1 Software Structure

TUFLOW AD is a computational engine that uses hydraulic information computed by TUFLOW on a timestep by timestep basis to simulate constituent fate and transport. Like TUFLOW, it does not have its own graphical user interface, but utilises GIS and other software for the creation, manipulation and viewing of data. These software platforms are:

- A GIS that can import/export .mif/.mid files (MapInfo Interchange Format files);
- 3D surface modelling software (e.g. Vertical Mapper) for importing 3D surfaces of model results into high quality reporting packages;
- SMS (Surfacewater Modelling System – www.aquaveo.com) or WaterRIDE (www.waterride.net) for the viewing of results and creation of animations;
- A text editor such as UltraEdit; and
- Spreadsheet software such as Microsoft Excel.

2.2 Data Input

2.2.1 Structure

Figure 2-1 illustrates the data input and output structure, and the relationship between TUFLOW and TUFLOW AD.

Text files are used for controlling TUFLOW AD simulations and simulation parameters. In general, the required inputs for TUFLOW AD are considerably simpler than for TUFLOW and this is primarily because all bathymetric, boundary condition location and 1D/2D network information is passed from TUFLOW to TUFLOW AD, avoiding the need for users to respecify this information within the AD module.

The figure also demonstrates the relationship between TUFLOW and TUFLOW AD in that (at this time) TUFLOW AD is called by TUFLOW as a dynamically linked library (dll) at every timestep.

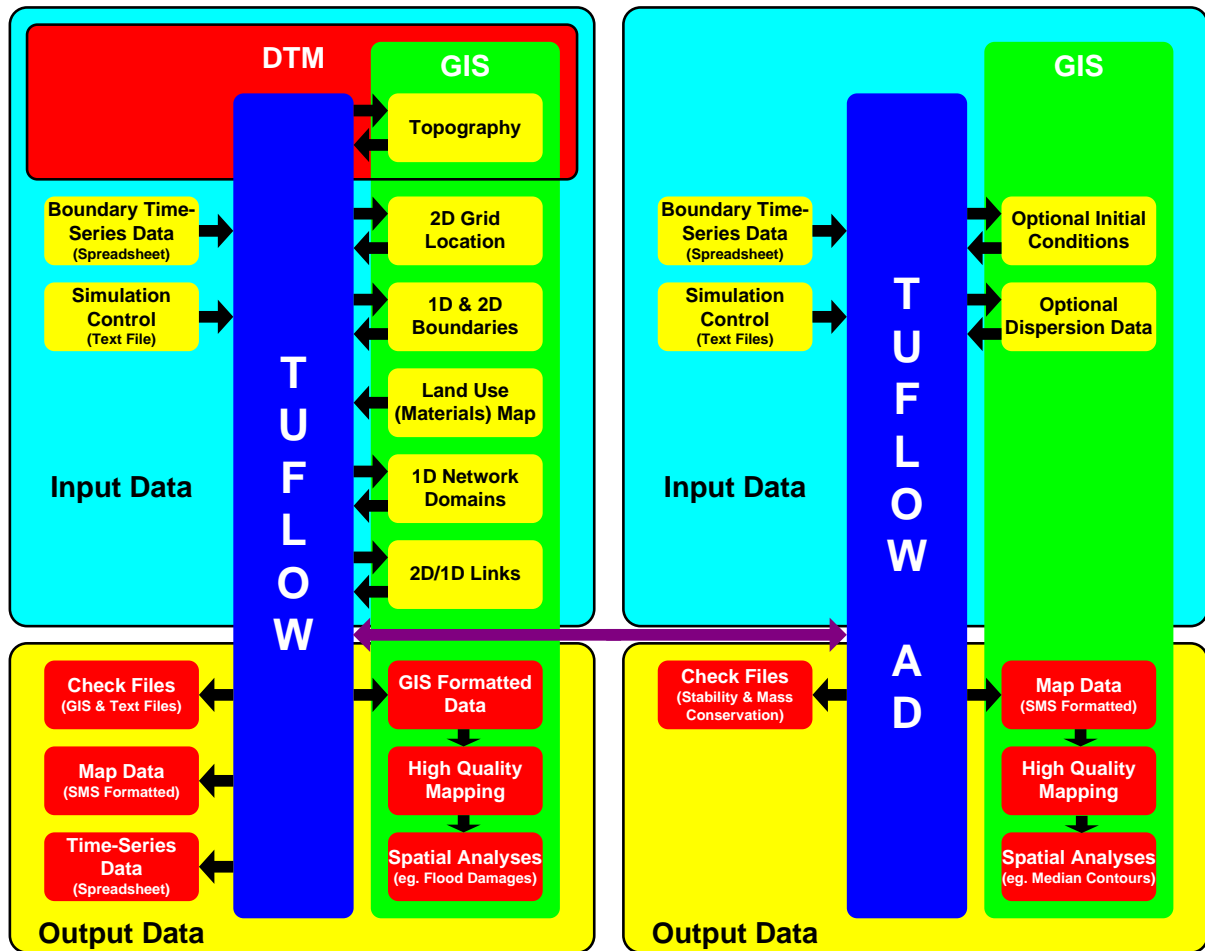


Figure 2-1 TUFLOW and TUFLOW AD Relationship and Data Input / Output

2.2.2 Suggested Folder Structure

Table 2.1 presents the recommended set of sub-folders to be set up for a 2D/1D TUFLOW and TUFLOW AD model. It is an extension of that suggested in the TUFLOW manual. Any folder structure may be used, however, it is strongly recommended that a system similar to that below be adopted. For large modelling jobs with many scenarios and simulations, a more complex folder structure may be warranted, but should be based on that below.

Note:

- **Files are located relative to the file they are referred from.** For example, the path and filename of a file referred to in AD Global Database is sourced **relative to the AD Global Database, not the .adcf or .tcf file**;
- Whilst TUFLOW AD accepts spaces in filenames and paths, other software may have issues with spaces. It is therefore recommended that spaces are not used in the simulation path and filename. Underscores are useful replacements; and
- Filenames and extensions are not case sensitive.

Table 2.1 Recommended Sub-Folder Structure

Sub-Folder	Description
Locate folders below on the system network under a folder named “tufLOW” in the project folder (e.g. J:\Project12345\tufLOW). These folders should be backed up regularly	
bc_dbase	Boundary condition database(s) and time-series data for TUFLOW (1D and 2D) and TUFLOW AD (2D) domains.
model	.tgc, .tbc, .tmf and other TUFLOW model data files, except for the GIS layers which are located in the model\mi folder (see below). No TUFLOW AD files are required here
model\mi	GIS layers that are inputs to the TUFLOW (2D and 1D) and TUFLOW AD (2D) model domains. Also GIS workspaces. These are only used for TUFLOW AD if spatially variable initial conditions and/or minimum dispersion coefficients are used.
runs	TUFLOW (.tcf or .ecf) and TUFLOW AD (.adcf) simulation control files.
runs\log	TUFLOW log files (.tlf or .elf and _messages.mif files) and TUFLOW AD log files (.adlf, _ADmass.csv and _ADcfl.csv) (use the TUFLOW Log Folder command)
For large models the folders below can be located on a local hard drive under a folder “tufLOW” under the project folder (e.g. C:\Project12345\tufLOW) These folders do not need to be backed up regularly as the data they contain is reproducible	
results	The result files (use the TUFLOW Output Folder command).
check	TUFLOW GIS and other check files to carry out quality control checks (use the TUFLOW Write Check Files command). Not used for TUFLOW AD at time of release.

2.2.3 File Types and Naming Conventions

For TUFLOW AD, files are generally classified as:

- Control Files;
- Data Input Files (including databases); and
- Data Output Files.

Control files are used for directing inputs to the simulation. The style of input is free form commands.

Data input files are primarily comma-delimited files generated using spreadsheet software. If needed, GIS files can also be read as appropriate, although these are not required to execute TUFLOW AD.

Data output files are primarily map output in SMS formats, text files and comma-delimited files (see Section 6).

The most common TUFLOW AD file types and their extensions are listed in Table 2.2.

Table 2.2 List of Most Commonly Used File Types

File	Extension	Description	Format
Control Files			
TUFLOW AD Simulation Control File	.adcf	Called by the .tcf file (AD Control File). Controls the data input and output for an AD simulation. Mandatory.	Text
Data Input			
Comma Delimited Files	.csv	<p>These files are used for:</p> <ul style="list-style-type: none"> • Global data bases that capture constituent details; • Boundary condition databases that itemise and cross reference boundary condition source tables; and • Boundary condition source tables themselves. <p>All are opened and saved using spreadsheet software such as Microsoft Excel.</p>	Text
GIS MIF/MID Files	.mif .mid	<p>MapInfo's industry standard GIS data exchange format. The .mif file contains the attribute data definitions and the geographic data of the objects. The .mid file contains the attribute data. Used for input of initial conditions or for specifying spatially variant dispersion characteristics. Optional, depending on level of sophistication within the AD model construction.</p> <p>The .mid files are of similar format to .csv files, so they can be opened by Excel or other spreadsheet software.</p>	Text
Data Output (see Section 6)			
SMS Super File (written by TUFLOW)	.sup	SMS super file containing the various files and other commands that make up the output from a single simulation. Opening this file in SMS opens the TUFLOW .2dm file and the primary .dat files, including both TUFLOW and TUFLOW AD results.	Text
SMS Data File	.dat	SMS generic formatted simulation results file. TUFLOW AD output is written using the .dat format.	Binary

2.2.4 GIS Input File Types and Naming Conventions

It is recommended that the prefixes described in Table 2.3 be adhered to for 2D GIS layers, where used. This greatly enhances the data management efficiency and, importantly, makes it much easier for another modeller or reviewer to quickly interpret the model. This approach is also consistent with that of TUFLOW.

Table 2.3 GIS Input Data Layers and Recommended Prefixes

GIS Data Type	Suggested File Prefix	Description	Refer to Section
2D Domain GIS Layers			
2D AD Initial Conditions	2d_ad_ic_	Layer containing polygons defining the spatial distribution of initial conditions for a given constituent. Optional,	4.8
2D AD Minimum Dispersion Coefficient	2d_ad_md_	Layer containing polygons defining the spatial distribution of minimum dispersion coefficients (D_w) for a given constituent. Optional.	4.9

2.3 Performing Simulations

TUFLOW AD simulations are started by running a TUFLOW simulation with the key command [AD Control File](#). The presence or absence of this command determines whether TUFLOW calls the AD module or not, respectively.

2.4 Installing a Dongle

Dongle installation instructions and operating rules are provided in the TUFLOW manual, and do not differ for TUFLOW AD.

2.5 Data Output

TUFLOW AD produces a range of outputs as presented below.

Output is structured into two categories:

- Text files for checking and quality control of models.
- Result files containing 2D results.

Text files (Section 6.1.2)

These files are produced so that modellers and reviewers can readily check the model set up and integrity. The files take the following forms:

- A log file describing the model construction process and execution;
- A file listing all CFL data for each timestep; and

- A file listing total constituent masses at each timestep

Result Files (Section 6.2.1)

Result files contain the computed spatial and temporal evolution of simulated constituents as SMS formatted files.

2.6 Limitations and Recommendations

TUFLOW AD is designed to model dissolved and particulate constituent advection and dispersion in coastal waters, estuaries, rivers, and floodplains. This is achieved through solution of the 2D transport equation using a variant of the ULTIMATE QUICKEST scheme first devised by Leonard (1991).

Limitations to note include:

- 1 Simulation of constituents through 1D SX connections is currently only on a mass balance basis. That is, it is assumed that the concentration of a constituent exiting an SX connection is the same as that at the entrance to the connection at the same timestep. This approach conserves mass to the limit that these inflows and outflows are approximately equal and that the transit time through the SX connection is small compared to the timescale at which constituent concentrations vary at the upstream end of the SX connection. As such, only relatively ‘short’ SX connections (using this timescale definition) should be simulated in the present release;
- 2 The dispersion scheme adopted by TUFLOW AD (Falconer et al. 2005) is such as to allow use of literature values for D_l and D_t . Users adopting literature values for these coefficients, however, should do so with extreme caution as they are known to vary widely, and by up to several orders of magnitude. **It is always preferable to use monitoring data to calibrate advection dispersion models (TUFLOW AD included) and this should be done whenever and wherever possible. If no such data is available, then literature values can be used for D_l and D_t , however results need to be appropriately caveated, and TUFLOW AD predictions (as for any AD model) should be seen as qualitative or indicative at best.**
- 3 Modelling predictions should also be cross checked with desktop calculations where possible. For example, this might include a hand calculation of expected salt masses in a given tidal system, with comparison made to TUFLOW AD text outputs.
- 4 TUFLOW AD allows for specification and computation of large dispersion coefficients, and with the automatic substepping implementation it should generally remain stable. However, specification of large (i.e. greater than approximately 100-500) dispersion coefficients may lead to results that are not physically real or defensible. As such, (in conjunction with 2 and 3 above) results should **always be sanity checked and correlated with measurements. Relying on uncalibrated model predictions is not recommended.**

3 The Modelling Process

Section Contents

3	The Modelling Process	3-1
3.1	Data Input Requirements	3-2
3.2	Calibration and Sensitivity	3-2
3.3	Model Resolution	3-2
3.3.1	2D Cell Size	3-2
3.4	Computational Timestep	3-3

3.1 Data Input Requirements

The minimum measured or literature data requirements for setting up a TUFLOW AD model are:

- 1 A properly constructed and stable TUFLOW hydraulic model (as detailed in Section 3.3 of the TUFLOW manual);
- 2 Boundary conditions for constituent concentrations (e.g. ocean salinities, catchment inflow pollutant concentrations etc.);

Initial conditions, dispersion coefficients, settling and decay rates will all be set to zero if not specified to be otherwise.

Preferable (and recommended) data requirements include:

- 1 Water quality calibration information as timeseries data at points. This is particularly important for dispersion coefficient calibration;
- 2 Spatially variant initial conditions;
- 3 Particulate matter settling rates (if any); and
- 4 Dissolved species decay/transformation rates (if any).

3.2 Calibration and Sensitivity

Advection dispersion models are usually calibrated against water quality observations. For example, salinity recovery data can be used to calibrate and validate models, with longitudinal and transverse dispersion coefficients being the primary free variables. Dissolved and/or particulate constituents can then be simulated using the derived dispersion coefficients, and can include use of settling and/or decay rates as needed.

Ideally, models should be calibrated for conditions similar to those under investigation (e.g. a catchment inflow to an estuary) although this is not always possible, particularly when data is limited. In these situations, sensitivity analyses could be carried out by increasing and decreasing calibration variables, but this not a preferred approach due to the large variability in the literature with respect to acceptable dispersion coefficients.

3.3 Model Resolution

3.3.1 2D Cell Size

The cell sizes of 2D domains need to be sufficiently small to reproduce advection dispersion behaviour. It is worth noting that, in general, the larger the cell size is with respect to the scale of mixing processes, the greater potential there is for numerical dispersion to play a role in the model execution process. Even though TUFLOW AD has in-built measures to reduce these effects, it is advisable to make sure that 2D cells are appropriately sized to minimise this effect, without seriously compromising simulation efficiency.

3.4 Computational Timestep

The selection of the timestep is important for the success of a model in that the run time is directly proportional to the number of timesteps required to calculate model behaviour for the required time period. Notwithstanding this, TUFLOW AD automatically substeps with respect to TUFLOW on the basis of maintaining both advective and dispersive stability (see Section 1.2) so the selection of timestep should be focused on ensuring hydraulic stability, as AD stability should follow, providing reasonable dispersion coefficients are set.

4 Data Input

Section Contents

4.10	UltraEdit	4-10
------	-----------	------

4.1 Control Files – Rules and Notation

Like the TUFLOW control file (.tcf) the TUFLOW AD control file (.adcf extension) is a keyword driven text file. The commands are entered free form, based on the rules described below. Comments may be entered at any line or after a command. The commands are listed in the index in [Appendix B](#).

An example of a command is:

```
AD GLOBAL DATABASE == ..\bc_dbase\2d_ad_globaldbase_run1.csv ! Simulation variables
```

which sets the simulation global parameters and their properties. The text to the right of the “!” is treated as a comment and not used by TUFLOW AD when interpreting the line.

The style of input is flexible but a few rules. The rules are:

- A few characters are reserved for special purposes as described in Table 4.1 and
- Only one command can occur on a single line.

Table 4.1 Reserved Characters – Text Files

Reserved Character(s)	Description
“#” or “!”	A “#” or “!” causes the rest of the line from that point on to be ignored. Useful for “commenting-out” unwanted commands, and for modelling documentation.
==	A “==” following a command indicates the start of the parameter(s) for the command.

The notation used to document commands and valid parameter values are presented in Table 4.2.

Table 4.2 Notation Used in Command Documentation – Text Files

Documentation Notation	Description
< ... >	Greater than and less than symbols are used to indicate a variable parameter. For example, the commonly used <file> example is described below.
<file>	Is a filename (can include an absolute or relative path, or a URL/UNC path). Examples are: 2d_ad_ic_Run1.mif (must be co-located with global database file) ..\model\2d_ad_ic_Run1.mif (this is a relative path – the “..” indicates to move up a level) P:\jb99\tuflow\model\2d_ad_ic_Run1.mif (this is an absolute path) \\wbm\catchments\jb99\tuflow\model\2d_ad_ic_Run1.mif (this is a URL or UNC path)
spaces	Spaces can occur in commands and parameter options. If a space occurs in a command, it is only one (1) space, not two or more spaces in succession. Spaces can occur in file and path names.

4.2 Simulation Control File

4.2.1 TUFLOW AD Control File (.adcf File)

The TUFLOW AD Control File or .adcf file points to the two mandatory files required for AD model execution. It is the top of the tree for the AD model and is called directly from TUFLOW via the .tcf ([AD Control File](#) command). The .adcf file must reference:

- one global database file using the [AD Global Database](#) command; and
- one boundary database file using the [AD BC Database](#) command.

No other commands are required in the adcf file.

In UltraEdit, the commands and comments can be colour coded for easier viewing (see Section 4.10).

```
# This is an example of an .adcf file
! Comments are shown after a "!" or "#" character.
! Blank lines are ignored. Commands are not case sensitive.

AD GLOBAL DATABASE == ..\bc_dbase\2d_ad_globaldatabase_Demo1.csv !global
AD BC DATABASE == ..\bc_dbase\2d_ad_dbase_Demo1.csv !boundaries
```

[Appendix B](#) lists and describes these commands and their parameters.

4.2.2 Run Time and Output Controls

Both run time and output controls are set within the TUFLOW .tcf and the parameters specified there apply also to the AD simulation. Section 4.2.2 of the TUFLOW manual describes these parameters.

4.3 GIS Layers

GIS data layers are transferred into TUFLOW AD using the MapInfo data exchange MIF/MID format. This format is documented and in text (ASCII) form, making it easy to transfer GIS data. It is also available for import and export from most mainstream CAD/GIS platforms.

AS per TUFLOW. all GIS layers imported to TUFLOW AD **must be in the same geographic projection**. Only polygon data is read by TUFLOW AD, where this data specifies regions for initial conditions (Section 4.8) and/or minimum dispersion coefficients (Section 4.9). Both are specified in the Global Database file (Section 4.6). GIS data is interpreted by TUFLOW AD in the same manner as TUFLOW. Section 4.3 of the TUFLOW manual describes this manner. Table 4.3 repeats an abridged version, as applied to TUFLOW AD.

Table 4.3 TUFLOW AD Interpretation of MIF Objects

Object Type	TUFLOW Interpretation
Used Objects	
Region (polygon)	<ul style="list-style-type: none"> Either effects any 2D cell or cell mid-side/corner (e.g. Zpt) that falls within the region. If the command is modifying a whole 2D cell, it uses the cell's centre to determine whether the cell falls inside or outside of the region. If the cell's centre, mid-side or corner lies exactly on the region perimeter, uncertain outcomes may occur. Holes within regions are accepted.
Unused (Ignored) Objects	
Point	Ignored.
Line (straight line)	Ignored.
Pline (line with one or more segments)	Ignored.
Arc	Ignored.
Collections	Ignored.
Ellipse	Ignored.
Multiple (Combined) Objects	Ignored.
none	Ignored. These most commonly occur when a line of attribute data is added that is not associated with an object. In MapInfo, this occurs when a line of data is added to a Browser Window.
Roundrect (Rounded Rectangle)	Ignored.

Rect (Rectangle)	Ignored.
Text	Ignored.

4.4 2D Geometries

All 2D domain information is specified with TUFLOW (.tgc) and sent to TUFLOW AD as required. No additional geometry information is required or read by TUFLOW AD.

4.4.1 Multiple 2D Domains

Multiple 2D domains are not currently supported by TUFLOW AD.

4.5 1D Geometries

All 1D information (at current release only SX data) is read and processed by TUFLOW and ESTRY and required information passed to TUFLOW AD. TUFLOW AD does not require or read any further 1D data.

4.6 Specification of Constituent Properties

Constituent properties are specified in the Global Database file, which is identified in the .adcf file using the [AD Global Database](#) command. This database file has a set structure, in much the same way as TUFLOW boundary database files, and can be created in software such as Microsoft Excel. The number of constituents simulated by TUFLOW AD is simply the number of line entries in this file (excepting the header data). Constituents can be removed from the simulation by prefacing rows in the global database file with the ‘!’ or ‘#’ character. The maximum number of constituents TUFLOW AD can simulate is 20.

The global database file must be .csv (comma delimited) formatted. The first row must contain the predefined keywords (in order) as listed in Table 4.4, separated by commas. Subsequent rows contain constituent data.

Table 4.4 Global Database Keyword Descriptions

Keyword	Description
Name	The name of a constituent. This might be ‘TN’ or ‘Salinity’ (without the inverted commas). The Name field is limited to 40 characters and must be alphanumeric characters only. Mandatory.
Heat Name	Not currently used. Leave blank. When the thermal module is released, this field will identify the constituent being simulated as heat (i.e. temperature) and will prompt TUFLOW AD to treat it differently in terms of required data inputs (i.e. atmospheric interaction) and limitations on its transport.
Decay Rate	The decay rate (k) of the constituent in units of day^{-1} . This value is used in a first order decay calculations at each timestep, i.e.

Keyword	Description
	$C(t) = C_0 e^{-kt}$ <p>where:</p> <ul style="list-style-type: none"> • $C(t)$ is constituent concentration at time t • C_0 is a reference concentration • k is the decay rate specified here; and • t is time <p>If no decay is required, then either enter 0 or leave the field blank.</p>
Settling Rate	<p>The settling rate of the constituent in units of m.day^{-1}. This value is used in a simple mass balance calculation that removes the constituent from the water column based on this rate.</p> <p>If no settling is required, then either enter 0 or leave the field blank.</p>
Longitudinal Dispersion Coefficient	<p>The value D_l for the constituent, as per Section 1.4. Allowing such variation between constituents permits simultaneous simulation of multiple constituents with varying dispersion properties. This is useful at the model calibration stage when a range of dispersion coefficients can be tested within one simulation to ascertain the best match to monitoring data. This feature can also be used in sensitivity testing.</p> <p>Notwithstanding this, this value should not be varied from constituent to constituent once the AD model is calibrated.</p> <p>If the field is blank or set to zero, then longitudinal dispersion is switched off.</p>
Transverse Dispersion Coefficient	<p>The value D_t for the constituent, as per Section 1.4. Allowing such variation can be exploited in the same manner as described above for longitudinal dispersion. This value should not be varied from constituent to constituent once the AD model is calibrated.</p> <p>If the field is blank or set to zero, then transverse dispersion is switched off.</p>
Initial Condition	<p>This can be set to either a single number or a path reference to a GIS .mif layer (2d_ad_ic_). If the former is specified, then that value is applied uniformly to all wet cells at initialisation.</p> <p>If a path to a GIS .mif layer is specified, then the layer must comprise of (only) polygons with a single attribute. The attribute must be of type Float. The field name is not used by TUFLOW AD, so can be set to a label that is meaningful to the user. The polygon data, with spatially varying attributes of initial concentration is applied to wet cells at simulation initiation. Wet cells not covered by any polygon in the specified .mif layer are set to a concentration of zero.</p> <p>If the field is left blank, then a concentration of zero is applied to all cells.</p>
Minimum	<p>Not currently used. Leave blank. When the thermal module is released, this field will set a minimum computed water temperature at each timestep. This is useful for avoiding unrealistic temperature predictions in very shallow waters.</p>

Keyword	Description
Maximum	Not currently used. Leave blank. When the thermal module is released, this field will set a maximum computed water temperature at each timestep. This is useful for avoiding unrealistic temperature predictions in very shallow waters.
Minimum Dispersion	<p>This sets the value of D_w as per Section 1.4. It can be set to either a single number or a path reference to a GIS .mif layer. If the former is specified, then that value is applied uniformly to all wet cells at each timestep.</p> <p>If a path to a GIS .mif layer is specified, then the layer must comprise of (only) polygons with a single attribute. The attribute must be of type Float. The field name is not used by TUFLOW AD, so can be set to a label that is meaningful to the user. The polygon data, with spatially varying values of D_w is applied to wet cells at each timestep. Wet cells not covered by any polygon in the specified .mif layer will have D_w set to zero.</p> <p>This field cannot be left blank. If a minimum dispersion of zero is required, then 0.0 must be entered in this field. Errors will result if this field is left blank.</p>

An example global database file is provided in the demonstration models.

4.7 Boundary Conditions

TUFLOW AD uses the same approach as TUFLOW to setting up boundary conditions in that two types of files are required:

- A boundary condition database; and
- Boundary condition data files (i.e. timeseries).

Like TUFLOW, TUFLOW AD also uses comma delimited format for both these file types.

TUFLOW AD does not require specification of any geographical information regarding the location of boundary conditions. All such required data is passed from TUFLOW to TUFLOW AD for TUFLOW boundary types HT, QT, HS, HQ, QC, VC, VT, and SA. SX data is passed as needed.

4.7.1 Boundary Condition (BC) Database

A boundary condition (BC) database is set up using spreadsheet software such as Microsoft Excel. It must be .csv (comma delimited) formatted and is identified in the .adcf file (see [AD BC Database](#)). The database contains a list of files and attribute names to search for within those files. The attribute names are then used to extract the desired boundary condition data.

The AD BC database is structured in the same way as a TUFLOW BC database in that it must contain a header line with subsequent rows of information. The header line must contain the keywords

```
Name, Source, Column 1, Column 2, Add Col 1, Mult Col 2, Add Col 2, Column 3, Column 4
```

in that order, with meanings as per Table 4.5.

Table 4.5 BC Database Keyword Descriptions

Keyword	Description
Name	<p>The name of a BC data set. It consists of two concatenated elements as follows:</p> <ul style="list-style-type: none"> • First: This must be the same ‘Name’ attribute used in the GIS 2d_bc layer(s) specified in TUFLOW. This is third attribute in the 2d_bc layer and follows ‘Type’ and ‘Flags’. It may contain spaces, but must not contain commas. It is not case sensitive. • Second: This must be the name of the appropriate constituent for which the boundary condition is being specified. This name must be one of those specified in the AD Global Database ‘Name’ field. <p>These two names are joined by a double underscore. As such, if there are “M” 2d_bc boundary condition objects specified in TUFLOW, and “N” constituents to be simulated by TUFLOW AD, then M*N entries are required in the AD BC Database.</p> <p>An example is Ocean__Salinity, where the TUFLOW 2d_bc file has a polyline with Name attribute “Ocean” and the AD Global Database has a variable called “Salinity” listed.</p> <p>Mandatory.</p>
Source	<p>The file from which to extract the BC data. It must be a .csv file. Paths are relative to the AD Global Database.</p> <p>Mandatory.</p>
Column 1	<p>The name of the first column of data (time values) in the .csv Source File.</p> <p>Mandatory.</p>
Column 2	<p>The name of the column of data in the .csv Source File. Values in this column are always concentrations, for all allowable BC sets. These are applied to cells corresponding to the appropriate locations of all types of BCs specified in TUFLOW 2d_bc GIS layers. These specified concentrations override any other computed concentrations at the boundary locations.</p> <p>The exception to the above is for SA boundaries, where the specified concentration is multiplied by the inflow corresponding to that concentration (as passed to TUFLOW AD from TUFLOW) and the mass load over the SA polygon computed. This mass load is then added to the mass of constituent within the wet computational cells within the SA polygon, and mass conservation used to compute a new resultant ambient concentration.</p> <p>Mandatory.</p>
Add Col 1	Not used. Leave Blank.
Mult Col 2	Not used. Leave Blank.

Keyword	Description
Add Col 2	Not used. Leave Blank.
Column 3	Not used. Leave Blank.
Column 4	Not used. Leave Blank.

4.7.2 BC Database Example

The Excel spreadsheet below illustrates a simple example of an AD BC database set up in a worksheet that is exported as a .csv file for use by TUFLOW AD. Four polyline boundaries have been specified via GIS in TUFLOW (with Name fields “West”, “North”, “East” and “South”) and two constituents have been specified in the AD Global Database (with Name fields “Tracer_01” and “Tracer_02”). Four boundaries and two constituents thus require eight entries in the BC file.

	A	B	C	D	E	F	G	H	I
1	Name	Source	Column 1	Column 2	Add Col 1	Mult Col 2	Add Col 2	Column 3	Column 4
2	!Tracer 1 data								
3	West_Tracer_01	Demo1_Concs1.csv	Time	W_Tracer_01					
4	North_Tracer_01	Demo1_Concs1.csv	Time	N_Tracer_01					
5	East_Tracer_01	Demo1_Concs1.csv	Time	E_Tracer_01					
6	South_Tracer_01	Demo1_Concs1.csv	Time	S_Tracer_01					
7	!Tracer 2 data								
8	West_Tracer_02	Demo1_Concs2.csv	Time	W_Tracer_02					
9	North_Tracer_02	Demo1_Concs2.csv	Time	N_Tracer_02					
10	East_Tracer_02	Demo1_Concs2.csv	Time	E_Tracer_02					
11	South_Tracer_02	Demo1_Concs2.csv	Time	S_Tracer_02					
12									

The Demo1_Concs.csv file was created by saving the below as a .csv file from Excel. All values are concentrations in mg/L, with the exception of the Time column, which has units of hours.

	A	B	C	D	E	F	G	H	I
1	Time	W Tracer 01	N Tracer 01	E Tracer 01	S Tracer 01	W Tracer 02	N Tracer 02	E Tracer 02	S Tracer 02
2	0	0	0	0	0	0	0	0	0
3	49.9	20	40	5	1	66	40	5	20
4	50	10	20	2.5	0.5	0.5	20	2.5	65
5	54.9	100	200	25	5	5	200	31	100
6	55	90	180	22.5	4.5	4.5	35	22.5	90
7	60	70	140	17.5	3.5	3	140	17.5	70
8	501	0	0	0	0	0	0	0	0

4.8 Initial Conditions

Initial conditions are specified for each constituent as either a constant value or spatially variant (see Table 4.4). The former is simply entered as a decimal (or integer) in the Initial Condition field of the AD Global Database. This value is applied to all wet cells at model initiation.

The latter is applied by entering a relative (or absolute) file path to a GIS layer in the Initial Condition field of the AD Global Database. The GIS file has the attributes described in Table 4.6.

Table 4.6 2D Initial Conditions (2d_ad_ic) Attribute Descriptions

GIS Attribute	Description	Type
Conc	The initial condition concentration.	Float

As many polygons as needed can be included in this layer. Any wet cells not covered by these polygons will be initialised to a concentration of zero. The naming convention prefix for this layer is 2d_ad_ic_. **The objects must be polygons – rectangles, round rectangles etc. are not read by TUFLOW AD.** The attribute name is not read by TUFLOW AD and can be anything meaningful to the user - “Conc” is used as an example above for clarity.

4.9 Minimum Dispersion Coefficient (D_w)

Minimum dispersion coefficients are specified for each constituent as either a constant value or spatially variant (see Table 4.4). The former is simply entered as a decimal (or integer) in the Minimum Dispersion field of the AD Global Database. This value is applied to all wet cells at all timesteps. The latter is applied by entering a relative (or absolute) file path to a GIS layer in the Minimum Dispersion field of the AD Global Database. The GIS file has the attributes described in Table 4.7.

Table 4.7 2D Minimum Dispersion Coefficient (2d_ad_md) Attribute Descriptions

GIS Attribute	Description	Type
MD	Minimum dispersion coefficient.	Float

As many polygons as needed can be included in this layer. Any wet cells not covered by these polygons will be assigned a minimum dispersion coefficient of zero. The naming convention prefix for this layer is 2d_ad_md_. **The objects must be polygons – rectangles, round rectangles etc. are not read by TUFLOW AD.** The attribute name is not read by TUFLOW AD and can be anything meaningful to the user - “MD” is used as an example above for clarity.

4.10 UltraEdit

UltraEdit (www.ultraedit.com) is recommended as the text editor for TUFLOW text files. UltraEdit has many excellent features, of which a few are noted here.

- 1 A file “Wordfile.txt” is provided with TUFLOW in the UltraEdit folder. Replace the equivalent file in the UltraEdit installation folder (typically “C:\Program Files\UltraEdit”) with the one provided with TUFLOW. UltraEdit will now colour code TUFLOW, ESTRY and TUFLOW AD text files. (Note: If you have modified the UltraEdit Wordfile.txt file for your own purposes, you will have to merge the two files.) You can change the colours in UltraEdit via Advanced, Configuration, Syntax Highlighting menus.

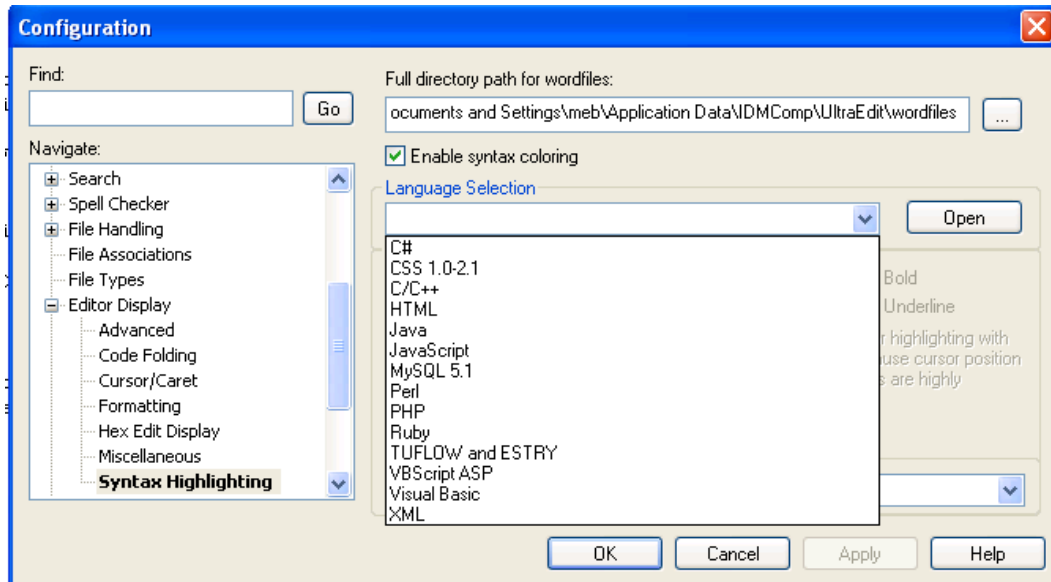
For more recent versions of UltraEdit, you may have to rename the “Wordfile.txt” provided to ‘tufLOW.uew’ and include it in the wordfiles directory that has other .uew files (such as ‘vbscript.uew’). This directory may be something like

C:\Program Files\IDM Computer Solutions\UltraEdit\wordfiles

You will then need to delete all content from the ‘tufLOW.uew’ file *except that relating to TUFLOW and ESTRY*. This information starts at the line:

“/L14”TUFLOW and ESTRY” Line Comment = “...

You will also need to change the number after the leading L to be the number of files in the directory containing your .euw files (including the tufLOW.euw file). The example above has thirteen other .euw files read by UltraEdit in the wordfiles directory, so the tufLOW.euw file leading line was changed to start with /L14. On startup, UltraEdit reads all 14 files, and then offers the associated colour coding options in a drop down menu in Advanced > Configuration > Editor Display > Syntax Highlighting as per the below



- 2 UltraEdit has a very useful feature that allows opening of a file that is specified in the active text file. Place the pointer anywhere over the text of the file you wish to open and click the right mouse button. The top menu item on the pop-up menu will open the file.

5 Model Development

Section Contents

5	Model Development	5-1
5.1	Example Models	5-2
5.2	Setting up a New Model	5-2

5.1 Example Models

An example TUFLOW AD model is available via the TUFLOW example model database hosted on the [TUFLOW Wiki](#).

5.2 Setting up a New Model

The steps below describe the process for setting up a TUFLOW AD model. It is assumed that the user is familiar with TUFLOW and that the folder structure for TUFLOW has been setup with all required files. The user should run the TUFLOW model without the AD module first to make sure that it is appropriately configured and stable.

Create a TUFLOW AD control file (.adcf)

- 1 Use a text editor to create an empty .adcf file and save it to the “runs” folder.

Set up AD global database (.csv file)

- 2 Set up TUFLOW AD global database in the “bc dbase” folder (see Table 4.4).
- 3 In the .adcf file use [AD Global Database](#) to set the location of the global database as follows.

```
AD Global Database == ..\bc dbase\my ad global dbase.csv
```

Setup up the boundary condition tables (.csv file(s))

- 4 Setup the boundary condition table(s) in the “bc dbase” folder (Section 4.7.2).

Setup up the boundary condition database (.csv file)

- 5 Setup the boundary condition database in the “bc dbase” folder (Section 4.7.1) that references the tables set up in the previous step.
- 6 In the .adcf file use [AD BC Database](#) to set the location of the bc database as follows.

```
AD BC Database == ..\bc dbase\my ad bc dbase.csv
```

Setup up TUFLOW to activate the AD module (.tcf file)

- 7 In the .tcf file use the command AD Control File to set the location of the adcf and activate execution of the AD module as follows.

```
AD Control File == ad_run.adcf
```

Run the model

- 8 Run TUFLOW as normal. The AD module will be called and results files written as described in Section 6.

6 Data Output

Section Contents

6	Data Output	6-1
6.1	General	6-2
6.1.1	Console (DOS) Window Display	6-2
6.1.2	TUFLOW AD Log Files	6-2
6.1.2.1	<i>Simulation Log File</i>	6-3
6.1.2.2	<i>CFL Log File</i>	6-3
6.1.2.3	<i>Mass Log File</i>	6-4
6.2	2D Domains	6-5
6.2.1	SMS (Map) Output (.dat or .xmdf Files)	6-5

6.1 General

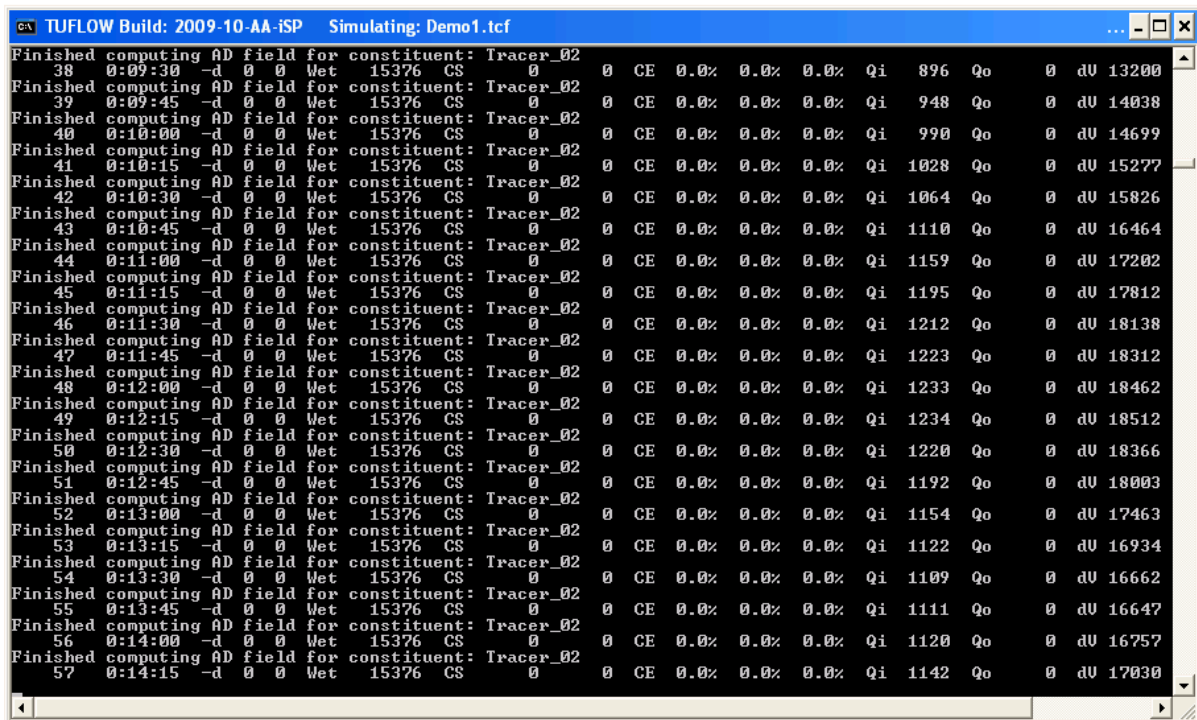
6.1.1 Console (DOS) Window Display

TUFLOW AD displays a lot of information to the Console (DOS) Window during the data input stages. If there are data input problems, trace back through the Window buffer (no buffer is available on Windows 98) to establish where in the input data process the problem occurs. Alternatively, search the .adlf file.

Once the simulation has started, the simulation status at each timestep is displayed. The AD module writes to screen as an additional line to the TUFLOW output as (for a constituent called 'Tracer_X'):

```
Finished computing AD field for constituent: Tracer_X
```

The Console Window appears as something similar to that shown below. The colours, size and other attributes of the window can be changed as required.



```
TUFLOW Build: 2009-10-AA-ISP Simulating: Demo1.tcf
Finished computing AD field for constituent: Tracer_02
38 0:09:30 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 896 Qo 0 dU 13200
Finished computing AD field for constituent: Tracer_02
39 0:09:45 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 948 Qo 0 dU 14038
Finished computing AD field for constituent: Tracer_02
40 0:10:00 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 990 Qo 0 dU 14699
Finished computing AD field for constituent: Tracer_02
41 0:10:15 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 1028 Qo 0 dU 15277
Finished computing AD field for constituent: Tracer_02
42 0:10:30 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 1064 Qo 0 dU 15826
Finished computing AD field for constituent: Tracer_02
43 0:10:45 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 1110 Qo 0 dU 16464
Finished computing AD field for constituent: Tracer_02
44 0:11:00 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 1159 Qo 0 dU 17202
Finished computing AD field for constituent: Tracer_02
45 0:11:15 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 1195 Qo 0 dU 17812
Finished computing AD field for constituent: Tracer_02
46 0:11:30 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 1212 Qo 0 dU 18138
Finished computing AD field for constituent: Tracer_02
47 0:11:45 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 1223 Qo 0 dU 18312
Finished computing AD field for constituent: Tracer_02
48 0:12:00 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 1233 Qo 0 dU 18462
Finished computing AD field for constituent: Tracer_02
49 0:12:15 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 1234 Qo 0 dU 18512
Finished computing AD field for constituent: Tracer_02
50 0:12:30 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 1220 Qo 0 dU 18366
Finished computing AD field for constituent: Tracer_02
51 0:12:45 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 1192 Qo 0 dU 18003
Finished computing AD field for constituent: Tracer_02
52 0:13:00 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 1154 Qo 0 dU 17463
Finished computing AD field for constituent: Tracer_02
53 0:13:15 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 1122 Qo 0 dU 16934
Finished computing AD field for constituent: Tracer_02
54 0:13:30 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 1109 Qo 0 dU 16662
Finished computing AD field for constituent: Tracer_02
55 0:13:45 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 1111 Qo 0 dU 16647
Finished computing AD field for constituent: Tracer_02
56 0:14:00 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 1120 Qo 0 dU 16757
Finished computing AD field for constituent: Tracer_02
57 0:14:15 -d 0 0 Wet 15376 CS 0 0 CE 0.0% 0.0% 0.0% Qi 1142 Qo 0 dU 17030
```

6.1.2 TUFLOW AD Log Files

TUFLOW AD text (i.e. not results) outputs are written to two log files in the location specified by 'Output Folder' in the .tcf file (or the "runs" folder if this command is not used):

- A simulation log file;
- A CFL condition log file; and
- A mass balance log file.

All are written to the location specified by 'Log Folder == ' command in the .tcf file, or the location of the .tcf itself if this command is not used.

6.1.2.1 Simulation Log File

This file is named 'SimulationX.adlf' for simulation (and .tcf file) name SimulationX. It contains commentary of input reading, constituent specification etc. as the simulation sets itself up. Following that, output is regular at each timestep as:

```
Simulation time (h)           0.0125

Finished constituent Tracer_01   at AD substep iteration number   1
Finished constituent Tracer_02   at AD substep iteration number   1
Finished constituent Tracer_02   at AD substep iteration number   2
Finished constituent Tracer_02   at AD substep iteration number   3
```

These lines show information regarding the simulation time for each constituent. In particular, the number of AD sub-steps needed to be executed to maintain stability under CFL and Peclet conditions is reported. In the above example, constituent Tracer_01 required no substepping, whilst constituent Tracer_02 required 3 substep iterations to maintain stability. This is caused by Tracer_02 being set up with greater dispersion coefficients than Tracer_01 in the AD global database. Additional rows are added as required by the number of constituents simulated.

6.1.2.2 CFL Log File

This file is named 'SimulationX_ADcfl.csv' for simulation (and .tcf file) name SimulationX. It contains commentary on CFL and Peclet numbers, maximum dispersion coefficients and number of substep iterations. An example is shown below.

	A	B	C	D	E	F	G	H	I	J	K
1	time (hrs)	Constituent Name	Max CFL u	Max CFL v	Max Peclet u	Max Peclet v	Max sum u	Max sum v	Max Disp x	Max Disp y	Num Iterations
2	0.00417	Tracer_01	0.00025	0	0	0	0.00025	0	0	0	1
3	0.00417	Tracer_02	0.00025	0	0.03003	0.03	0.03029	0.03	5.00535	5.00027	1
4	0.00833	Tracer_01	0.00095	0	0	0	0.00095	0	0	0	1
5	0.00833	Tracer_02	0.00095	0	0.036	0.036	0.036	0.036	6	6	1
6	0.0125	Tracer_01	0.00174	0	0	0	0.00174	0	0	0	1
7	0.0125	Tracer_02	0.00174	0	0.036	0.036	0.036	0.036	6	6	1
8	0.01667	Tracer_01	0.00246	0	0	0	0.00246	0	0	0	1
9	0.01667	Tracer_02	0.00246	0	0.036	0.036	0.036	0.036	6	6	1

Specifically, the column data is as per Table 6.1:

Table 6.1 _ADcfl.csv File Columns

Column	Description
time (h)	The simulation time in hours.
Constituent Name	The name of the constituent as specified in the AD global database.
Max_CFL_u	The maximum CFL for u velocities anywhere in the computational domain at that timestep.
Max_CFL_v	The maximum CFL for v velocities anywhere in the computational domain at that timestep.
Max_Peclet_u	The maximum Peclet number for u dispersion anywhere in the computational domain at that timestep.
Max_Peclet_v	The maximum Peclet number for v dispersion anywhere in the computational domain at that timestep.
Max_sum_u	The maximum of the sum of CFL and Peclet numbers in the x (u) direction anywhere in the computational domain.
Max_sum_v	The maximum of the sum of CFL and Peclet numbers in the y (v) direction anywhere in the computational domain.
Max_Disp_x	The maximum dispersion coefficient in the x (u) direction anywhere in the computational domain.
Max_Disp_y	The maximum dispersion coefficient in the y (v) direction anywhere in the computational domain.
Num_iterations	The number of iterations required by TUFLOW AD to remain stable. This can vary from constituent to constituent if different dispersion coefficients are applied.

6.1.2.3 Mass Log File

This file is named ‘SimulationX_ADmass.csv’ for simulation (and .tcf file) name SimulationX. It contains commentary on mass conservation. An example is shown below.

The screenshot shows a Microsoft Excel spreadsheet titled 'Demo1_ADmass.csv'. The spreadsheet has columns labeled A through O. The data is organized as follows:

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	time (hrs)	Tracer_01	Tracer_02												
2	0.004167	20160	14112.69434												
3	0.008333	20160	14112.69434												
4	0.0125	20160	14112.69434												
5	0.016667	20160	14112.69434												
6	0.020833	20160	14112.69434												
7	0.025	20160	14112.69336												
8	0.029167	20160	14112.69141												
9	0.033333	20160	14112.69043												

Specifically, the column data is as per Table 6.2:

Table 6.2 _ADmass.csv File Columns

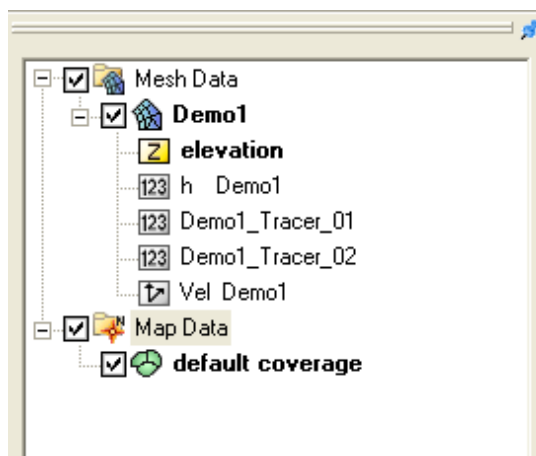
Column	Description
time (h)	The simulation time in hours.
Constituent Name 1	The total mass of that constituent in the computational domain. TUFLOW AD assumes that the constituent concentrations are specified in mg/L, and this number is then in tonnes of constituent. If the concentration is g/L, then this number should be multiplied by 1000 to be in units of tonnes.
Constituent Name 2	As per constituent 1. Column repeated until all constituents have been accounted for

6.2 2D Domains

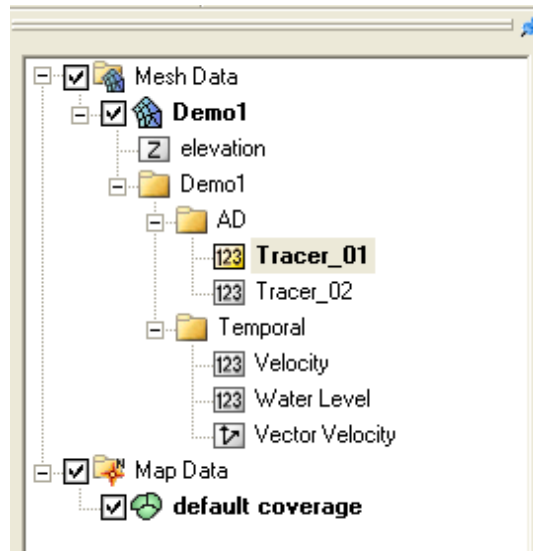
6.2.1 SMS (Map) Output (.dat or .xmdf Files)

TUFLOW AD produces one of two (or both) output formats, and these are set in the tcf file by using the Map Output Format command. These are:

- SMS formatted (*.dat) output files. The .ALL.sup (SMS) file created by TUFLOW is altered by the AD module to load the .dat AD results files automatically. One .dat file is produced for each constituent listed in the AD global database, in that order. These can also be loaded directly into SMS using the .2dm file produced by TUFLOW as a geometry. An example of the data sets loaded by the .ALL.sup structure in SMS is shown below.



- XMDF formatted output file. This file format offers a range of advantageous features:
 - All map output is in the one file (ie. all .dat files become one .xmdf file and this .xmdf file is the same as that produced by TUFLOW – i.e. all TUFLOW and AD data sets are written to the same file).
 - Much faster to access and instant load up when first opened due to an indexing system located in the file header.
 - Data are stored in a folder structure that software such as SMS can use to access the data. Specifically, the AD data sets within the TUFLOW .xmdf file are all included within a folder named “AD”. See image below as an example.



- Data stored as either static or temporal (time) based.
- Format is an industry standard and recognised by other software. Executable code available to write applications that access the data.

Two existing TUFLOW tools are relevant to the post-processing of .dat files (if required).

The TUFLOW utility TUFLOW_to_GIS can be used to convert these files to GIS files (*.asc) as per standard TUFLOW files. For example, the following command will create an ASCII grid at 5m resolution at time = 10 hrs from the file Demo2_TSS.dat

```
TUFLOW_to_GIS.exe -asc -grid5 -k10 Demo2_TSS.dat
```

Similarly, dat_to_dat.exe can be used to create a dat file at one timestep only, e.g.

```
dat_to_dat.exe-k10 Demo2_TSS.dat
```

The main reason not to use .xmdf files at this stage is these utility programs are not yet updated to work with .xmdf files.

To output in the .xmdf format use Map Output Format == XMDF in the tcf. TUFLOW AD will automatically follow suit in output file format.

7 References

- Falconer, R.A., Lin, B. and Kashefipour, S.M. (2005)** *Modelling Water Quality Processes in Estuaries* Computational Fluid Dynamics: Applications in Environmental Hydraulics, Eds P.B. Bates, S.N. Lane and R.I. Furguson. John Wiley and Sons.
- Leonard, B.P. (1991)** *The ULTIMATE Conservative Difference Scheme Applied to Unsteady One-Dimensional Advection* Computer Methods in Applied Mechanics and Engineering **88**:17-74.
- Leonard, B.P. and Niknafs, H.S. (1991)** *Cost-Effective Accurate Coarse-Grid Method for Highly Convective Multidimensional Unsteady Flows* NASA Centre for Aerospace Information Report 91N21075.
- Leonard, B.P., MacVean, M.K. and Lock, A.P. (1993)** *Positivity-Preserving Numerical Schemes for Multidimensional Advection* NASA Centre for Aerospace Information Report 93N27091.
- Wu, Y. and Falconer, R.A. (2000)** *A Mass Conservative 3-D Numerical Model for Predicting Solute Fluxes in Estuarine Waters* Advances in Water Resources **23**:531-543.

Appendix A .tcf File Commands

[AD Control File](#)

AD Control File == <.adcf_file>

(Mandatory to trigger AD module)

Triggers TUFLOW to execute AD simulation and specifies the TUFLOW AD control file name.

Example:

AD Control File == Demo1.adcf

Appendix B .adcf File Commands

[AD Global Database](#)

[AD BC Database](#)

AD Global Database == <file>

Mandatory

A pointer to a file containing constituent information (e.g. name and dispersion coefficients) – see Section 4.6.

AD BC Database == <file>

Mandatory

A pointer to a file containing boundary database information (e.g. names of boundary files as mapped to GIS data sets read by TUFLOW) – see Section 4.7.2.