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*for a sustainable future*

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**TOGETHER**  
*for a sustainable future*

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POLLUTION CONTROL RESEARCH INSTITUTE, HARDWAR (U.P.)

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INDIA

Technical report: Software engineering in  
environmental pollution control\*

Prepared for the Government of India  
by the United Nations Industrial Development Organization,  
acting as executing agency for the United Nations Development Programme

Based on the work of Dr. Kurt Fedra, UNIDO consultant

Backstopping officer: S. P. Maltezou, Section for  
Integrated Industrial Projects

United Nations Industrial Development Organization

Vienna

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## 1. SUMMARY AND RECOMMENDATIONS

During the first days of the assignment at PCRI and after a series of introductory discussions, the author participated and contributed to a National Workshop on: "Pollution in Industrial Environment", chairing one technical session and presenting a one hour lecture on Hazardous Substances and Industrial Risk Management.

During the following weeks, the author worked very closely with a group of six young scientists/engineers, namely Mr. S.N. Sah, P.K. Singh, A. Jain, A. Kumar, P. Malik, and A. Goel, who were assigned to the computer/modeling group for the duration of the authors stay at PCRI.

Discussions on more general and strategic questions of the use of electronic data processing and modeling at PCRI were held with Prof. S.P. Mahajan (Head, PCRI) and Mr. A.K. Gupta (Manager).

Work with the software group involved a series of lectures and discussions (see chapter 4), the transfer and implementation of a number of PC based models and auxiliary software (see chapter 3). Basic characteristics, data requirements, and scope of application for these models were discussed with the project team. In total, 40 diskettes with PC software (executable models, source code, input and data files, example output files, and partial documentation) were given to PCRI staff.

Finally, following up on a suggestion at the national Workshop, the team designed, developed and implemented an interactive model for indoor (workplace) air pollution, e.g., for foundries. This exercise involved the entire cycle from problem analysis to software implementation and testing, and was used, in conjunction with the above mentioned lectures and related discussions, to teach in a practical and directly relevant example, basic principles and techniques of Environmental Impact Assessment and software engineering with extensive hands-on sessions on the computer.

As a second practical exercise, graphical output subroutines (for screen and lineprinter) for an already existing Gaussian air pollution models and for time series display were developed and tested in several versions to exemplify basic principles of (raster) graphics programming.

The practical work, however, was severely hampered by the fact that only one PC XT (640 kB, one floppy, 20 MB disk, monochrome VDU, without math processor) was available for the entire group.

Given the ambitious but certainly realistic and manageable plans and objectives for computer based analysis and modeling at PCRI, the equipment currently available (1 PC XT) or on order (1 PC AT), is grossly inadequate.

It is strongly recommended that every effort is made to make available adequate computing facilities, based on a network of super-micro engineering and graphics workstations as soon as possible. A proposal for a technically and economically feasible configuration, discussed extensively with the PCRI management and the project team, is presented in chapter 6. Also, it appears important to stress that such computer equipment will require very careful control and maintenance of its operating environment, and in particular careful dust control, for reliable long-term functioning.

In summary, while the team of young engineers was eager to learn, and in fact did learn very quickly on the basis of their good engineering backgrounds, the overall level of computer literacy and experience is still low. More long-term training of some of the most promising young engineers in appropriate institutions

abroad or in India, that also provide sufficient and modern equipment to gain practical experience, is highly recommended.

Further training at PCRI should ideally be project oriented to allow the immediate practical application of software transferred and methods and techniques studied. One very attractive possibility would be an involvement of PCRI in the second phase of the so-called Doon Valley Project (85/82(US/GLO/85/039) in collaboration with the International Institute for Applied Systems Analysis (IIASA), Austria. This project would allow meaningful and directly useful on-the-job training in a familiar and in fact local problem context. It would allow to combine further training in environmental systems analysis and modeling with PCRI's recognized strength in monitoring and analysis of environmental parameters.

Finally, given an analysis of problem areas that PCRI is addressing or intends to address in the future, a short list of recommended (public domain) software appropriate for these problem areas are discussed in section 5.

## 2. TIME TABLE AND ITINERARY

1987	10	19	briefing at UNIDO, Vienna
1987	10	20	departure from Vienna
1987	10	21	arrival in Delhi, India
1987	10	22	public holiday in India (Diwali)
1987	10	23	briefing at UNDP, Delhi; departure for Hardwar and arrival in Hardwar
1987	10	24	first working day at PCRI
1987	10	28	National workshop on
1987	10	29	Pollution in Industrial Environment
1987	11	10	last working day at PCRI and departure for Delhi
1987	11	11	debriefing at UNDP, Delhi
1987	11	12	departure from Delhi, and arrival in Vienna
1987	11	13	scheduled debriefing in Vienna
1987	11	15	completion of report.

## **2.1 DETAILED WORKPLAN AT DUTY STATION**

### **Overall Objective:**

- 1) assess the computer related needs and capabilities of PCRI to suggest possible improvements in terms of training, software, and hardware;
- 2) train the PCRI project team in the concepts, development, and practical application of model-based information and decision support systems for environmental impact analysis or assessment (EIA) of relevant industrial projects.

### **Specific Tasks:**

- 1 Assess and analyze the scope of PCRI tasks that need software/model support and design/propose integrated software (and possibly hardware) solutions with special reference to existing public domain and third party software.
  - 1.1 Develop a catalog of generic industrial pollution problems for which computer based methods and models can be used. This problem catalog should include information as to the source characteristics, major indicators, external variables, required (decision relevant) output information etc. It can then serve as the starting point for the identification of appropriate models and software packages.
  - 1.2 Identify data requirements and design a system of data bases for
    - hazardous substances (pollutants)
    - industrial waste streams
    - waste treatment technologies, treatability manual
    - industrial process technologies (including pollution abatement)
  - 1.3 Identify a set of models for the above problem catalog, including aspects of risk assessment and waste management, and related support software (statistical packages, database management software, geographical information systems (GIS), etc.
  - 1.4 Design/specify an appropriate hardware environment for the above.
- 2 Installation (together with the PCRI team) of selected PC software for EIA (e.g., PCGEMS, ISC, DYNTOX, WASP, QUAL-II, etc.) and a set of utility programs;
- 3 Train the PCRI project team in the use of the above; this will include:
  - 3.1 development and implementation of a concrete example case study (indoor (workplace) air pollution control using a simple box model);
  - 3.2 lectures, training exercises & discussions on relevant topics such as EIA, specific models and their data requirements, interactive simulation, computer graphics, decision support systems (DSS), software engineering, artificial intelligence (AI);

### 3. Models and Software transferred

As part of the training exercises and to directly provide PCRI with a set of operational models, a number of PC based models from the US Environmental Protection Agency (EPA) were delivered and installed, as far as technically feasible, on the PCRI PC. However, since most of the models do require a mathematical coprocessor which was not available on the PC XT currently used, only a few of the models could actually be tested.

Printed documentation, as far as available to the author and not yet delivered to PCRI, will be made available through UNIDO in Vienna. Additional literature describing the theory and operation of the models transferred is referenced in the respective sections and in section 7.

With the availability of a PC AT (including a mathematical coprocessor) in a few weeks, all the models should be made operational.

The following models, all in the public domain and originating from the United States Environmental Protection Agency (EPA) were delivered:

1. **PCGEMS: EPA's Graphic Exposure Modeling System.**

20 diskettes and printed user manual.

PCGEMS is the personal computer version of EPA's Graphic Exposure Modeling Systems, residing on the Office of Toxic Substances (OTS) VAX 11/780 at Research Triangle Park in North Carolina. PCGEMS offers greater access and ease than the original mainframe GEMS, being ported to the IBM PC XT or AT. Since the future is towards greater use of personal computers, PCGEMS will expand in capabilities as the hardware improves.

A copy of the PCGEMS User's Guide was made available to PCRI.

- 1.1 **ENPART: ENvironmental PARTitioning model**, based on the fugacity approach. It is a first level screening tool for pre-manufacturing notices and existing chemicals. It uses simple physical chemical data to estimate equilibrium concentration ratios of a chemical between different environmental media.
- 1.2 **PCLOGP: chemical property estimation (octanol/water coeff.)** PCLOGP estimates the partition coefficient, i.e., the equilibrium concentration of a solute in a non-polar solvent (water) divided by the concentration of the same species in a polar solvent (octanol). All the input required is the Simplified Molecular Line Entry System (SMILES) notation for the chemical. For an introduction to the SMILES notation system, see the PCGEMS User's Guide p 3-3 and 3-4.
- 1.3 **PCCHEM: automatic chemical property estimation.** Based on input of the SMILES notation and the log Kow values (known or estimated with PCLOGP), PCCHEM estimates: melting point; water solubility; boiling point; vapor pressure; Henry's Law constant; bioconcentration factor; organic carbon adsorption. Many of these parameters are required by subsequent environmental impact models.
- 1.4 **PCHYDRO: chemical property estimation (hydrolysis).** This module is still under development. The current version is limited to a few of the carboxylic acid esters.
- 1.5 **PCFAP: fate of atmospheric pollutant.** Models such as ENPART, ISC, or TOX-SCREEN can use, as part of their input, the rate of degradation and loss of a chemical in air. The FAP model estimates the rate of atmospheric oxidation from structural information (SMILES notation) alone.

- 2 **ANNIE: Interactive Pre-processor for QUAL2 and DYNTOX**  
1 diskette  
ANNIE/QUAL2 is an interactive preprocessor for QUAL2E. It assists users in the development and modification of input sequences for QUAL2E.
- 3 **QUAL2E: Water quality simulation model**  
2 diskettes  
The Enhanced Stream Water Quality Model is a steady state model for conventional pollutants in branching streams and well mixed lakes. It includes conservative substances, temperature, coliform bacteria, biochemical oxygen demand, dissolved oxygen, nitrogen, phosphorus and algae. QUAL2E is widely used for waste load allocation and permitting in the United States and other countries.
- 4 **WASP: Water quality simulation model**  
5 diskettes  
The Water Analysis Simulation Program WASP is a dynamic model for organic toxics and eutrophication simulation. The model system contains two distinct programs, TOXIWASP for organic toxic substances, and EUTRWASP for eutrophication (inorganic nutrients) problems.
- 5 **DYNTOX: stochastic toxic waste allocation model**  
5 diskettes  
The Dynamic Toxics Model (DYNTOX) is a waste load allocation model using a probabilistic modeling technique. Three procedures are readily available which estimate a broad range of conditions. These are:
  - Continuous Simulation
  - Monte Carlo Simulation
  - Log Normal Analysis Dyntox is a simple interactive program, also using ANNIE as the user interface program.
- 6 **DYNHYD: general hydrodynamics**  
2 diskettes  
DYNHYD (version 3.0) is a Hydrodynamic Simulation Program for rivers, lakes, and tidal areas. DYNHYD3 can be linked with WASP3V2 to provide the necessary hydrodynamic input data.
- 7 **ISCST: Industrial Source Complex (short term) air pollution model**  
1 diskette  
The ISC is a state-of-the-art version of the basic Gaussian air pollution model, including several extensions and modifications that allow a versatile use for a broad range of industrial problems, estimating concentration as well as deposition values. The model can handle multiple point and area sources, describes temperature and stack dependent plume rise, particle size dependent settling characteristics, secondary entrainment of settled particles through spatially variable reflection coefficients, effects of topography, and wake effects in the neighborhood of tall buildings.  
Together with the source code of the major model routines, a copy of the input data description was made available to PCRI.

A more detailed description and installation instructions for the above models is given in the following sections.

### **3.1 PCGEMS: EPA's Graphic Exposure Modeling System.**

PCGEMS is the personal computer version of EPA's Graphic Exposure Modeling Systems, residing on the Office of Toxic Substances (OTS) VAX 11/780 at Research Triangle Park in North Carolina. PCGEMS offers greater access and ease than the original mainframe GEMS, being ported to the IBM PC XT or AT. Since



the future is towards greater use of personal computers, PCGEMS will expand in capabilities as the hardware improves.

PCGEMS is designed to communicate (through KERMIT), for the running of some of the larger models, with the OTS VAX in North Carolina. While this is clearly infeasible at PCRI, PCGEMS also includes the possibility to integrate PC versions of these or equivalent models (such as the ones described below) into its menu and record management system and thus make them integrated components of a user configured PCGEMS version.

PCGEMS allows for an entire library of related environmental software to be incorporated within one coherent framework. To support and manage all the data that accumulates, PCGEMS contains a catalog manager as well as transformation routines that allow to transform data to and from DIF, dBASE and LOTUS 1-2-3 format. Also, other utility programs like a screen editor (vi) can be incorporated in the PCGEMS menu environment.

### **SYSTEMS REQUIREMENTS**

IBM XT/AT with hard disk and/or Bernoulli boxes DOS Version 2.2 or higher 8087 (80287) math Co-Processor Two floppy disk drives A minimum of 6 MB free space on the hard disk

### **SYSTEMS INSTALLATION**

To load PCGEMS on the hard disk,

- 1) insert the PCGEMS systems disk into drive A:
- 2) set the drive/directory to A: by typing "A."
- 3) enter "PCGEMS"
- 4) an interactive installation procedure will take over (see PCGEMS USER'S GUIDE p 1-2).
- 5) to load the remaining PCGEMS modules, invoke them via the main menu system; PCGEMS will then prompt for loading the appropriate diskettes and guide you through the installation procedure.

#### **3.1.1 Environmental Partitioning Model (ENPART)**

Theory and function of ENPART are extensively explained in the PCGEMS USER'S GUIDE p. 2-2 - 2-7.

To access ENPART, position the cursor over the Environmental Partitioning option in the main menu, and press the PgDn key.

#### **3.1.2 Octanol Water partition coefficients (PCLOGP)**

To access PCHEM, position the cursor over the corresponding option in the Chemical Property Estimation Selection Menu and press the PgDn key.

#### **3.1.3 Automatic chemical property estimation (PCCHEM)**

To access PCHEM, position the cursor over the corresponding option in the Chemical Property Estimation Selection Menu and press the PgDn key.

### 3.1.4 Hydrolysis Estimation (PCHYDRO)

To access PCHYDRO, position the cursor over the corresponding option in the Chemical Property Estimation Selection Menu and press the PgDn key.

### 3.1.5 Fate of Atmospheric Pollutants (PCFAP)

To access PCFAP, position the cursor over the corresponding option in the Chemical Property Estimation Selection Menu and press the PgDn key.

### 3.2 ANNIE/QUAL2 Program

ANNIE/QUAL2 is an interactive preprocessor for QUAL2E. It assists users in the development and modification of input sequences for QUAL2E.

This version requires an IBM/PC with 256K and 1 floppy disk drive.

#### INSTALLATION

1. make a copy of the distribution floppy disk on your hard disk or another floppy disk. (If you have a hard disk you may want to make a directory for ANNIE/QUAL2)
2. run the test runs by typing the following:  
DEMO (carriage return:cr)  
(cr)  
Y (cr)  
(cr)  
Y (cr)
3. run QUAL2E with file TEST.OUT as input, the results should be the same as those from Example Run #8

#### FILES ON DISTRIBUTION DISK

ANNIEQ.EXE	executable for ANNIE/QUAL2
ANNMESS.DA	message file for ANNIE/QUAL2
TEST1.INP	input for test run 1
TEST2.INP	input for test run 2
DEMO.DAT	batch run to test ANNIE/QUAL2
README.1ST	this file

#### FILES USED BY ANNIE/QUAL2

ANNINP.SEQ	optional file containing user responses to ANNIE/QUAL2 questions
ANNLOG.TMP	file containing echo of user responses to ANNIE/QUAL2 questions

### 3.3 ENHANCED STREAM WATER QUALITY MODEL (QUAL2E)

IBM PC Version 3.3 July 1986

Source:

Center for Water Quality Modeling  
U.S. Environmental Protection Agency  
Environmental Research Laboratory  
College Station Road

Athens, Georgia 30613

(404) 546-3123  
(FTS) 250-3123

#### **INTRODUCTION**

The Enhanced Stream Water Quality Model is a steady state model for conventional pollutants in branching streams and well mixed lakes. It includes conservative substances, temperature, coliform bacteria, biochemical oxygen demand, dissolved oxygen, nitrogen, phosphorus and algae. QUAL2E is widely used for waste load allocation and permitting in the United States and other countries.

#### **DOCUMENTATION**

A copy of the following publication should be obtained from the source above:  
Computer Program Documentation for the Enhanced Stream Water Quality Model QUAL2E. Linfield C. Brown and Thomas O. Barnwell, Jr., August 1985 EPA/600/3-85/065.

The following documents are also recommended. However, they are only available on request. These are loan copies that should be copied and returned to the Center for Water Quality Modeling as soon as possible. If any of these documents are on loan when your request is returned, your name will be placed on a waiting list and the document(s), as requested, will be mailed to you at the earliest possible date.

Workshop Manual for Stream Quality Routing Model QUAL2E. Thomas O. Barnwell, Jr., June 1985 (Loan copy).

NCASI Technical Bulletin No. 391.

Note: The NCASI document contains extensive commentary on an earlier release of the source code that may be useful to your staff programmers.

#### **DISTRIBUTION DISKETTES**

PCRI has been provided with 2 IBM PC DOS formatted diskettes that contain release 3.3 of the Enhanced Stream Water Quality Model (QUAL2E) for the micro-computer environment. The files on each diskette were created with the DOS COPY command and may be copied to your hard disk if you select to install the model on a hard disk drive (see INSTALLATION section), or copied to other diskettes for backup.

The file name and content section that follows provides a brief functional description of each file by name or file name extension type. Other sections in this document contain information on program development, installation, source code, program modification, and execution.

#### **FILE NAME AND CONTENTS**

The first diskette (EXECUTE Q2E) contains the QUAL2E executable task image and test input and output data files that may be used to test your installation of the model. The second diskette (SOURCE Q2E) contains the FORTRAN source code and all command files that may be used to re-compile and link edit the program should the user wish to make changes in the model. Diskette number 2 is not required to run the model.

**Diskette Number 1 - Label = EXECUTE Q2E**

**QUAL2E.EXE** QUAL2E executable task image.  
**OUACHL.DAT** This is a test input data set that may be used to test your installation of the QUAL2E model on your PC.  
**WORKSHOP.DAT** Other test input data sets.  
**X8.DAT**  
**OUACHL.OUT** This is a sample output file for a QUAL2E test run using OUACHL.DAT as input. When your test run with OUACHL.DAT as input is complete, the output file you designate at run-time (ex. OUACHL.TST - see EXECUTION OF QUAL2E) should be compared with this file to test your installation of the QUAL2E model.

**Diskette Number 2 - Label = SOURCE Q2E**

**README.1ST** This document.  
**QUAL2EMS.BAT** This is a DOS batch command file that may be used to compile and link edit the QUAL2E program to incorporate changes that you made to the source code. This command assumes that all Microsoft FORTRAN (MSFORT) commands and files are stored in a root sub-directory MSFORT. It also assumes that all QUAL2E batch commands, source code, and FORTRAN INCLUDE source code files are stored on the same diskette or in the same root sub-directory (ex: C:QUAL2E). The DOS PATH should contain the MSFORT directory - example PATH x::MSFORT;... where 'x' is the diskette or hard disk drive that contains the MSFORT sub-directory.  
**QUALMS.BAT** This is a DOS batch command file that may be used to link edit the QUAL2E program. This command assumes the same storage format and PATH as shown above. All source code must be compiled without error and object files produced before executing this command.  
**\*.FOR** All FORTRAN source code files.  
**QUAL2E.LNK** This is a link edit command file used by the MSFORT linkage editor. This file contains the overlay structure and all MSFORT LINK command options used for QUAL2E. Its contents are piped to the LINK command automatically in the batch command files QUAL2EMS.BAT and QUALMS.BAT.  
**QUAL2E.OPT** This file contains MSFORT FORTRAN compile options (Metacommands) that are used when compiling the QUAL2E model on the IBM PC. These commands are brought into the FORTRAN source code by the FORTRAN INCLUDE statement.  
**\*.VAR** COMMON area declaration statements that are brought into the FORTRAN source code files at compile time by the FORTRAN INCLUDE statement.

## DEVELOPMENT SYSTEM

The following list provides the language and program development tools used to build the PC distribution version for release 3.3 of the QUAL2E model. Also shown is the recommended minimum hardware and software configuration for the implementation of the model. Make sure that your IBM PC or "compatible" system meets these specifications before installation.

### Development System:

Language: FORTRAN 77  
Operating System: 1PC DOS v3.1 (Version 2.12 or higher may also be used.)  
Compiler: Microsoft FORTRAN (MSFORT) v3.31  
Linkage Editor: Microsoft FORTRAN v3.31  
Overlay Structure: Yes (see QUAL2E.LNK).

### Storage Requirements:

Random Access Memory: 256k bytes of RAM  
Diskette Drive: Model may be executed from diskette drive.  
Hard Disk Drive: Optional.  
Installation Size: Approximately 514k bytes in 62 files.

Numerical Coprocessor: Optional.

## INSTALLATION

If you plan to execute the QUAL2E model from a diskette drive, no installation is required (see EXECUTION OF QUAL2E). To install the QUAL2E model on a hard disk, transfer the contents of at least the run-time diskette to your hard disk. The source code diskette (Label = SOURCE Q2E) may also be copied if you plan to modify the model.

Description	Command
Set the default drive to the hard disk (e.g., hard disk "n"):	n:
Create a QUAL2E directory:	MKDIR QUAL2E
Change default directory:	CDQUAL2E
Transfer files from diskette (e.g.,	COPY m:*. * n:*. * /V drive "m") to the hard disk with verification of copy (optional).
List directory contents:	This step may be repeated for both diskettes: DIR

## EXECUTION OF QUAL2E

### Execution from Diskette:

The QUAL2E model may be executed from a diskette drive by inserting the run-time d'skette (Label = EXECUTE Q2E) and typing designation (ex. C:>B:QUAL2E). In this example you could also have designated drive 'B' as the default drive (enter 'B:' then press the 'Enter' key) then enter QUAL2E at the prompt B:> to execute the model.

After an opening screen, the program will prompt you for the input data set (ex: X8.DAT). Drive letters may be used in the file name (ex: B:X8.DAT). Next the program will prompt you for an output destination for which three options are available:

- 1) Enter a file name. Drive letters are allowed (ex. X8.OUT or A:X8.OUT)
- 2) Enter 'CON:'. This will direct the output to your screen.
- 3) Enter LPT1: or PRN. This will direct output to a printer. If using 8-1/2" paper, execute the DOS command MODE LPT1:132,8 before running QUAL2E to set your printer to 132 columns and 8 lines an inch. Note: Output is set for 8 lines per inch and 88 lines per page. This may be changed by modifying the variable 'PGSIZE' near the end of the source code file QUAL2E.FOR. If changed, the user will be required to recompile and link the model.

**Execution from Hard Drive:**

First, complete the instructor shown in the INSTALLATION section that makes the QUAL2E program resident on the hard disk. To start the QUAL2E program, change to the QUAL2E sub-directory on the hard disk by entering 'CDQUAL2E' at the system prompt. Next enter 'QUAL2E' to begin program execution. The program will follow the same execution sequence as outlined in the previous section.

If you would like to be able to execute the QUAL2E program from the root directory or any sub-directory on your system, then modify the DOS PATH to contain the QUAL2E sub-directory name.

Ex: PATH C:;QUAL2E;MSFOR;.....(etc.)

**MODIFICATION**

The QUAL2E executable task image QUAL2E.EXE as well as the source code files for IBM PC and compatible systems, source code include files, batch command files to compile and link edit, and link edit overlay structure and command/option files are included with the distribution diskette set. Please note that the Microsoft FORTRAN compiler and link editor are NOT required to execute the model as received on diskette. However, if the user wishes to modify the model, it will be up to the user to supply the appropriate FORTRAN program development tools to recompile and link edit the model.

**TECHNICAL CONTACT**

If you have any questions concerning the installation of the QUAL2E model on your IBM PC or compatible system, please contact David Disney in the Athens ERL ADP Section at 404/546-3123 or (PTS) 250-3123. Questions concerning model content, application, or theory should be addressed to Tim Wool at the same number.

**3.4 WATER ANALYSIS SIMULATION PROGRAM (WASP)**

IBM PC Version 3.3 October 1986

**Source:**

Center for Water Quality Modeling  
U.S. Environmental Protection Agency  
Environmental Research Laboratory  
College Station Road  
Athens, Georgia 30613  
404/546-3123

## INTRODUCTION

You have been provided with 5 IBM PC formatted diskettes which contain version 3.3 of the Water Analysis Simulation Program for organic toxics and eutrophication simulation. The files on each diskette are stored in BACKUP format and will therefore require the use of the RESTORE command in order to install them on your system (see instructions below).

The file content section provides a brief functional description of each file by name. Other sections in this document contain information on program installation and modification.

## FILE NAME AND CONTENTS

README.1ST	This document.
COMPLINK.BAT	A batch command file to compile and link edit either the toxics or eutrophication WASP source code. See program for documentation.
TOXIWASP.BAT	A batch command file to execute toxics WASP. To execute, type: TOXIWASP "file name" where "file name" is the name of an input data set (ex. TOXIWASP POND.INP).
EUTRWASP.BAT	A batch command file to execute eutrophication WASP. To execute, type: EUTRWASP "file name" where "file name" is the name of an input data set (ex: EUTRWASP 2DLAKE.INP).
TOXIWSP3.LNK EUTRWSP3.LNK	These are link edit command files used by the PLINK86 linkage editor in COMPLINK.BAT.
POND.OUT 2DLAKE.OUT	These are sample output files for TOXIWASP and EUTRWASP test runs using POND.INP and 2DLAKE.INP as input. Compare these to WASP.OUT after executing the appropriate version of the model.
POND.INP 2DLAKE.INP	These are data sets which may be used as input for the TOXIWASP and EUTRWASP models in order to test your installation of the WASP system. POND.INP is a simple pond and sediment system where toxic degradation and mobility are simulated. 2DLAKE.INP simulates eutrophication attributes in a stratified lake system.
WASP3V3.FOR	This is the FORTRAN source code file for the WASP driver program. This program solves the mass balance equation and controls the time step function.
TOXIWASB.FOR	This is the kinetic subroutine that is linked with WASP3V3.FOR to simulate organic toxics.
EU03WASP.FOR	This is the kinetic subroutine that is linked with WASP3V3.FOR to simulate eutrophication attributes.
TOXIWSP3.CMN EU03WSP3.CMN	If you select to compile and link edit WASP3V3 without using the batch command file COMPLINK.BAT as described above, then you will be required to either - copy TOXIWSP3.CMN to WSPCMN.F4P before compiling WASP - copy EU03WSP3.CMN to WSPCMN.F4P before compiling WASP

for organic toxics, or

for eutrophication simulation.

This step is required because of different FORTRAN common blocks for each simulation system. Remember, this step is needed only if you select to compile WASP WITHOUT using the batch command file COMPLINK.BAT. If you choose to use the command file, then it must be edited in order to select the appropriate common block which will be copied automatically for each compile and link edit (see COMPLINK.BAT for further detail).

EU03WSPB.CMN  
TOXIWSPB.CMN

These are the common blocks that are required by the kinetic subroutines (EU03WASP.FOR and TOXIWASP.FOR).

TOXIWSP3.EXE  
EUTRWSP3.EXE

Executable task image codes.

### INSTALLATION

Before installation, make sure that your IBM/XT, /AT, or "compatible" system measures up to the following recommended hardware configuration and software specifications:

- 640 kilobyte Random Access Memory (RAM)
- 360 kilobyte diskette drive
- 5/10/20 megabyte hard disk drive
- 8087 math coprocessor
- DOS version 2.12 or higher
- dot matrix printer with 132 column capability

To install the WASP model, transfer the contents of all diskettes to your hard disk:

Description	Command
Set the default drive to the hard disk (e.g., hard disk "n"):	n:
Create a WASP3P directory:	MKDIR WASP3P
Request verification of copy:	VERIFY ON
Change default directory:	CD/WASP3P
Transfer files from diskette (e.g., drive "m") to the hard disk:	RESTORE m: n:
Remove verification:	VERIFY OFF
Verify directory contents:	DIR

### MODIFICATION

Executable task images for TOXI and EUTRO WASP for IBM PC and compatible systems have been included on the distribution diskettes. Please note that the IBM Professional FORTRAN compiler (PROFORT v1.0) and the Phoenix Software Associates link editor (PLINK86 v2.11) are not required to run either WASP program. However, if any modification of the FORTRAN source code is required, then both of these software development tools will be required.



### **3.5 DYNAMIC TOXICS MODEL (DYNTOX)**

PC Version 1.0 July 1986

Source:

U.S. Environmental Protection Agency  
Environmental Research Laboratory  
College Station Road  
Athens, Georgia 30613

(404) 546-3123

(FTS) 250-3123

#### **INTRODUCTION**

The Dynamic Toxics Model (DYNTOX) is a waste load allocation model using a probabilistic modeling technique. Ideally, it would be desirable to assess the impacts of toxic discharges on receiving water quality over the entire range of historical and future conditions. These conditions would then be analyzed to define frequency and duration of exposure above specified limits. Unfortunately, on a practical basis this approach is impossible. However, three procedures are readily available which estimate this range of conditions. These are:

1. Continuous Simulation
2. Monte Carlo Simulation
3. Log Normal Analysis

All three are included in the DYNTOX program.

DYNTOX is a simple interactive program using ANNIE as the user interface program. ANNIE will take the user through the DYNTOX program step by step and assist the user in executing the program.

This microcomputer implementation of DYNTOX was done by Mr. David Dilks of Limno-Tech Inc. and the ANNIE routines were developed and modified by Mr. Jack Kittle of Aqua Tera Inc.

#### **DOCUMENTATION**

A copy of the DYNTOX User's Manual accompanies each response for the model and will be forwarded to PCRI in due course.

#### **DISTRIBUTION DISKETTES**

You have been provided with 5 IBM PC DOS formatted diskettes that contain release 1.0 of the Dynamic Toxics Model (DYNTOX) for the PC operating environment. The files on each of the disks are stored in BACKUP format and will therefore require the use of the DOS RESTORE command to install them on your system (see instructions in INSTALLATION section).

The file name and content section that follows provides a brief functional description of each file by name. Other sections in this document contain information on program development, installation, execution, and modification.

## FILE NAME AND CONTENTS

README.1ST	This document.
COMPLINK.BAT	This is a batch command file that is used to compile, link and test execute the Long and Short version of DYNTOX. (See DEVELOPMENT SYSTEM for differences between the two versions—see file listing for documentation on how to use this command.)
DYNTOX.EXE	The executable task image for the Long version of DYNTOX.
DYNTOXS.EXE	The executable task image for the Short version of DYNTOX.
DAMAKE.EXE	The executable task image to create the ANNIE direct access message file ANNMESS.DA.
*.FOR	These are the FORTRAN source code files for the DYNTOX model.
ANUTIL.FOR	This is a group of FORTRAN source code that comprises the ANNIE interface program.
DAMAKE.FOR	A FORTRAN program that creates the ANNIE direct access message file from ANNMESS.SEQ.
ANNMESS.SEQ	The ANNIE sequential message file that is read by DAMAKE.EXE to create the direct access file ANNMESS.DA.
*.COM	The associated FORTRAN common block files for ANNIE and DYNTOX that are included in the appropriate FORTRAN program during compilation.
DYN.LNK DYSN.LNK	The PLINK86 link edit command files that contain the overlay structure for the Long and Short versions of DYNTOX.
STORET.DAT	This is an STORET data base example that can be read into DYN10X by running TEST1.INP.
TEST*.INP	These are example data sets that can be used to illustrate the various simulation techniques used in DYNTOX.

## DEVELOPMENT SYSTEM

The following list describes the language and program development tools used at CWQM to build the microcomputer distribution version for release 1.0 of the DYNTOX model. Also shown is the recommended minimum hardware and software configuration for implementation of the model. Make sure that your IBM PC or "compatible" system meets these specifications before installation.

### Development System:

Language:	FORTRAN 77
Operating System:	MS DOS v2.12 (Higher versions of MS/PC DOS may also be used.)
Compiler:	IBM Professional FORTRAN (PROFORT v1.0)
Linkage Editor:	Phoenix Software Associates, LTD (PLINK86 Plus v2.11)
Overlay Structure:	Yes
Numerical Coprocessor:	8087 or 80287 required
Installation size:	Approximately 2.0 megabytes

### Storage Requirements:

---

#### SHORT VERSION:

Random Access Memory: 256k bytes of RAM  
Diskette Drive: Required for installation only  
Hard Disk Drive: 5 megabytes or larger (10M recommended)  
Run-Time Size: Up to approximately 3 megabytes of  
hard disk storage may be required

#### LONG VERSION:

Random Access Memory: 512k bytes of RAM  
Diskette Drive: Required for installation only  
Hard Disk Drive: 5 megabytes or larger (10M recommended)  
Run-Time Size: Up to approximately 3 megabytes of  
hard disk storage may be required

### INSTALLATION

To install the DYNTOX model on your IBM PC or compatible system, transfer the contents of all diskettes to your hard disk:

Description	Command
Set the default drive to the hard disk (e.g., hard disk "n"):	n:
Create a DYNTOX directory:	MKDIR DYNTOX
Request verification of copy:	VERIFY ON (optional)
Change default directory:	CDDYNTOX
Transfer files from diskette (e.g., drive "m") to the hard disk. Make sure you have at least 2 megabytes of free space:	RESTORE m: n:
Remove verification: (optional)	VERIFY OFF
List directory contents:	DIR

### EXECUTION OF DYNTOX

You have been supplied with two executable task images for the DYNTOX model, a long and short version. The major differences between these versions is that the short version can be executed on a PC that has only 256k bytes of random access memory, where as the long version requires 512k of random access memory. The short version of DYNTOX is limited in the length of the simulations that can be run.

Please note that program execution may not display the exact same screens as shown in the documentation. This is due to co-development of the code and documentation.

Before executing the DYNTOX model, you may be required to modify the DOS system configuration file CONFIG.SYS. This file should be under the DOS root directory on your hard disk (CONFIG.SYS) and should at least contain the statements

```
BUFFERS=10  
FILES=7
```

to execute the DYNTOX model on your PC. If these statements are not present then modify the CONFIG.SYS file accordingly. Or, create this file and add these statements with a text or word processor, the DOS COPY or ECHO commands, or the DOS line editor EDLIN. See the DOS Operating System Reference Manual for command

and statement structure and usage.

If you were required to edit or add the CONFIG.SYS file for these commands, then you will need to perform a system cold start (power off/power on) or a warm start (Ctrl/Alt/Del) for these changes to become effective. This step must be completed successfully before attempting to execute the DYNTOX model.

Before executing the DYNTOX model you must execute DAMAKE which will create the ANNIE direct access message file called ANNMESS.DA. To do this change to the DYNTOX sub-directory on the hard drive by entering CDDYNTOX. Then type DAMAKE and press the Return or Enter key. This should take about 5 minutes to execute.

To execute the DYNTOX model, change to the DYNTOX sub-directory (CDDYNTOX) on your hard drive. Then type:

DYNTOX /R2048 (For the Long Version) or

DYNTOXS /R2048 (For the Short Version)

The /R2048 is to inform DOS to initialize the maximum record length to be equal to 2048.

After the DYNTOX program of your choice begins execution you will be greeted by a welcome screen. Once there you may select one of two options: 1) start an interactive session or 2) run a test data set. If you elect to run a test data set, you should answer the first question with a "Y" response then press the enter key. You will next be asked for an "Input File Name". You should respond by typing in the name of a test data set. It is suggested that you start with test data set 1 (TEST1.INP) and work sequentially through the test data sets. This order is suggested since latter data sets may access files that are created by the earlier test data sets. An example is the Time Series files.

If you elected to have an interactive session follow the prompts given by ANNIE. When using the interactive version, you may terminate execution at any time. Your responses during the session are saved in the log file ANNIE.LOG. This file may be renamed and read back in as a data set that will resume program execution where the previous run stopped.

PLEASE NOTE: One limitation of the SHORT version is that it cannot do the Time Series simulation.

#### MODIFICATION

The executable task images DYNTOX.EXE and DYNTOXS.EXE for the IBM PC and compatible systems has been included with the distribution diskette set. Please note that the IBM Professional FORTRAN compiler and the Phoenix Software Associates linkage editor are NOT required to execute the model as received on diskette. However, if the user wishes to modify the model, it will be up to the user to supply the appropriate FORTRAN program development tools required to recompile and link edit either version of the model.

#### TECHNICAL CONTACT

If you have any questions concerning the installation of the DYNTOX model on your IBM PC or compatible system, please contact David Disney in the Athens ERL ADP Section at 404/546-3123 or (FTS) 250-3123. Questions concerning model content, application, or theory should be addressed to Tim Wool at the same number.

### 3.6 HYDRODYNAMIC SIMULATION PROGRAM (DYNHYD3)

IBM PC Version 3.0 August 1986

Source:

Center for Water Quality Modeling  
U.S. Environmental Protection Agency  
Environmental Research Laboratory  
College Station Road  
Athens, Georgia 30613  
404/546-3123

#### INTRODUCTION

You have been provided with 2 IBM PC formatted diskettes which contain version 3.0 of the Hydrodynamic Simulation Program DYNHYD3 for rivers, lakes, and tidal areas. The files on each diskette should be copied to your hard disk using the DOS COPY command. (See instructions below.)

The file content section provides a brief functional description of each file by name. Other sections in this document contain information on program installation and modification.

#### FILE NAME AND CONTENTS

README.1ST	This document.
DYNHYD3.FOR	This is the FORTRAN source code file for the DYNHYD3 program.
DHYD.COM	This is the COMMON block source code that is brought into the main source code by the FORTRAN INCLUDE statement.
DYNHYD3.EXE	Executable task image.
COMPLINK.BAT	A batch command file to compile and link edit the DYNHYD3 program. See file for documentation.
DYNHYD.BAT	A batch command file to execute DYNHYD3. To execute, type: DYNHYD3 "file name" where "file name" is the name of an input data set (ex. DYNHYD3 COEF2.INP).
COEF2.INP	This is a data set which may be used as input for the DYNHYD3 model in order to test your installation of the DYNHYD3 system. COEF2.INP is a simple hydrodynamic run for a 13 segment estuary.
COEF2.OUT	This is a sample output file for DYNHYD3 and represents a test run using COEF2.INP as input. Compare this to DYNHYD3.OUT after executing the model.
CANAL.INP	CANAL.INP is a special sample input data set for the DYNHYD3 model. This data set provides an example of how DYNHYD3 can be linked with WASP3V2. To use this you must first run DYNHYD3 with the supplied data set COEF2.INP. DYNHYD3 will produce a formatted file called SUMRY2.OUT. Upon executing WASP for eutrophication (via EUTRWASP CANAL.INP - see PC WASP3V2 documentation) with the CANAL.INP as the input dataset, WASP3V2 will read in the flows and volumes from SUMRY2.OUT. CANAL.OUT is supplied for
CANAL.OUT	

comparison with WASP.OUT which is produced by executing EUTRWASP.

**PLEASE NOTE:**

If it is desired to link flows and volumes data (SUMRY2.OUT), as produced during the execution of DYNHYD3, with either of the WASP3V2 programs (TOXICS or EUTRPHICATION), you must first set the appropriate switches in your input data sets for DYNHYD3 and WASP3V2. The input data set (ex: COEF2.INP) for DYNHYD3 must have a "2" in column five of the SUMMARY CONTROL DATA card group. A value of "2" will cause DYNHYD3 to produce a formatted file called SUMRY2.OUT. This modification has already been made to the COEF2.INP data file as supplied with this diskette set.

**Example:**

```
***** SUMMARY CONTROL DATA *****  
2 0 0100 10 3 10 5 9 13 1 9 4 8 13
```

A WASP3V2 data set (ex: CANAL.INP) must have a "5" in line one, column five of card group D: FLOWS. A value of "5" indicates to WASP3V2 during execution that it should look for a formatted file called SUMRY2.OUT. When these modifications are made correctly, WASP3V2 will read volumes and flows and continue execution of the TOXICS or EUTRPHICATION program, depending upon which model the data set was built to be used with. For additional information on the linkage see the model documentation. This modification has already been made to the CANAL.INP data file as supplied with this diskette set.

**Example:**

```
5 13 D:FLOWS
```

**INSTALLATION**

Before installation, make sure that your IBM/XT, /AT, or "compatible" system measures up to the following recommended minimum hardware configuration and software specifications:

- 256 kilobyte Random Access Memory (RAM)
- 360 kilobyte diskette drive
- 5/10/20 megabyte hard disk drive
- 8087 math coprocessor
- DOS version 2.12 or higher
- dot matrix printer with 132 column capability

To install the DYNHYD3 model, transfer the contents of all diskettes to your hard disk:

Description	Command
Set the default drive to the hard disk (e.g., hard disk "n"):	n:
Create a DYNHYD3 sub-directory:	MKDIR DYNHYD3
Change default directory:	CDDYNHYD3
Transfer files from diskette (e.g., drive "m") to the hard disk with verification of copy.	COPY m:*. * n:*. * /V
Verify copy by listing directory contents:	DIR

### MODIFICATION

The executable task image DYNHYD3.EXE for IBM PC and compatible systems has been included on one of the distribution diskettes. Please note that the IBM Professional FORTRAN compiler and linkage editor (PROFORT and LINK v1.0) are not required to run the DYNHYD3 program. However, if any modification of the FORTRAN source code is desired, then both of these software development tools will be required.

### 3.7 ISCST: Industrial Source Complex (short term)

The ISC is a state-of-the-art version of the basic Gaussian air pollution model, including several extensions and modifications that allow a versatile use for a broad range of industrial problems, estimating concentration as well as deposition values. The model can handle multiple point and area sources, describes temperature and stack dependent plume rise, particle size dependent settling characteristics, secondary entrainment of settled particles through spatially variable reflection coefficients, effects of topography, and wake effects in the neighborhood of tall buildings.

The *ISC Short-Term Model (ISCST)* is designed to calculate ground-level concentration or deposition from stack, volume or area sources. The receptors at which the concentration or deposition are calculated are defined on a x-y, right-handed Cartesian coordinate system grid. Discrete or arbitrarily placed receptors may be defined. Average concentration or total deposition may be calculated in 1-, 2-, 3-, 4-, 6-, 8-, 12-, and/or 24-hour time periods. An 'n'-day average concentration (or total deposition) or an average concentration (or total deposition) over the total number of hours may also be computed. Concentrations (depositions) may be computed for all sources or for any combination of sources the user desires. Other options include input of terrain heights for receptors, tables of highest and second highest concentrations or depositions at each receptor and tables of the fifty maximum values calculated.

Other extensions of the Gaussian Model include: the influence of urban or rural area on the weather; plume rise (Briggs 1971, 1975); variable topography of the area, influencing the variation of wind and temperature; the influence of buildings close to the source (Huber and Snyder, 1976; Huber 1977), affecting the coefficient of dispersion; the exponential decomposition of chemicals; a simple deposition model (Dumbauld et al., 1978; Cramer et al., 1972).

### DISTRIBUTION FILES

The following subroutines are on the distribution diskette:

disc	disk output subroutine
dyout	prints the daily concentration (deposition) for a given time period for a given day. this routine also prints the highest or second highest tables of concentration (deposition) for a given averaging time. finally, this routine prints the 'n'-day table or prints the elevation heights for all receptor points. if iavg = 99, print elevation heights. if iavg = 75, print 'n'-day table. if iflag = 1, print daily table. if iflag = 2, print highest table. if iflag = 3, print second highest table.
erfx	error function: calculate $\text{erf}(a) - \text{erf}(b)$ . hpl = lower limit, hpu = upper limit.
gitout	grid output

hp dummy main program  
inchk this routine reads the rest of the input variables and provides default values if required. also tables listing the input variables are controlled by this routine.  
inday input a day of met data and compute wind speed category in order to load default value for p or dthdz.  
insorc input variables related to particulate sources.  
intopo this subroutine reads the terrain elevation for the receptor grid and/or the discrete receptors.  
iscst this is the main subroutine of the epa industrial source complex short term model. this routine's purpose is to calculate the amount of storage required for tables, receptor grid and source information. in order for these calculations to be made the 'isw' array, the variables which determine the number of receptors and the number of sources are read.  
max50 this routine holds the highest 50 concentrations (depositions) for a given time period.  
maxot this routine lists the highest 50 concentrations (depositions) for a given time period.  
model this routine contains the model equations for calculating ground-level concentration or deposition including the plume rise equations. this routine also controls the calculation and output of all tables the program produces.  
sigmaz this routine calculates the vertical sigma given the effective downwind distance xb in kilometers and stability category ist.  
if iflag = 1, calculate sigma z.  
if iflag = 2, calculate average 'b' only.  
if iflag = 3, calculate effective downwind distance index ixdist as a function of xb, xz and stability.  
spezout grid output routine.  
vert this routine compiles the summation term in the vertical term for gravitational settling categories.

#### 4. Major topics of training and lectures

##### 4.1 EIA, Modeling, and Software Engineering

A series of more or less daily morning and afternoon lectures was given on a number of topics related to the PC software delivered as well as several more general topics.

Lectures on Environmental Impact Assessment, Environmental Modeling, and Software Engineering were largely based on Munn (1979), Gordon (1985), and Kernighan and Plauger (1978).

As one concrete example of a comprehensive environmental impact study, a case study for the Ganga river with special reference to industrial pollution was discussed. For this study, data requirements, major models, and the overall framework and form of presentation of the results were elaborated with the group.

##### 4.2 Exercise: air pollution modeling with a box model

As a concrete programming example, using FORTRAN77 on the PC XT, an indoor air pollution model for industrial production sites, e.g., foundries, was developed and implemented. The model is based on the so-called Box-model (see, e.g., Gordon 1985, p 84-85), and was developed together with an interactive, menu based user interface including context dependent default parameters, input



feasibility checks, and error correction functions.

The model computes indoor air pollution levels as a function of building geometry, ventilation, fugitive emissions, and operating schedules and calculates pollution concentrations for a 24 hour cycle. Model output was also presented in a simple graphical format as a time-series diagram.

#### 4.3 Exercise: line-printer graphics for model output

As an immediately useful software tool to better visualize and present model output graphically, a set of simple raster-based routines was developed with the project team. They include one-dimensional time series display (used for the concentration time series of the box model exercise) and 2D concentration field displays (with implicit isoline contours) for a Gaussian air pollution model.

#### 4.4 Introduction to models and software transferred

##### PCGEMS: EPA's Graphic Exposure Modeling System

theory, principle of operation, installation, inclusion of additional user-specified software, with extensive reference to the PCGEMS USER'S GUIDE.

##### ENPART: Environmental partitioning model

basic principle of the fugacity approach (McKay) and equilibrium modeling.

##### PCLOGP: chemical property estimation (octanol/water coeff.)

##### PCCHEM: automatic chemical property estimation

##### PCHYDRO: chemical property estimation (hydrolysis)

##### PCFAP: fate of atmospheric pollutant

principles of regression based empirical estimation procedures.

##### ANNIE: Interactive Pre-processor for QUAL2 and DYNTOX

basic principle and advantages of interactive, menu driven programs with reference to the box model example which uses the same techniques.

##### QUAL2E: steady-state water quality simulation model

##### WASP: dynamic water quality simulation model

##### TOXIWASP: for toxic substances

##### EUTRWASP: for eutrophication problems

##### DYNTOX: stochastic toxic waste allocation model

introduction to water quality modeling, basic steady state models such as Streeter-Phelps, dynamic models, spatially distributed (multi-compartment) models, relationship of water quality and air models (in particular the box model discussed extensively).

##### DYNHYD: general hydrodynamics (preprocessor for WASP)

use of DYNHYD as a preprocessor for WASP, importance of hydrodynamics for water quality modeling.

##### ISCST: Industrial Source Complex air pollution model

basic theory of Gaussian air pollution modeling, special features and extensions of the ISC model, examples of model implementation including interactive input generation and graphical output.

#### 4.5 Further project assignments

On special request of Mr. A.K.Gupta, a set of further problems and project assignments, based on the training material and the software delivered and developed, was designed with and for the project team for continuing work.

These projects/assignments include:

- 1) Installation of PCGEMS on the new PC AT;
- 2) Integration of all available models into the PCGEMS framework: this should include all the EPA models delivered, models already available and operational on the PCRI PC (simple Gaussian air pollution model), the box model developed during the assignment, the graphics subprograms (modified to stand-alone utilities, see below) developed for screen/lineprinter graphics, and the screen editor vi as well as the data base management and editor/utility programs dBase and Wordstar available at PCRI;
- 3) Develop the lineprinter graphics subroutines for one- and two dimensional data display (time series and concentration fields) into stand-alone utility programs, reading their respective inputs from disk files, for inclusion into PCGEMS.
- 4) Further development of the Box model; this should include:
  - a rerun and output comparison option for multiple runs;
  - coupling the time series plot program with the model for simple or multiple plots of concentration profiles;
  - add rule based components that suggest strategies to reduce workplace concentrations, based on either increase in ventilation, different operation/ventilation schedules, or reduction of fugitive emission depending on cost and technical feasibility criteria;
  - add simple engineering cost estimation to the suggested strategies;
  - develop a report generator that prints a summary of the problem, model run results, and suggestions including graphics in an attractive and directly useful report format.
- 5) Add interactive and menu-driven input routines including error correction and a report generator including the graphical output routine developed to the existing Gaussian air pollution model.
- 6) Extend the Gaussian model to multiple source situation, using basic matrix addition of individual source results.

#### 5. A Catalog of Typical Problem Situations

To assess the training, software, and hardware requirements of PCRI, an effort was made as part of the work program to compile a catalog of typical problem situations that PCRI wants to develop and apply computer based analysis methods for. These problems have been grouped into the following categories:

- 1) Air Pollution
- 2) Water Pollution
- 3) Soil and Food Chain
- 4) Toxic Substances and Waste
- 5) Risk Assessment

As a cross-cutting theme, the topic of geographical data management, e.g., for spatial impact analysis, emerged.

Under the above categories, only points 1) and 2) are currently addressed by PCRI. In the air pollution field, single-source emissions from thermal power stations with suspended solids and SO<sub>2</sub> as the main parameters of interest are of dominant importance. Analysis of cement industries shows similar model relevant characteristics. However, in both cases deposition of dust and fly ash, respectively, should also be taken into consideration. Currently modeling exercises are

restricted to single-source and SO<sub>2</sub> simulations. In addition, topics such lime kilns (several point and/or area sources), foundries (several point or area sources), and the special case of accidental atmospheric emissions (such as in Bhopal) were brought up.

In the area of water pollution, organic waste pollution (BOD) in rivers (in particular the Ganges), from several municipal and/or industrial point sources are the major concern.

Other related topics such as groundwater pollution, solid waste sites (atmospheric as well as water pollution), bioaccumulation of heavy metals from fly ash are in part treated by laboratory methods and field studies, but not yet with parallel model based analysis.

For the range of the above topics, a set of well established and relatively simple to use models with modest data requirements can be suggested:

Atmosphere:	ISC (Industrial Source Complex Model) simple box models for first screening
Water:	QUAL2 for BOD studies in rivers (steady state) EUTRWASP for dynamic (transient) analysis direct implementation of a simple Streeter-Phelps model WODA (a self-calibrating Streeter-Phelps model)
Toxics:	TOX-SCREEN for multi-media (air-water-soil) analysis including the soil model SESOIL ENPART for basic multi-media screening WASP and DYNTOX for water pollution by organic toxics
Food Chain:	TERMOD (adapted from a radionuclide uptake model)
Risk Analysis:	the World Bank fault tree analysis package direct implementation of engineering formulas, e.g., from the "yellow books" of the Dutch ministry for Housing, physical Planning, and the Environment, VROM.
Geographical Information Systems:	GRASS (US Army Corps of Engineers)

Most models mentioned in the air and water categories as well as several in the toxics group have been made available to PCRI during the current assignment (see section 3).

A short description of these models, their availability, contact addresses, and related literature is given in the appendix.

In addition the following software and information system projects were discussed as being of great interest and potential usefulness to PCRI. It should be noted here, however, that most of the proposed projects listed below are certainly of more general interest and would therefore warrant some consideration on the part of UNIDO.

- 1) data base on (hazardous) chemicals and industrial pollutants
- 2) data base on industrial waste streams
- 3) data base on waste treatment technologies

- 4) data base on industrial process technologies
- 5) data base on pollution control equipment and technologies
- 6) model and software inventory.

The compilation and development of these data bases as well as compiling, adapting, or developing a coherent set of, in view of their intended distribution in developing countries, primarily PC based models and software tools for industrial pollution control, environmental impact analysis, and risk assessment would be a worthwhile project for UNIDO to consider. Ongoing and planned work at PCRI could certainly contribute as well as greatly profit from such an international research and development as well as dissemination effort.

#### **6. Proposal for an Integrated Hardware/Software Environment**

It seems obvious that an upstarting institution like PCRI should be able to take advantage of the large amount of available software in the field of environmental impact assessment, risk analysis, and related areas.

Thus, one of the most important functional characteristics for an in-house computer installation has to be a flexible and powerful software development environment that will allow for the easy and cost efficient adaptation of available software to the specific conditions required.

It is therefor strongly recommended that any hardware/software solution be based on the UNIX operating system, which is rapidly emerging as the de-facto industry standard for scientific and engineering computing on mini- and supermicro computers.

At the same time, the large volume of PC based software for auxiliary administrative tasks such as text processing, data management etc. suggest a solution that can fully integrate a number of IBM PC (compatible) personal computers.

Major features required are:

- 1) Sufficient computing power for at least two workstations for large numerical models (e.g., large finite element models or optimization packages); Current industry standard for engineering workstations is in the order of 2 to 4 MIPS. Also, the workstations should provide sufficient RAM capacity for large programs (space requirements of most graphics packages such as Core or GKS are large), and modern programming languages such as LISP; industry standard for RAM capacity for engineering and graphics workstations is in the range of 4 - 32 MB.
- 2) Sufficient mass storage to keep models, data bases, and in particular space demanding graphics images (stored segments or metafiles) on line; for an installation with up to ten simultaneous users, this should be in the order of 400 - 500 MB initial disk storage.
- 3) High resolution color graphics capabilities (19" screens, minimum of 60 Hz refresh rates non-interlaced, 256 simultaneous colors)
- 4) Corresponding peripheral devices, in particular a larger digitizing table for the entry of (geo)graphical data, and printer/plotter devices capable of color hardcopy from raster devices.

For the basic software requirements, the standard UNIX OS and utilities together with the (usually included in the OS software) basic compilers for the high-level languages C, FORTRAN, and Pascal provide a good starting point for a powerful software development environment. This also must include basic graphics packages such as ACM Core, ISO GKS, ISO CGI, and possibly emerging standards such as PHIGS. In addition, a LISP (CommonLisp) development system and a SQL standard

data base management system are highly recommended as additional basic software. Also, a geographical information system (GIS) for the storage and manipulation of geographical data (maps) and land impact analysis is an important component of EIA software; such systems are also available in the public domain. A mathematical subroutines package (e.g., IMSL, NAG) and a versatile problem solver for mathematical programming problems (e.g., MINOS, also available together with a matrix generator in a PC version) are highly recommended.

As an additional technical detail, given the very high ambient dust level in Hardwar, extreme precautions will have to be taken for reaching and maintaining a sufficiently dust-free environment required for the reliable long-term operation of computer facilities. Sealing of windows and doors, a well filtered air conditioning system, no food, tea, or smoking in the computer room, changing of shoes when entering the computer room, and the regular (daily) use of vacuums cleaners are all essential measures and practices to maintain the necessary clean working environment.

#### **A Hardware Configuration Proposal**

As one concrete configuration proposal, the following system is suggested:

- 2 SUN 3/60C-8 high-resolution color workstations 20 MHZ 68020 (3 MIPS), 68881 arithmetic coprocessor, 8 MB RAM,  
19" color monitor 1152\*900 pixels, 256 simultaneous colors,  
2 \* 140 MB winchester disks, 60 MB streamer cartridge tape.

The two workstations are interconnected vi Ethernet. The same Ethernet can be used to integrate several IBM PCs (or compatibles) through the PC NFS (network file system) throughout the PCRI campus. This local area network allows the PCs to access the SUN workstation resources, in particular disks and printers. Each PC can also function as a terminal to the SUN workstations.

Additional software should include:

SUN UNIFY/SIMPLIFY, a relational (SQL industry standard) data base management system

SUN GKS graphics Kernel System (widely compatible graphics package)

SUN CommonLisp development system (optional)

Additional peripherals should include:

- 1 lineprinter
- 1 laser or color electrostat printer/plotter (e.g., HP LaserJet or Kontron color Plotter) for raster screen dumps (graphics) and high quality text processing output; for large format (vector graphics) hardcopy, a multicolor pen plotter is recommended;
- 1 digitizing table (min 120 by 90 cm, e.g., GTCO).

Total estimated cost of above configuration including software and a starting supply of material (tapes, ribbons, etc.) is estimated at about US\$ 100,000.

Please note that the configuration includes two parallel identical systems and thus offers a high degree of reliability even under difficult maintenance conditions. It also allows for the complete and very efficient integration of the (partially already available) PC XT and AT personal computers.

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