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SIMSYS2D: A TWO-DIMENSIONAL FLOW AND WATER QUALITY SIMULATION S--ETC(U)
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SIMSYS2D: A TWO-DIMENSIONAL FLOW AND WATER QUALITY SIMULATION SYSTEM*

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SIMSYS2D: A TWO-DIMENSIONAL FLOW AND WATER QUALITY SIMULATION SYSTEM

by

J. J. Leendertse*

ABSTRACT

The SIMSYS2D system is designed for the two-dimensional simulation of hydrodynamics and water quality in well-mixed estuaries, coastal seas, harbors, and inland waters. The system can simulate the hydrodynamics in complicated geographical areas and the land/water boundary is determined by the model during simulation. The system accounts for sources of discharges, for tidal flats, for islands or dams, for time varying or time invaryinq flow restrictions in which sub or super critical flow occurs and such as generated by openings in dams, sluices, or stormsurge barriers. The system is designed for planning, design and execution of engineering works and for the assessment of the impact thereof. The input and results of simulations are well documented in printed reports and graphical displays. The latter are of high quality and can be incorporated in engineering reports.

The investigator has the choice of numerous finite difference approximations of the vertically integrated hydrodynamic equations. He is able to graph many variables and their derivatives as time histories or charts, thus displaying model input and results in a highly visible way.

The system is in daily use by a number of engineering groups in the United States and the Netherlands.

The SIMSYS2D system consists of nine programs; data is passed between these programs. In addition to these programs, a number of programs for extended data processing and data input preparation are being used.

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I. INTRODUCTION

The SIMSYS2D system is a system of interlocking computer programs for the two-dimensional simulation of hydrodynamics and water quality in well-mixed estuaries, coastal seas, harbors and inland waters.

It has its origin in a study[1] for the computation of long-period water waves and a Rand study[2] of water quality in Jamaica Bay for the City of New York. For these studies ad hoc programs were written and published, and are still widely used by many other investigators who make these modifications for their particular use.

Hand-in-hand with ongoing engineering investigations, in particular for the Netherlands Rijkswaterstaat, a system of programs has been developed which permits an investigator to make rapid model studies. The investigator has the flexibility to choose the finite difference approximation method he thinks is most suitable for his purpose, and if in doubt, he can perform sensitivity analysis by using other approximations by simply changing a few flags in the input.

The investigator has numerous choices of displaying and printing computation results. All these possibilities are easily accessible by simple instructions and, in our practice, it is common to receive hundreds of graphs already one day after the simulation. These possibilities, all thoroughly tested in ongoing investigations, also indicate new developments.

Due to imposed limitations on the size of this paper, only the main feature of the system will be presented. Similarly, we have to limit the presentation of results to a few examples of the many models which have been made.

An overview of the gross data flow in SIMSYS2D is presented in Fig. 1. This diagram shows the programs, the tape and disk storage of data, the reports, and graphical displays with different symbols. The data flow diagram assumes that all data which will be used is available on disk. From this data set we assemble, generally in blocks, the input data for a model. A very good guide for this is a report printed by the Input Data Processor, which we will discuss next. The assembly of data for the input is by far the largest job in an investigation. The thoroughness by which this task is executed will be greatly reflected in the accuracy of the results of a simulation.

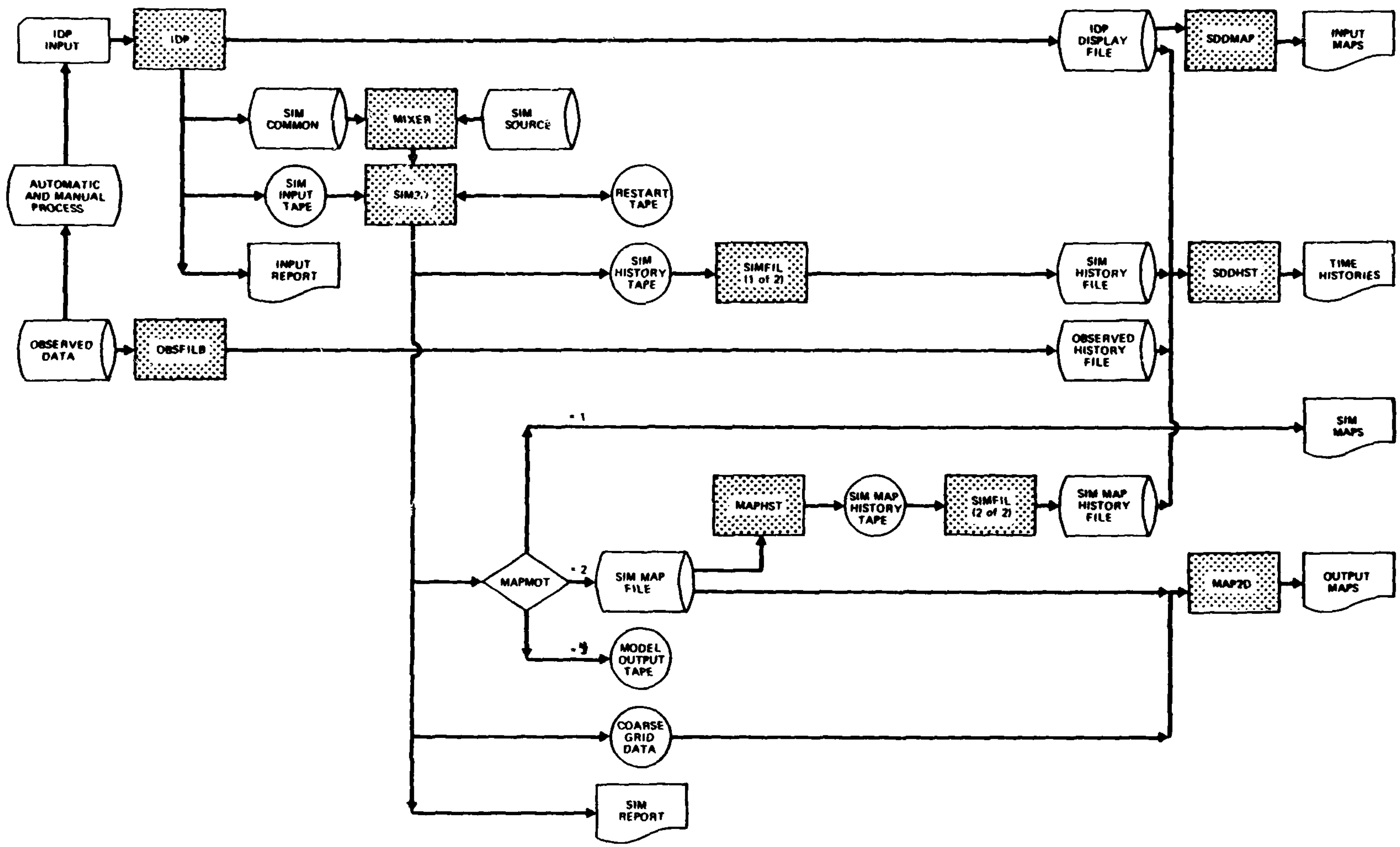

Fig. 1--Data flow in SIMSYS2D

II. THE PROGRAMS OF THE SYSTEM

IDP, The Input Data Processor

The Input Data Processor (IDP) reads a preliminary version of the input for the main simulation program which is called SIM2D. IDP checks the data for consistency, print error and warning messages. It prints the input data and the Input Report. In the latter every variable of the input data is explained. This report is kept for documentation and is generally the basis for modifications for the next experiment. The IDP program generates data dependent array definitions in the form of COMMON statements for inclusion in the compilation of the actual simulation program SIM2D. IDP writes the IDP Display File for the generation of charts on the two- dimensional input array variables and for the generation of time histories of the time varying data. Time varying data is inserted as data sequences for location. IDP processes this data and makes it available to SIM2D as data sets for each timestep or multiple of timesteps of the simulation. In the practice of numerical model studies, the actual simulations are generally made during the night when computation centers offer favorable rates for large computing jobs. The IDP program job step significantly reduces failures in the execution of the simulation or errors in the input data which would make the simulation of no value. Errors in input data can easily be checked by graphical display of the spatial and time varying inputs.

The IDP input report of a simulation is, in our practice, archived on microfiche together with pertinent graphical displays of the input data produced by SDDMAP on SDDHST programs.

SDDMAP

The Simulation Data Display of MAP's, SDDMAP, reads the IDP Display File and plots maps or charts of requested combinations of the input data. Data, such as the land boundary outline and titles, can be displayed and we are able to present contour charts of depth, the initial constituent concentrations, diffusion, and other coefficients. It is also possible to mark the location of the position of water level, current, and concentration stations, positions of dams, and tide openings barriers. On all of these graphs the computational grid can be indicated in many different ways. Figure 2 shows a graph made by SDDMAP. In this case, the outlines and titles were plotted together with the locations of different stations, outfalls, tide openings and the ranges through which the transports are computed.

A much used feature of SDDMAP is the plotting of computation points which participate in the simulation when the water is at a certain level. Application of this feature to a large series of water levels gives an insight to how tidal flats and marshes will flood during the

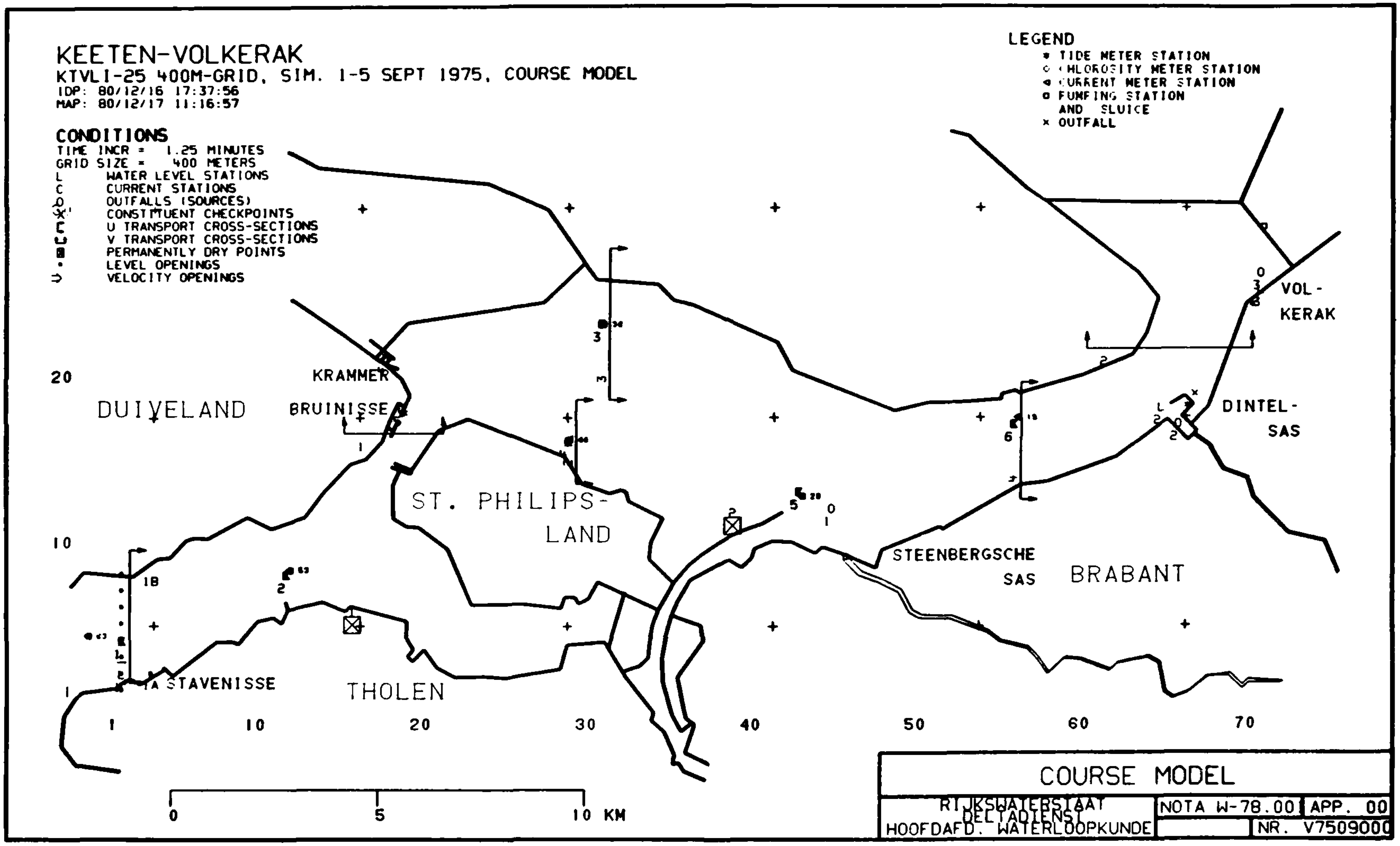

Fig. 2--Chart produced by SDDMAP to verify model inputs

simulation.

The graphic language used for all displays is IGS, the Integrated Graphic Language, developed by Rand in the 1960's. This language is quite commonly used and available for many computers and graphic devices. It is fast in execution of instructions and very powerful. Only ten basic instructions in this language are used in our system which makes interfacing with other graphic languages relatively uncomplicated, if the need arises.

SDDHST

The Simulation Data Display of Histories, SDDHST, plots time histories of data from different files. Generally one or two history files are plotted. Most plots take the conventional form of variable versus time and some variables may be plotted as time interval vector plots. The program can display data from different files simultaneously, thus we are able to compare, for example, observed data with computed data, or input data with observed data.

The program also allows for certain processing of data. Simple filters can be applied, adjustments for means can be made and standard deviations between two curves can be computed. It is also possible to plot differences between two data sets.

This program is extensively used for comparing overall results of different simulations and for making comparisons with prototype data. Data plotting can be done in intervals of one day to 30 days per graph. In the default mode, the scale of the variable is chosen on the basis of the maximum and minimum value of the data set to be plotted. Optionally the intervals can be set.

SIM2D

The Two-Dimensional simulation program (SIM2D) is the central computational program on the SIMSYS2D system. SIM2D receives input that has been processed by IDP. As IDP may have signaled warnings or errors or if we have a small change in plans, some variables of IDP may be overridden.

Using the bathymetry and physical characteristics described in the input, SIM2D computes water levels and currents as well as optionally the concentration and dispersion of constituents resulting from the time- varying effects of tide levels, wind, discharges, concentrations, and barriers. The computations can be made in many different ways, as described in the next chapter.

SIM2D will provide various outputs to the user upon request. These include printed tables of variables during the course of the run, plotted charts, and various data sets including the History tape, the Map tape, and the Restart tape. The latter is used to enable SIM2D to restart using data computed during an earlier run. This allows a run to continue from any point at which restart information was saved, so that a normal run may proceed from some specified time, or a run that failed due to computer problems can be restarted without total loss.

Printed data can be put on different files. For example, one file is used for progress data, warning messages, and another file is used for tables of variables at particular times. In our practice this data is archived on microfiche.

During simulation the two-dimensional array data can be plotted as maps with velocity vectors or transport vectors. These maps can also be made by use of the Map tape described later, but this is much more costly in our computation environment due to more extensive input/output processing.

SIM2D, including IGS, requires about 450K bytes of core in addition to the amount needed for data-dependent COMMON generated by IDP and the input/output of buffer requirements. The amount of core needed for data- dependent COMMON is printed by IDP. Since IGS takes considerable core, its usage can be omitted during a simulation which eliminates the core requirements of IGS.

MAP2D

The post-simulation MAP display program reads the Map tape to draw constituent concentration distributions, velocity, mass transport rate, and water level contour charts similar to those produced during the simulation. MAP2D also draws charts of particle path or plots of a cloud of particles simulating the dispersion of a dye release.

This program can also compute and plot residual currents and transports and compute and plot the vectors of the semidiurnal, quarter-diurnal, and sixth-diurnal tide at a particular time.

OBSFILB

The OBServed history data FILing program version B, OBSFILB, takes observed data given in regular time interval series form and writes an OBServed history FILe to be read by the SDDHST program for plotting of observed time histories in conjunction with computed histories.

MAPHST

The MAP data for HiSTory data program, MAPHST, extracts data at selected grid points from the data on the Map tape to produce the MAP History tape. Since the Map tape is not written as often as the History tape, the resultant time histories are represented by sparse data and the line representation is less smooth than generally produced from the History Tape.

III. MODEL CHARACTERISTICS

The finite difference approximation of the model is made upon a staggered grid. Velocities are computed at locations between the water level points and the depth is determined at a location centered between four water level points. This approach has the advantage that we are accurately computing velocities as they are occurring in cross-sections, which is very desirable for engineering investigations (Fig. 3). The error by the finite difference approximation in the sections through which the flow is computed appears smaller than when the depth point is taken at the location of the water level. In making the depth schematization, an effort must be made that all cross sections are well represented. The solution technique is an alternating direction implicit method with a large choice of approximation of difficult terms of the hydrodynamic equations.

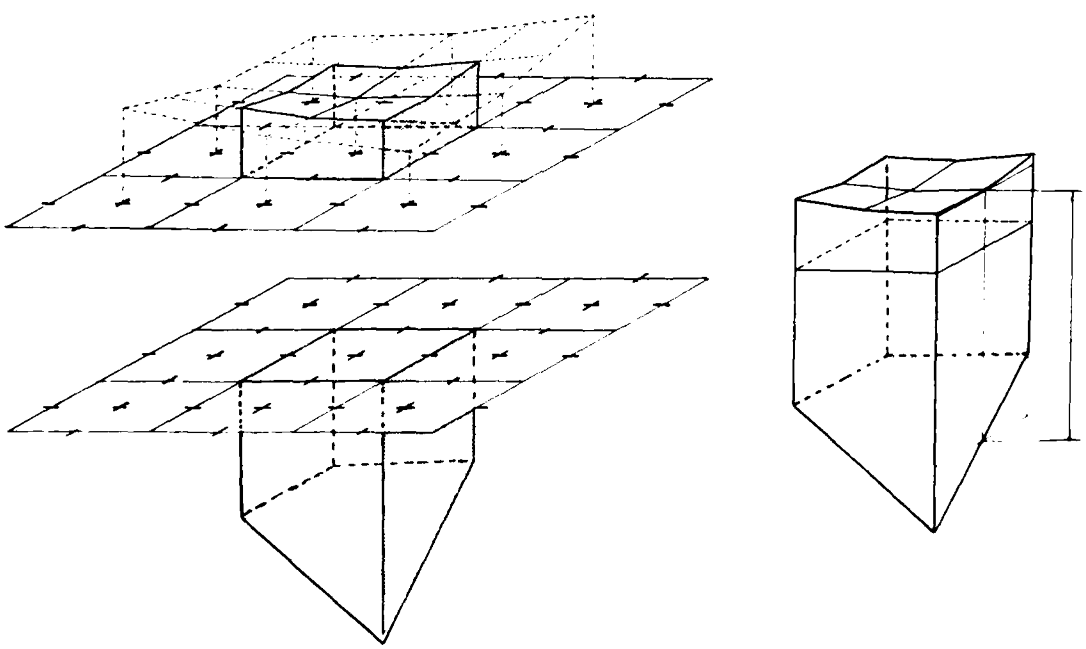

Fig. 3--Finite difference volume unit used for computation of the equation of continuity. Water level is computed in the center of the unit

Choices in Terms of the Hydrodynamic Equations

Advection. The advection can be taken on different time levels or forward and backward alternatively. Advection can be omitted and we can compute with schemes which have certain conservative properties such as velocity, vorticity, or the squared vorticity. The latter option is of great importance when jet type streams enter into water bodies with increasing depth. In such a case the vorticity per grid space increases and cannot be represented by the more simple advection representations.

By special means we are able to represent the effect of secondary flows and curves of channels and we can account for energy losses when the flow is diverging.

At a land/water boundary for flow parallel to the boundary several approximations can be selected such as the no slip and free slip condition. In total we can choose from five different approximations for flow parallel to the boundary and also from five different approximations for flow perpendicular to the boundary.

Bottom Stress. The bottom stress term can be taken at different time levels and can be a function of the Manning's n value, the Chezy C value or the K roughness value. The stress can be computed directly from the mean velocity or from a function of the local turbulent energy.

In practice it appears that the bottom stress value is not constant in regions with a salinity gradient but dependent on the direction of the flow. We have introduced an empirical correction factor which depends on the direction of the flow in relation to the salinity gradient and the value of the salinity gradient.

Salinity Pressure Gradient. When the salinity distributions are computed, the hydrodynamic equations can be coupled to the transport equation of the salinity. The pressure differential is computed from the density differences and the densities are computed with double precision from the computed salinities by an equation of state. The equation of state is valid for a very large range of the temperatures.

Viscosity. The viscosity can be introduced as a spatial variable, in addition to a value computed from the deformation of the flow field. Like the advection, five different approximations can be made for flow parallel to a land/water boundary and also five different approximations perpendicular to the land/water boundary.

Boundary Conditions

Two-Dimensional. Two-dimensional arrays of depth, Manning's n (or others), and viscosity define the usual two-dimensional input conditions for the hydrodynamic flow equations. The program allows for flooding and drying according to the water levels in the field. These procedures take care of a complete conservation of mass. In addition to these inputs, a spatial varying stress can be applied. This stress can be due to a spatially varying wind, e.g., by a hurricane or due to a radiation stress from short waves. This stress can be periodically given and is interpolated lineally between the time data is given.

One-Dimensional. One-dimensional array data is required every timestep at the open boundaries of the model. For water levels, a linear interpolation of the water levels is made when water levels at each section of the open boundary is supplied as a time series. If a Fourier series is given at each end of the boundary section a linear interpolation of amplitude and phase is used between the points specified. The interpolation of the phase occurs over the smallest angle. Similar procedures are used for velocities and transports. A radiative boundary condition for the water level is also programmed. Components of the incoming wave need to be supplied; the outgoing wave is computed from information in the flow field.

Singular points. At selected locations we are able to discharge water in a time varying way, thus simulating outfalls. At other points we are able to introduce barriers. The flow can be sub- and supercritical freesurfaceflow conditions and sub- and supercritical gateflowconditions. The sill depth and the gate height can be time varying. The horizontal opening dimension can also be varied in time. Between the different basic flow conditions, which are determined from the upstream and downstream water levels, the gate height and the sill depth, we have made flow transitions so that no discontinuity is generated in the flow when a transition from one flow condition to another occurs. The barrier characteristics can be made dependent on the flow direction to allow for non-symmetrical structures. The barrier can flow in u or v direction or both. It is possible to take a single point or a series of points out of the computation. This then represents a dam.

The Transport Equations

Transport of Dissolved Substance. Optionally, together with the integration of the finite difference approximations of the hydrodynamic equations, the transport of constituents can be computed. Like the hydrodynamic equations, the transport equations have a second order accuracy and conserve mass. A large number of constituents can be computed simultaneously. The constituents can be conservative or have a decay. Interaction between constituents is possible. Typical constituents used in the investigations are salinity, BOD and DO and coliform bacteria.

The dispersion coefficient can be set for each point of the grid and/or can be computed from information of the flow field. The dispersion in the direction of the flow can be taken different from that perpendicular to the flow.

In the sources the concentration can be variable in time.

In addition to the transport of dissolved substances, computations of heat and the turbulent energy can be made. For the energy computations, the energy loss due to the bottom stress over one timestep is added to the vertically average subgrid scale energy and simultaneously energy losses occur which are a power function of the energy intensity.

Transport of Particles or Particle Clouds

The system permits the release of single particles or groups of particles at arbitrary times. Following such a release the movement of each particle is computed with each timestep of the simulation. When particle clouds are released, each particle obtains, in addition to the advective transport, a random movement. The intensity of the movement is different in the direction of flow and perpendicular to the flow. The intensity is also dependent on the intensity of the computed subgrid scale energy.

Diagnostic Computations

During the simulation, special diagnostic computations can be optionally requested. It is standard practice in numerical model studies to compute discharges through ranges and simultaneously compute the mass transport through these ranges. The advective and diffusive transport through these ranges are being computed. The total flow from the beginning of the computation is also computed.

When the special diagnostic computations are made, it is possible to extract the contributions of the different terms of the momentum equation at selected points in order to assess their relevance. In cross-sections we are able to compute optionally the energy transport. All of this information can be graphed and is easily available to the investigator.

Run Log. The system keeps a log of every usage of a program and makes note of files and tapes, model version used. Job statistics are logged such as the number of graphs produced from each model run. Also warning and error messages are logged when failures occur. The Run Log appears to be indispensable in the management of computer simulation studies and it provides vital inputs for improvements and operation of the system.

IV. APPLICATIONS

In addition to the extensive series of publications of the first water quality simulations with a two-dimensional model for a study of Jamaica Bay [2]), the system is now being used for studies in the Delta Region of the Netherlands where a storm surge barrier is being built. An overview of these model studies is published in a few papers.[3,4] A very extensive report on these studies is being prepared. Large models are being used, as shown in Figs. 4, 5. These models contain about 20,000 points. Excellent agreement between observed and computed data has been obtained in the calibration and verification steps (Figs. 6, 7).

It has become evident that much time is spent on developing the operational and analytical experience of working with these models. The investigative teams found innovative methods for the adjustment of models and new ways of determining boundary conditions.[5]

To disseminate the experience gained, the principal investigators and the model development staff on both sides of the Atlantic have now given several training courses to engineering personnel of the sponsor, which has resulted in a very extensive usage of the system.

V. ASSOCIATED PROGRAMS

In addition to the programs of SIMSYS2D, a number of programs are routinely being used for processing of data. Very extensively we are using a programmed system for optimal linear estimation of relations between timeseries. The resultant estimates are used, for example, for the adjustment of parameters. Extensive use of these results is also made in a program which prepares the open boundary conditions of models for times that no detailed field data is available.

Very extensive use is made of a program which constructs procedures for filtering data. With this program we can design non-recursive filters, make graphs of the filter characteristics and apply the filter.

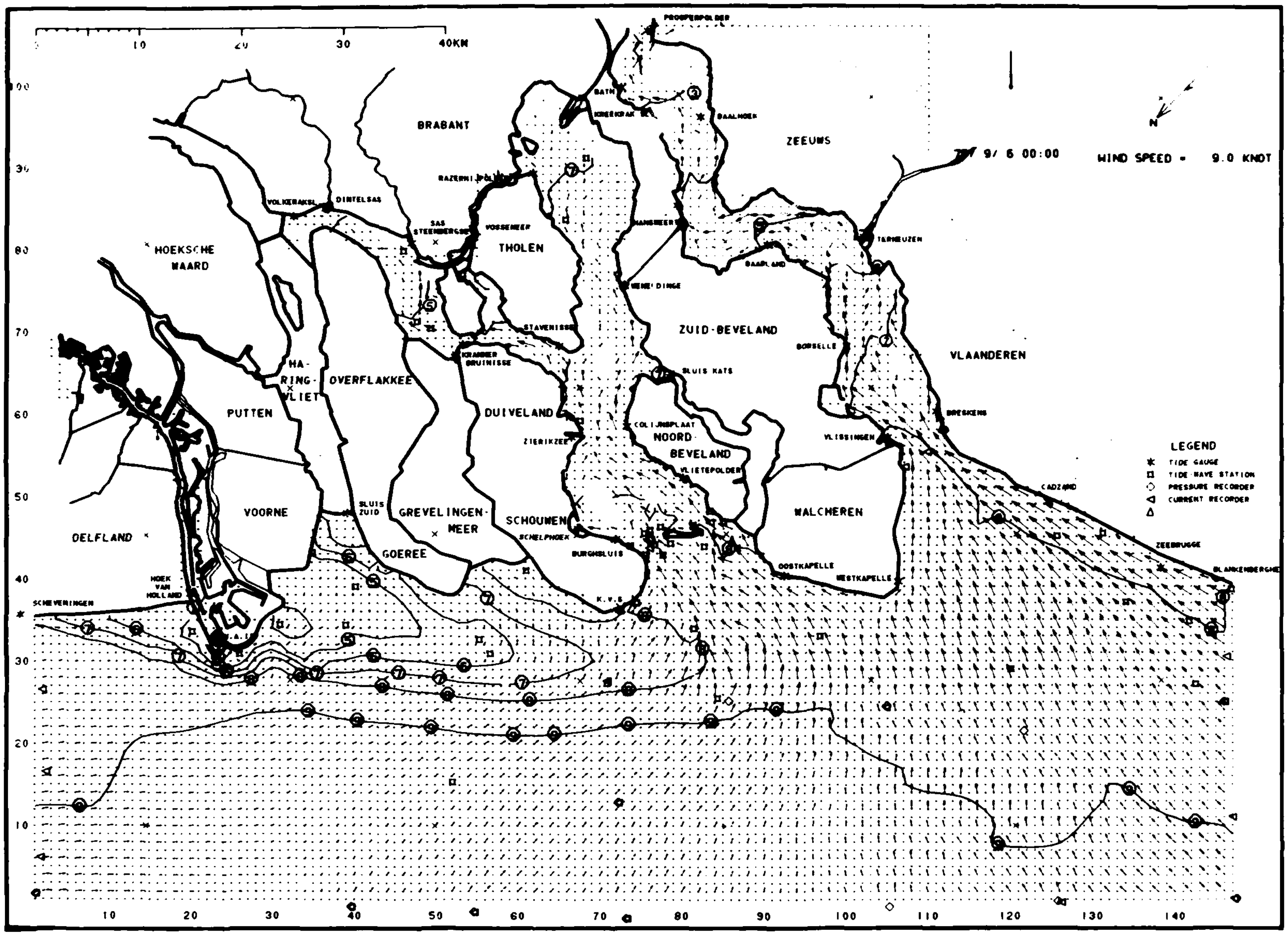

Fig. 4--Computed salinity distribution after 5-day simulation. Locations which are flooded are indicated by (•). Velocity vectors plotted every other grid point in each direction. The velocity vector scale is one grid unit for a velocity of 0.5 m/sec. The salinity isocontours are: (1) 8 kg/m^3, (2) 12 kg/m^3, (3) 16 kg/m^3, (4) 20 kg/m^3, (5) 24 kg/m^3, (6) 26 kg/m^3, (7) 28 kg/m^3, (8) 30 kg/m^3, (9) 31.5 kg/m^3.

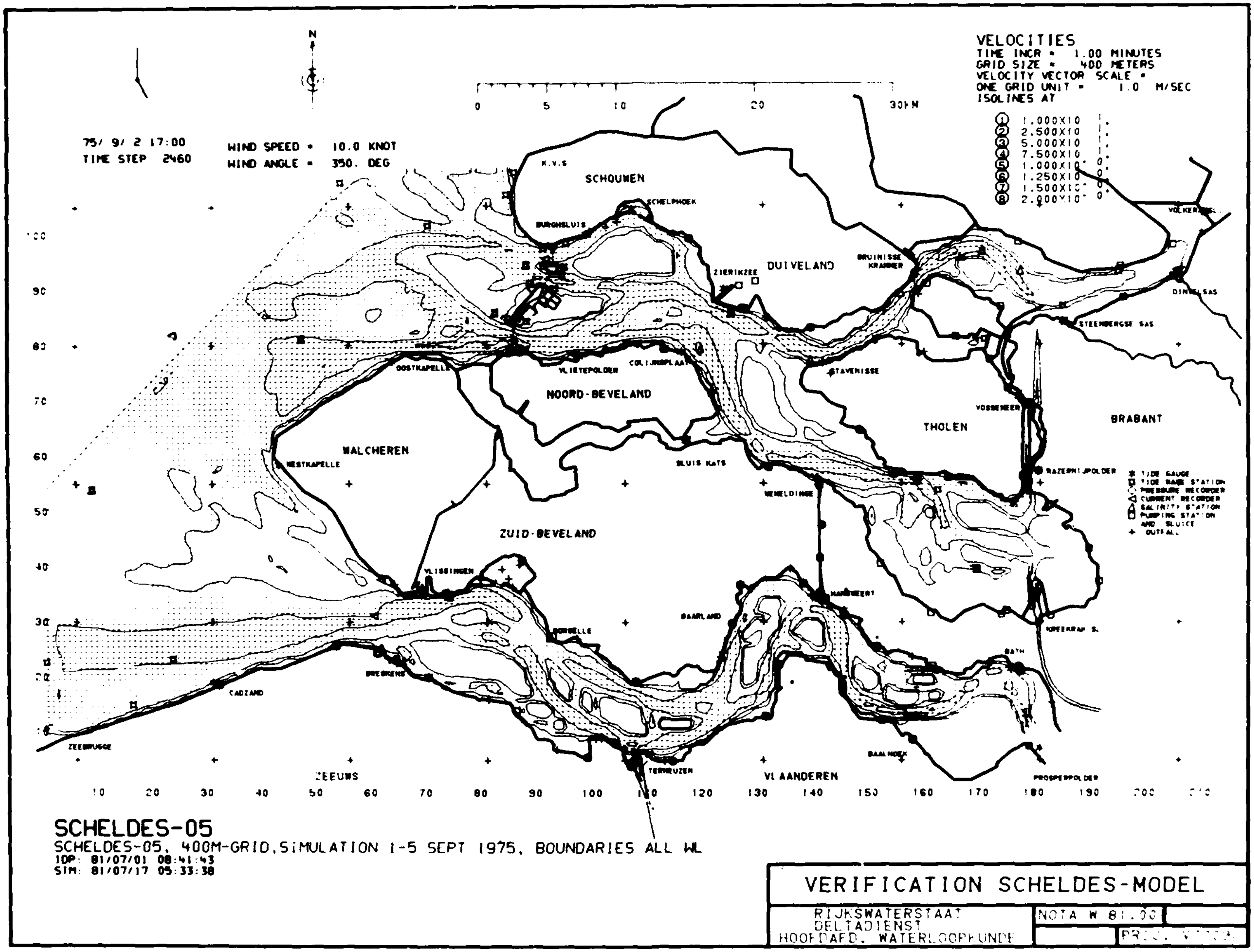

Fig. 5--Computed velocity vector field of the Scheldes model.

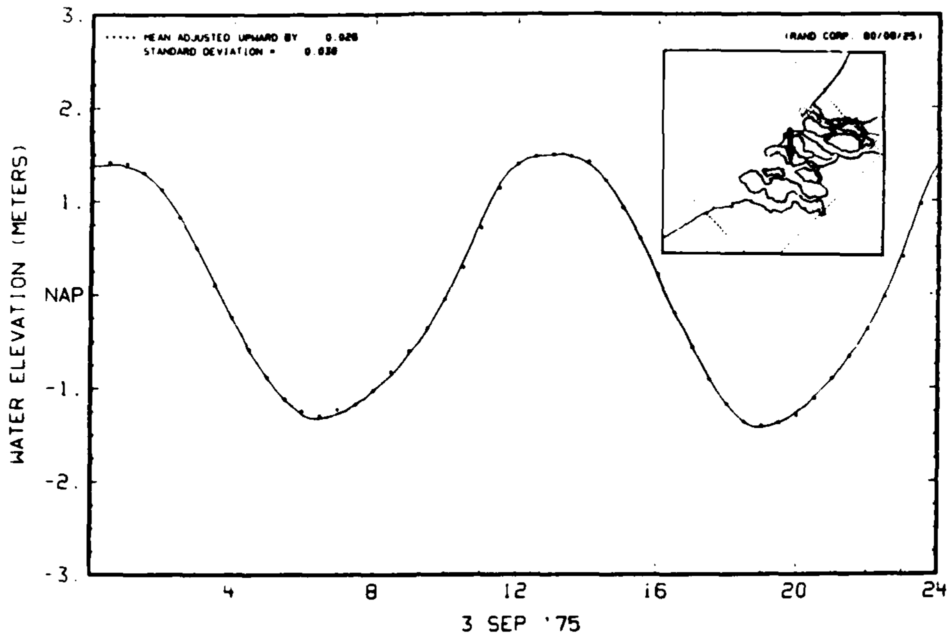

Fig. 6--Observed and computed water levels at a station in the Eastern Scheldt

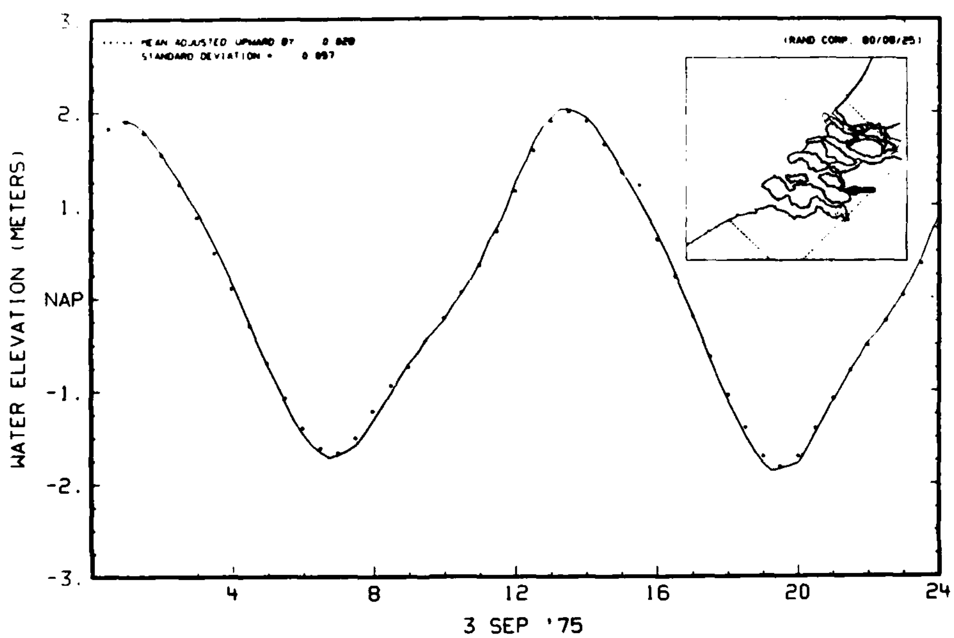

Fig. 7--Observed and computed water levels at a station in the Eastern Scheldt

V. FUTURE DEVELOPMENTS

Even though we still expect growth of the present version of SIMSYS2D, we consider the system now quite well matured.

A major effort is presently underway to streamline the computation procedures and make the main program easily accessible for maintenance.

Simultaneously, with 2D simulation studies and the development of SIMSYS2D, three dimensional modeling studies are made. Three dimensional models are now routinely being used and a simulation system is gradually being developed.

The three dimensional model is actively being used in the partly stratified waters of the Bering Sea. For this application the movement of ice fields has been added. Results of the hydrodynamic simulations in that area are used in computations with wind models to predict the movement of oil spills, if these would occur during oil exploitation.[6]

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