User's Guide

WAQPRO

Rijkswaterstaat
Ministerie van Infrastructuur en Waterstaat

User's Guide

WAQPRO

WAQPRO is the WAQUA-in-SIMONA processor.

Version	:	10.45, July 2009
Maintenance	:	see www.helpdeskwater.nl/waqua
Copyright	:	Rijkswaterstaat

Contents

1 About the User’s Guide

The text of this User’s Guide partly originates from the Rand Corporation Working Draft WD-822-Neth, written by A.B. Nelson, C.N. Johnson, and J.J. Leendertse. The parts provided by the Rand Corporation have already been rearranged by A. Staakman, Th. L. van Stijn and G.J. Bosselaar for an earlier version of the WAQUA user’s guide.

This guide depends on the general introduction for some general information about the system. It depends to an even greater extent on the ’user’s guide pre-processor WAQPRE’ for a detailed description of the input and limitations on the input.

2 The processor WAQPRO

2.1 General description

The two-dimensional simulation program WAQPRO is the central computational program in the WAQUA system. It is used to simulate hydrodynamic processes and water quality in well-mixed estuaries, coastal seas and rivers.

WAQPRO receives input that has been processed by the pre-processor WAQPRE and been stored on the SDS file. Using the bathymetry and physical characteristics described in the input, WAQPRO computes water levels and currents as well as the concentration and dispersion of constituents resulting from the time-varying effects of tide levels, wind, discharge, concentration, movable barriers and weirs, using either a rectilinear or a curvilinear grid.

RGF file

In case of a curvilinear computation, an 'RGF file' can be used. The RGF file contains the x- and y-coordinates of the grid, generated by a grid generator. The name of the file is given in the WAQPRE input file.

output

WAQPRO will provide various outputs to the user upon request. These include printed tables of variables during the course of the run (WAQPRO message file), and various data sets that are written to the SDS file.

Input

The input to the simulation is described in detail in the user's guide pre-processor WAQPRE.

run costs

WAQPRO is usually very expensive to run; therefore, great care should be taken in setting up the input and in selecting the output options. The cost of running WAQPRO depends upon the computer system used and upon the specific accounting algorithm in effect. The amount of CPU time required for a run depends mainly upon the size of the area being modelled (the number of points within the computational grid), the number of integration steps (length of time simulated / half time step) and the number of constituents in the model. Other factors affect the time to a lesser extend: e.g. the number of times that points flood or dry, and the amount of data saved for later analysis.

data storage

The simulation mentioned above uses considerable storage on disk. Users are urgently requested to monitor the dimensions of their files on disk closely and to copy these files onto tapes as soon as possible.

2.2 Limitations and reminders

input limitations

Limitations on the data input are described in the User’s Guide pre-processor WAQPRE.

computational limitations

With selection of too large an area to be modelled or of too small a grid size within the area, it is possible to exceed the core size of any computer.

reminders

Because the simulation can generate almost unlimited amounts of output, some restraint should be used in selecting the frequency and amount for the writing of data to the SDS file. Printed output can also become excessive if all options are exercised and the print requested too frequently.

2.3 User routine WASUST

2.3.1 Purpose

Subroutine WASUST offers users a facility to program additional mathematical/physical processes into the transport equation of the WAQUA system. It is possible for a user of the WAQUA system to change coefficients during the simulation by means of the subroutine WASUST.

$$\frac{\partial}{\partial t}(hC) + \frac{\partial}{\partial x}(huC) + \frac{\partial}{\partial y}(hvC) + \frac{\partial}{\partial z}\left(h(w - w_{val})C\right) =$$
$$= \frac{\partial}{\partial x}\left(D_x \frac{\partial}{\partial x}(hC)\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial}{\partial y}(hC)\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial}{\partial z}(hC)\right) +$$
$$+ S_+ - LC$$

The advection diffusion equation, solved by the WAQUA system is:

The user routine WASUST has to be programmed by the user. In WASUST the following coefficients can be changed:

D_x, D_y	refer to parameter DIFUV;
D_z	refer to parameter DIFW;
S_+	refer to parameter SEXP;
L	refer to parameter SIMP.

Note: the user transportroutine can also be used in parallel runs and in runs with domain decomposition. However, when the routine uses horizontal derivatives or otherwise requires data from neighbouring grid points in the computation of one grid point, special attention must be paid to the exchange of information (communication) between neighbouring subdomains. Please contact the SIMONA helpdesk for assistence or further information.

2.3.2 User interface

2.3.2.1 Heading

```
subroutine wasust(    irogeo, kf    , guuvv , xydep , rp    ,
                      vel   , wind  , wval  , zk    , difuv ,
                      difw  , vicow , rho   , user  , iuser ,
                      fvalue, spainp, spatim, solusr, work  ,
                      simp  , sexp  , iparll, mypart, numprc,
                      mydom , ndom  , npart , myprc , mcordt,
                      ncordt, icocad, dum2  , dum3  )
```

2.3.2.2 Parameters

```
Integer   irogeo(3,noroco),    kf(nmax,-2:mmax+3,2),
          iuser(lenius),       icocad(*)
real      guuvv(nmax,-2:mmax+3,4),        xydep(nmax,-2:mmax+3,2),
          rp(nmax,-2:mmax+3,kmax,lmax), user(lenusr),
          vel(nmax,-2:mmax+3,kmax,*),     wind(nmax,-2:mmax+3,2), zk(nmax,-
          2:mmax+3,0:kmax),     wval(lmax),
          difuv(nmax,-2:mmax+3,kmax),     fvalue(lentim),
          difw(nmax,-2:mmax+3,kmax),      value(lentim),
          vicow(nmax,-2:mmax+3,0:kmax),
          rho(nmax,-2:mmax+3,kmax),
          spainp(nmax,-2:mmax+3,leninp),
          spatim(nmax,-2:mmax+3,lentdf),
          solusr(nmax,-2:mmax+3,lensol),
          work(nmax,-2:mmax+3,lenwrk),
          simp(nmax,-2:mmax+3,kmax,lmax),
          sexp(nmax,-2:mmax+3,kmax,lmax),
          dum2(*),    dum3(*)
```

where:

difuv i/o Horizontal diffusion coefficients (in $m^2 s^{-1}$), refer to user's guide WAQPRE, chapter GENERAL, DIFFUSION.

difw i/o Vertical diffusion coefficients (only filled for 3D approach (IAPDIM = 3)).

dum2 i Dummy argument for later usage.

dum3 i Dummy argument for later usage.

fvalue i Function value *f* at time TIMNOW of TIMEFUNCTIONS (refer to user's Guide WAQPRE, chapter TRANSPORT, USERDATA_TRANSPORT).

guuvv i Contains:
- GUU: transformation coefficients at u-points;
- GVV: transformation coefficients at v-points.

icocad i/o Administration array for COCLIB. This array is necessary for communications with COCLIB.

irogeo i All computational grid rows and columns.

In the first part of IROGEO the computational grid is described by NOROWS rows, consisting computational grid points. The first index of IROGEO contains:
pos. 1: n = n-coordinate of the computational grid row;
pos. 2: m1 = m-coordinate of the first u-velocity point of the computational grid row;
pos. 3: m2 = m-coordinate of the last u-velocity point of the computational grid row.
The second index of IROGEO contains the row number.

In the second part of IROGEO the computational grid is described by NOROCO - NOROWS columns, consisting computational grid points. The first index of IROGEO contains:
pos. 1: m = m-coordinate of the computational grid column;
pos. 2: n1 = n-coordinate of the first v-velocity point of the computational grid column;

		pos. 3: n2 = n-coordinate of the last v-velocity point of the computational grid column. The second index of IROGEO contains the column number.
iparll	i	flag for indicating type of run: 0=sequential, 1=parallel, 2=ddvert, 3=ddhor,4=ddhor+vert
iuser	i	Array IUSER containing integer data (refer to the user's guide WAQPRE, paragraph USERDATA).
kf	i	Contains: - KFU (= KF(1:NMAX,-2:MMAX+3,1)) status flag for drying/flooding at u-velocity points: 1 : wet u-velocity point; 0 : (temporarily) dry u-velocity point; - KFV (= KF(1:NMAX,-2:MMAX+3,2)) status flag for drying/flooding at v-station points: 1 : wet v-velocity point; 0 : (temporarily) dry v-velocity point;
mcordt	i	coordinate transformation parameter x/xi-direction
mydom	i	number of domain to which current subdomain belongs
mypart	i	own subdomain number
myprc	i	own process number
ncordt	i	coordinate transformation parameter y/eta-direction
ndom	i	number of (global) domains in current run
npart	i	logical number of parts in the parallel run
numprc	i	total number of processes in run
rho	i	Densities.
rp	i	Constituent concentrations throughout the field for all constituents.
sexp	i/o	Global source values throughout the grid for all constituents (in $[C] \cdot m \cdot s^{-1}$; [C] denotes the used dimension for the constituent). At input SEXP is filled with the global source values valid at the previous time step.
simp	i/o	Global sink values throughout the grid for all constituents (in $m \cdot s^{-1}$). At input SIMP is filled with the global sink values valid at the previous time step.
solusr	i/o	Array containing the OUTPUT_SPATIAL_DATA as defined in the input (refer to the user's guide WAQPRE, paragraph USERDATA_TRANSPORT).
spainp	i	Array containing the INPUT_SPATIAL_DATA (refer to the user's guide WAQPRE, paragraph USERDATA_TRANSPORT).

spatim i Array containing the TIMEDEPENDENT_SPATIAL_DATA valid for time TIMNOW (refer to the user's guide WAQPRE, paragraph USERDATA_TRANSPORT).

user i Array USER containing real data (refer to the user's guide WAQPRE, paragraph USERDATA_TRANSPORT).

vel i Contains:
- UP (= VEL (1 : NMAX, - 2 : MMAX + 3, 1 : KMAXS, 1)): u-velocities throughout the field;
- VP (= VEL (1 : NMAX, - 2 : MMAX + 3, 1 : KMAXS, 2)): v-velocities throughout the field;
- WP (= VEL (1 : NMAX, - 2 : MMAX + 3, 1 : KMAXS, 3)): physical w-velocities throughout the field. Note: WP is only filled for 3D approach (IAPDIM = 3).

vicow i Vertical (eddy-)viscosity coefficients (only filled for 3D approach (IAPDIM = 3)).

wind i Array with the space-varying wind data; contains:
- WINDX(= WIND (1 : NMAX, - 2 : MMAX + 3, 1): u-components of wind velocity throughout the field in the u-points;
- WINDY (= WIND (1 : NMAX, - 2 : MMAX + 3, 2): v-components of wind velocity throughout the field in the v-points;

work - Work array.
Warning: This is a temporary array; the data of this array will be lost after exiting the user routine.

wval i Fall velocities of the constituents.

xydep i Contains:
- XDEP (= XYDEP (1 : NMAX, - 2 : MMAX + 3, 1): x-coordinates of depth points in the physical plane;
- YDEP(= XYDEP (1 : NMAX, - 2 : MMAX + 3, 2): y-coordinates of depth points in the physical plane.

zk i Position of the layer interfaces in water level / concentration locations with respect to the reference level; positive direction is pointed upwards. ZK contains:
- ZK (1 : NMAX, - 2 : MMAX + 2, 0): water level with respect to the reference level; positive is directed upwards;
- ZK (1 : NMAX, - 2 : MMAX + 2, 1 : KMAX - 1): positions of the layer interfaces;
- ZK (1 : NMAX, - 2 : MMAX + 2, 1 : KMAX): position of the bathymetry.

Note: the positive direction for array zk is pointed **upwards**, while the bathymetry as it is specified in the input is defined with respect to the reference level and the positive direction is pointed **downwards**.

Within WASUST the common block CWAUST is available. The user programming mathematical/physical processes can use parameters from this common block (refer to the chapter in this user's guide on common CWAUST).

2.4 Common CWAUST

```
integer nmax, mmax, kmax, lmax, norows, noroco, kurflg,             nst, iapdim,
lenusr, lenius, lenwrk, leninp,                    lentim, lentdf, lensol, iurtyp, ldengr,
isvwp,                  iflval, irfmsg, irfrep, itrudm
real  dx, dy, dtsec, tempw, salw, ag, pi, vico, windc,              windac, rhomm3,
timnow, grdang, angrad, tstart

common /cwaust/ nmax, mmax, kmax, lmax, norows, noroco,                    kurflg,
nst, iapdim, lenusr, lenius, lenwrk, leninp,          lentim, lentdf, lensol, iurtyp, ldengr,
isvwp,                  iflval, irfmsg, irfrep, dx, dy, dtsec, tempw, salw,           ag, pi,
vico, windc, windac, rhomm3, timnow, grdang,
     angrad, tstart, itrudm (300)
```

ag Gravity acceleration (in $m \cdot s^{-2}$).

angrad Conversion factor degrees -> radians.

dtsec Full integration step duration (in seconds)[1].

dx Grid size in the x-direction (in m).

dy Grid size in the y-direction (in m).

grdang Angle between the y-axis and the north rotating clockwise from the y-axis to the direction of the north (in degrees).

iapdim Number of dimensions involved in the approach of the transport problem (WAQUA: 2, TRIWAQ: 3).

iflval Flag: 0 = no, 1 = yes, WVAL-array filled.

irfmsg Dataset-reference number of the message print file.

irfrep Dataset-reference number of the report print file.

isvwp Flag: 0 = no, 1 = yes space-varying wind & pressure array (WIND) filled.

itrudm Dummy array for later usage.

iurtyp Type number of user routine.

kmax Number of layers.

kurflg Flag for curvilinear computation (0 = no, 1 = yes, curvilinear).

ldengr Flag for density gradient (0 = no, 1 = yes, density gradient (RHO) array filled).

leninp Number of fields in array SPAINP.

[1] The WAQUA-system performs the time integration in two equidistant steps; therefore WASUST is called two times in one WAQUA time step.

lenius	Size of array IUSER.
lensol	Number of fields in array SOLUSR.
lentdf	Number of fields in array SPATIM.
lentim	The maximum of NVAL and LENFOU (used for array FVALUE), where NVAL = number of function values per time instance in time series; LENFOU = number of Fourier series.
lenusr	Size of array USER.
lenwrk	Number of fields in array WORK.
lmax	Number of constituents.
mmax	M-size (x-direction) of WAQUA grid.
nmax	N-size (y-direction) of WAQUA grid.
noroco	Number of computational grid rows + columns.
norows	Number of computational grid rows.
nst	Full integration step counter, relative towards simulation starting time TSTART.
pi	Pi.
rhomm3	Ambient density of the sea water surrounding the model (in $kg \cdot m^{-3}$).
salw	Default salinity for the equation of state (in $kg \cdot m^{-3}$).
tempw	The water temperature in the equation of state (in °C).
timnow	Time now in elapsed minutes (relative towards simulation starting date, starting at midnight) for which forcings are given.
tstart	Simulation starting time in elapsed minutes (relative towards simulation starting date, starting at midnight).
vico	Horizontal eddy viscosity coefficient (in $m^2 \cdot s^{-1}$).
windc	Current global wind speed (in $m \cdot s^{-1}$).
windac	Current global wind angle (radians, relative towards y-axis).