# User Manual for EXPRESS, the

# "EXAMS-PRZM Exposure Simulation Shell"

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by

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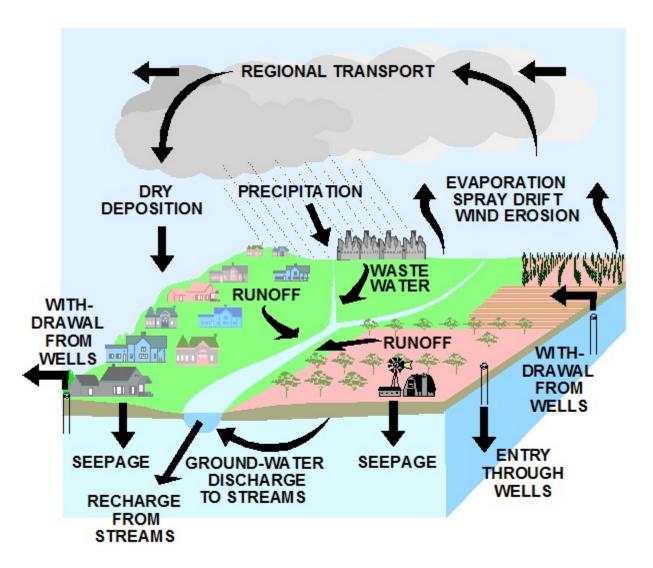Ecosystems Research Division
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**NOTICE**

**ABSTRACT**

The Environmental Fate and Effects Division (EFED) of EPA's Office of Pesticide Programs (OPP) uses a suite of ORD simulation models for the exposure analysis portion of regulatory risk assessments. These models (PRZM, EXAMS, AgDisp) are complex, process-based simulation codes that combine chemical and physical data required by EPA of industry with agronomic, physiographic, and limnological descriptions of the environmental settings into which pesticides are released. This complexity, while providing significant sophistication and specificity in analysis, has posed difficulties in maintaining a transparent, reproducible process clearly devoid of arbitrariness in parameter selections, exposure metrics, and interpretation of ecological and human health risks.

This project was undertaken to develop a Graphical User Interface (GUI) to combine regulatory simulation models, their supporting databases, regulatory "scenarios" for major crops, and data input screens for chemical properties into a user-friendly "simulation shell" lending itself to consistent analytical practices and reproducible exposure and risk assessments. The resulting computer software – Express (the EXAMS - PRZM Exposure Simulation Shell) – is a joint project of EFED and ORD. EFED designed and funded an initial draft of the Express software, and retains responsibility for developing and maintaining crop-specific modeling scenarios for regulatory analyses. ORD is responsible for continuing development, quality control, maintenance, and public availability of the software and its constituent models and analytical modules.

With the completion of Express, exposure metrics (peak, 4-day, 21-day, 60-day, annual) for ecological and human health risk assessments can be easily and conveniently and, as importantly, reproducibly, developed for any or all of the agronomic scenarios developed by EFED. Probabilistic analyses (Weibull distribution) of these exposure metrics are derived by coupling 30-year time-series of meteorological data to linked PRZM/EXAMS simulation studies. Express significantly reduces the variability, lack of reproducibility by external analysts, and perceived arbitrariness of EPA's regulatory processes for determining the safety and appropriate uses of registered pesticides.

## Table of Contents

**Transport Pathways of Pesticides**

### 1.0 Introduction to EXPRESS

The Office of Pesticide Programs (OPP) Environmental Fate and Effects Division (EFED) has developed a tiered approach to determine the appropriate level of modeling needed to perform a risk assessment for a pesticide. This tiered approach is designed to minimize the amount of analysis required to evaluate any given chemical. Each of the tiers is designed to screen out pesticides by requiring higher, more complex levels of investigation only for those compounds that have not passed the previous tier. Each tier screens out a percentage of pesticides from having to undergo a more rigorous review prior to registration or reregistration. "Passing" a given assessment tier indicates that there is a low possibility of risk to the aquatic environment. "Failing" an assessment tier does not, however, necessarily mean the chemical is likely to cause environmental problems, merely that the assessment should continue on to the next higher assessment tier. The intent of this tiered modeling system is to produce only as thorough an analysis as is necessary for each pesticide, and thereby focus greatest resources and efforts toward areas of greatest potential ecological threat. As a matter of policy, OPP does not take significant regulatory action based solely upon the results of screening models.

"Tier I" models provide simplified, highly conservative initial screening risk assessments of pesticides. For Tier I analyses, the Environmental Fate and Effects Division (EFED) of the U.S. Environmental Protection Agency's Office of Pesticides Programs (OPP) uses, *inter alia*, two "meta-models," GENEEC2 (Parker et al. 1995) and FIRST, developed by summarization of standardized linked simulations using the EPA PRZM and EXAMS models. Dynamically (file transfer-) linked Pesticide Root Zone Model (PRZM) and Exposure Analysis Modeling System (EXAMS) simulations are used for a "refined" (Tier II) estimation of pesticide concentrations in surface waters used as drinking water sources and for aquatic ecosystem exposure assessments. PRZM is a one-dimensional, dynamic, compartmental model used to simulate chemical movement in unsaturated soil systems within and immediately below the plant root zone (Carsel et al. 1984, Carsel et al. 1985, Suárez 2005). EXAMS contains a set of process modules that link fundamental chemical properties to the limnological parameters that control the kinetics of fate and transport of chemicals in aquatic ecosystems (Burns et al. 1982, Burns and Cline 1985, Burns 2000). Multiple-year pesticide concentrations in the water column and benthic sediments, generated by the PRZM-EXAMS simulations, are analyzed to produce, for each year, the single-day peak concentration, the maximum 24-hour, 96-hour, 21-day, 60-day, and 90-day mean concentrations, and the mean annual concentration. From simulation results encompassing the period of record for the available meteorological data, upper 10th percentile concentrations are made available in tabulations and

graphics for comparison with ecotoxicological and human health levels of concern (LOC). Documentation and access for these models can be found at:

- GENEEC2: http://www.epa.gov/oppEFED1/models/water/index.htm
- FIRST: http://www.epa.gov/oppEFED1/models/water/index.htm
- PRZM: http://www.epa.gov/ceampubl/gwater/PRZM3/index.htm
- EXAMS: http://www.epa.gov/ceampubl/swater/EXAMS/index.htm

The standard PRZM-EXAMS runoff modeling scenario captures the properties and dimensions of an agricultural field draining into water bodies for subsequent drinking water safety and aquatic exposure assessments. PRZM links two subordinate models (PRZM *per se* and VADOFT), that combine differing root zone and vadose zone characteristics into a single simulation to predict pesticide transport and transformation in the crop root and unsaturated zones, and edge-of-field losses in runoff waters and eroded sediment. Each PRZM modeling scenario represents a unique combination of climatic conditions, crop-specific management practices, specific soil properties, site-specific hydrology, and pesticide-specific application and dissipation (fate and transport) processes. Each PRZM simulation is conducted for multiple years (usually 30, spanning the years 1961-1990) using historical weather data (Burns 2001) to provide a probabilistic exposure characterization for a single site. Daily edge-of-field loadings of pesticides dissolved in runoff waters and sorbed to entrained sediment, as predicted by PRZM, are discharged into a standard water body simulated by the EXAMS model. The EXAMS model accounts for subsequent hydrologic transport, volatilization, sorption, hydrolysis, biodegradation, and photolysis of the pesticide.

EXPRESS (the EXAMS - PRZM Exposure Simulation Shell) has been created to facilitate a rapid and consistent Tier II assessment of aquatic pesticide exposure for multiple geographic and agronomic settings. EXPRESS was a joint project of the U.S. Environmental Protection Agency's Office of Pesticide Programs (OPP) and its Office of Research and Development (ORD). OPP contracted with Waterborne Environmental, Inc., for initial development of the shell code, and retains responsibility for development and maintenance of the crop-specific modeling scenarios. ORD developed and maintains the constituent Tier II models (PRZM and EXAMS) and the meteorological databases. Although EXPRESS provides access and output file management for GENEEC2 and FIRST, EXPRESS does not provide a Graphical User Interface (GUI) to facilitate use of these models for exposure assessment. Users wishing to run these Tier I models may wish to download their respective user manuals from the http sites cited above; the EXAMS and PRZM user manuals are provided with EXPRESS.

EXPRESS, developed using the Winteracter GUI development system (version 7.1a) from ISS Ltd., provides the following features:

- User-friendly scenarios and parameters in a *Microsoft Windows* environment.
- Simulation of an unlimited number of crop "scenarios" in a single run in less than 15 seconds per crop.
- Automatically runs both the ecological farm pond and the drinking water index reservoir scenarios.
- Provides options for simulating selected groupings of scenarios for special purposes (e.g., cumulative assessments).
- Provides flow/no-flow and steady/unsteady flow options for the farm pond and index reservoir, respectively.
- Simulates parent pesticide and degradates.
- Provides options for mixing types of applications, spray drift calculations, incorporation depth, etc., in the same simulation.
- Runs alternative versions of PRZM with the same initial setup to permit comparisons.
- Provides graphical and tabular ranked summary results for all scenarios together.
- Provides graphical and tabular output for each individual scenario.
- Provides graphical and tabular output for water column and benthic sediment zones.
- Provides a graphical and tabular PRZM water balance summary for each scenario run.
- Each graph and table can easily be printed or exported to reporting software.
- Time-series files for transmission to OPP's Health Effects Division (HED) for analysis of drinking water source contamination are automatically generated and inventoried. These files are in comma-separated-value (csv) format suitable for direct import into, for example, Excel for further analysis and plotting.
- New scenarios can be added or existing scenarios quickly and easily changed through a password-protected facility.
- Saves all run information in a single, email-able file from which the entire, multi-crop simulation can be recreated. This master file can be shared among multiple modelers working on the same problem set, or archived so that runs can be reproduced later or with future versions of PRZM and/or EXAMS.
- EXPRESS also includes the Tier I screening models FIRST and GENEEC2 (Section 9), but does not facilitate their use beyond providing project results file management and access.
- Optional production of detailed times-series (.ZTS) files from PRZM

## *2.0 Acquiring and Installing EXPRESS*

The EXPRESS user interface software can be obtained (gratis) from the EXPRESS main page at EPA's Center for Exposure Assessment Modeling (CEAM):

http://www.epa.gov/ceampubl/swater/EXPRESS/.

EXPRESS uses standardized files of weather data that are automatically installed in the "...\EXPRESS\stdmet\" directory. These thirty-year (1961-1990) data files of U.S. meteorological data are also available separately via the "Meteorological Data" link at the EXPRESS main page. The format of these data files is provided in Appendix A.

EXPRESS runs on PCs under the Windows operating system (installation has been tested on Windows 98, NT, 2000, and XP). To install, click on the "Install_EXPRESS.EXE" file and follow the on-screen directions. All required files will be installed automatically along the user-selected installation path ...\EXPRESS\.  EXPRESS requires a screen area setting of 1024x768 or higher, and will issue an error message if it is invoked from a lower resolution display. The free Adobe Reader is required to access model User Guides and location maps. EXPRESS is removed using the standard Windows uninstall procedure, i.e., via "Settings – Control Panel – Add/Remove Programs", followed by deletion of the directory structure along with any remaining user-modified project or meteorological data files.

To manually move the installation to a different directory or disk drive follow these steps:

1)  Use Windows Explorer to either copy or move EXPRESS in its entirety to the desired drive. The directory structure must remain exactly as installed, using "EXPRESS" as its base.

2)  Create a new (or modify the existing) Windows shortcut to point to the new drive (a modifiable shortcut file is supplied in the ...\EXPRESS\EXPRESS\ folder).

The latest PRZM release notes are available at http://www.epa.gov/ceampubl/gwater/PRZM3/prz3reln.htm; the latest EXAMS release notes are available at http://www.epa.gov/ceampubl/swater/EXAMS/examreln.htm.

### 3.0 Starting EXPRESS

Following installation, EXPRESS is started by double-clicking on EXPRESS.EXE or by using any shortcut to the EXPRESS executable. The starting screen (Figure 1) appears, depicting a stream flowing through an agricultural landscape, providing access to EXPRESS' main functionalities.



**Figure 2**. EXPRESS opening display screen

The functions available from EXPRESS' initial screen are:

Start a new project by creating a project folder: New Project

Navigate to an existing project folder, or to an existing directory created using functionality of the operating system (containing, e.g., a master project file created by a colleague: Find Project

Recall, annotate, or delete existing projects: [Project Management]

> (organized in chronological order, includes chemical name, file location, and user annotation/remarks)

Check software and database version numbers and dates; access EXPRESS , EXAMS, and PRZM User Guides: [Help]

Operate EXPRESS in regulatory mode for submission of studies to EPA's Office of Pesticide Programs: [OPP]

Operate EXPRESS in ORD (Office of Research and Development) mode with additional flexibility and input data control (see Appendix B for details): [ORD]

 - access the FIRST Tier I model

 - access the GENEEC2 Tier I model

 - prepare chemical and agronomic input data

 - start PRZM/EXAMS simulations

 - analyze and display PRZM/EXAMS results

### 3.1 Project Directories and the Master Project File

The first step in using EXPRESS is to select (or create) an active project directory. All relevant input/output data of a simulation run is saved in this directory; EXPRESS requires full read/write permission for the specified directory. New project folders can be created on hard disks



**Figure 2.** Create or select the active project directory

or network drives using EXPRESS itself, *Windows Explorer,* or other tools. Long filenames are supported. The default directory upon initiation of EXPRESS is undefined or "unset." When the

<p align="center">[ New Project ]    [ Find Project ]</p>

button is pushed, an input screen as in Figure 2 is displayed.

The initial project directory display is always the default project folder "...\express\projects." To select an existing directory, use the scroll bar to move to the desired drive\directory (if it is not already visible in the selection window), and then double-click on it. The selected folder (The terms "drive\directory" and "folder" are equivalent) will then replace the "...\express\projects" text initially displayed (see Figure 2). Pressing the **OK** button sets the selected drive\directory to be the current project directory. To create a new project directory, type a "\" followed by the new project directory

name on the line in Figure 2 labeled "create new directories here." For example, typing "\newchem1" at the end of the folder selection window creates a new project directory called "...\express\projects\newchem1." Only one subdirectory can be created in a single step; entering, for example, "\newchem1\app1", is not supported. To create dependent subdirectories (i.e., folders within folders), first create \newchem1, press the "OK" button, then reselect the [ New Project ] button and enter "\app1." This will create the "...\express\projects\newchem1\app1" project directory.



**Figure 3.** Options if Master Project File exists in currently selected directory

This option also serves to switch between previously created projects (which can contain multiple crop scenarios). (Section 3.3 describes the "project manager," a facility for cataloguing previously created scenarios.) Each simulation scenario can be modified, re-run, or re-analyzed by choosing a project directory in which simulations have previously been executed. A master project file (MPF), named "master.fpj," is created within each active project directory. This file contains all scenario-specific information necessary to characterize the entire simulation project in the active project directory. After an active project directory has been chosen, EXPRESS checks to see whether an MPF is present in this directory. If an MPF is present, EXPRESS returns an output window (Figure 3) for choosing the action to be taken. The available options are: *Copy, Edit, Browse, Reselect, EMail, Rerun*, and *View*. The function of each of these options is further described in Figure 3. If no MPF is found, EXPRESS starts the input generator program, initiating a new project. New project development can be facilitated by copying an existing project to a new directory, or by recalling a stored chemical dataset from the EXPRESS chemicals database.

The Master Project File contains **all** the information needed to identify and replicate an EXPRESS analysis. The MPF enables convenient exchange of EXPRESS simulation scenarios among EXPRESS users. Once an MPF received from another user has been copied into a valid

folder, it is available to the receiving analysts as an active project directory. This (MPF) feature makes it possible to easily re-create each crop-use scenario, pesticide chemistry, and the application-specific model inputs used to generate a particular EXPRESS analysis. Because every master project file is named "MASTER.FPJ," only one MPF can be stored in a project folder.

### 3.2 Format of the Master Project File

The definitions of the scenario, pesticide chemistry, and application-specific parameters are compiled according to formats used in the PRZM input parameter file (*.inp) (Suárez 2005). A typical example of a Master Project File is given in Figure 4. This sample Master Project File was created for a parent compound, a single scenario, and a single application. The information included in the Master Project File is complete, but omits EXPRESS default settings to save space. The individual lines of the Master Project File specify:

Line 1:     Date on which the file was created by the EXPRESS.
Line 2:     Version and date of EXPRESS
Line 3:     Name of the parent compound
Line 4:     Identification of Group File, if any
Line 5:     Scenario type (3 = Standard Tier II)
Line 6-9:   Index of selected scenarios (1 = used; 0 = not used for this project)
Line 10:    Chemical input data controls
Line 11:    EXPRESS operational mode (OPP or ORD)
Line 12-24: Chemical properties (parent and metabolites)
Line 25:    Number of specific application sequences
Line 26:    Application input data controls
Line 27-34: Application parameters for each crop
Line 35:    EXAMS chemistry and flow process controls
Line 36-47: EXAMS process parameters

**This file must not be modified by hand in any way. This description of the MPF is provided solely for informational purposes. Attempts to modify this file will in all probability result in loss of data and EXPRESS execution failure.**

The MPF is not designed to provide a complete input summary of model parameters with complete descriptions of all input values and their units. The MPF does, however, provide complete documentation of EXPRESS input values used for a specific analysis.

```
 1 Master Project File Created: 2006-12-21 at 13:02:43
 2 EXPRESS     v. 1.03.00    (2006-12-20)
 3 Parent Compound: Chemical A
 4          Scenario Group File:   0  No GroupFile
 5                Scenario Type:  3
 6          PRZM Crop Selector: 000001000000000000000000000000000000000000000000000
 7          PRZM Crop Selector: 000000000000000000000000000000000000000000000000000
 8          PRZM Crop Selector: 000000000000000000000000000000000000000000000000000
 9          PRZM Crop Selector: 000000000000000000000000000000000000000000000000000
10 Chemical Input Data Controls:  1 1 0 1 0
11     EXPRESS Operational Mode: OPP
12 Chemical Name(s):  Chemical A          |
13               Molecular Weight:  300.0
14          Plant Uptake Factor:  0.000
15 Partition Coefficient Method:           1           1
16  Partition Coefficient Value:  30.00       60.00
17               Vapor Pressure:  0.1000E-05
18               Solubility   :  100.0
19   Soil Degradation Half-Life:  30.00
20            % Degradate formed:  0.000       0.000       0.000
21             Foliar Half-Life:  0.000
22   Foliar Washoff Coefficient: 0.5000
23    Air Diffusion Coefficient:  4300.
24     Enthalpy of Vaporization:  20.00
25 Application DataSets Number:  1
26        Application Parameters:  1  1  2  2  1  0  0    87.00  0
27   Days Relative/Absolute    :        -   1
28               Month        :           0
29               CAM          :           2
30             Depi (cm)    :  4.000
31             Rate         :  0.5000
32         Drift Farm Pond % :  5.000
33     Drift Index Reservoir % :  16.00
34             Efficiency % :  95.00
35   Product chem./hydr. status: 1 1 1
36 Aerobic Dissipation (days) :   20.00
37      Q10 Base Temperature :   25.00
38      Q10 Limnetic Bacteria:   2.000
39 Anaerobic Dissipation(days):   100.0
40      Q10 Base temperature:   25.00
41      Q10 Benthic Bacteria:   2.000
42 Photolysis Half-Life (days):   10.00
43   Number of Hydrolysis Obs.:           3
44    Hydrolysis Temperatures:   25.00
45  Hydrolysis C1:  3.000E+01 3.000E+01 3.000E+01
46  pH Hydrol. C1:      5.00      7.00       9.00
47               Melting Point: -99.00
```

### 3.3 Project Manager

The "Project Manager" tracks and maintains EXPRESS simulation scenarios. Information for each project created is stored in a user database that includes the location of the project folder, the date and time the project was created, the name of the primary chemical, and optional user-supplied commentary/annotation (Figure 5). A record is added (or updated) in the Project Manager database each time the *Write* option is executed in the input generator. The "Action" operator (third column; options "Keep" or "Delete")), when "Delete" is chosen, deletes all files in the project folder and the folder itself. The user is prompted to confirm the deletion of each project selected for elimination.
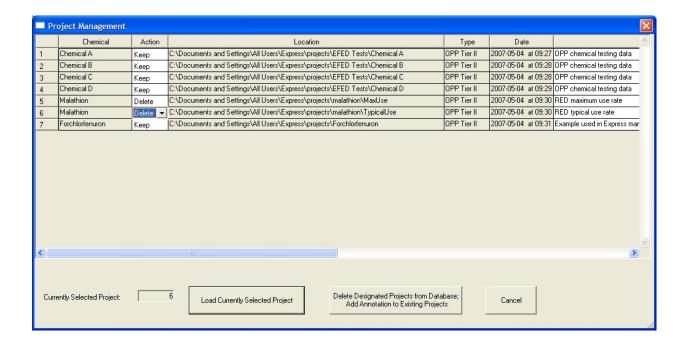


| | Chemical | Action | Location | Type | Date | |
|---|---|---|---|---|---|---|
| 1 | Chemical A | Keep | C:\Documents and Settings\All Users\Express\projects\EFED Tests\Chemical A | OPP Tier II | 2007-05-04 at 09:27 | OPP chemical testing data |
| 2 | Chemical B | Keep | C:\Documents and Settings\All Users\Express\projects\EFED Tests\Chemical B | OPP Tier II | 2007-05-04 at 09:28 | OPP chemical testing data |
| 3 | Chemical C | Keep | C:\Documents and Settings\All Users\Express\projects\EFED Tests\Chemical C | OPP Tier II | 2007-05-04 at 09:28 | OPP chemical testing data |
| 4 | Chemical D | Keep | C:\Documents and Settings\All Users\Express\projects\EFED Tests\Chemical D | OPP Tier II | 2007-05-04 at 09:29 | OPP chemical testing data |
| 5 | Malathion | Delete | C:\Documents and Settings\All Users\Express\projects\malathion\MaxUse | OPP Tier II | 2007-05-04 at 09:30 | RED maximum use rate |
| 6 | Malathion | Delete | C:\Documents and Settings\All Users\Express\projects\malathion\TypicalUse | OPP Tier II | 2007-05-04 at 09:30 | RED typical use rate |
| 7 | Forchlorfenuron | Keep | C:\Documents and Settings\All Users\Express\projects\Forchlorfenuron | OPP Tier II | 2007-05-04 at 09:31 | Example used in Express man |

Currently Selected Project: 6    [Load Currently Selected Project]    [Delete Designated Projects from Database; Add Annotation to Existing Projects]    [Cancel]

**Figure 5.** EXPRESS Project Manager

### 4.0 Creating Input Files for PRZM-EXAMS Simulation

The input generator (Figure 6) creates an exposure model input data set in five consecutive steps. Start the input generator by pressing the **inputs** button on the main EXPRESS screen (Figure 1). (Recall that the project directory must be selected prior to starting the input generator.) The input data tabs (Figure 6) have the following functions.
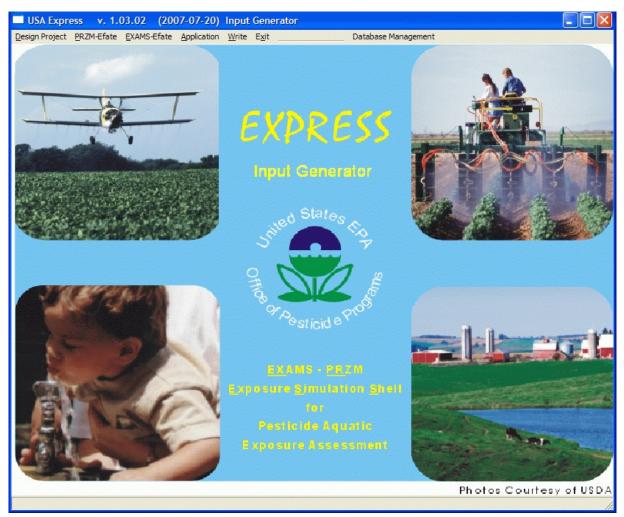


**Figure 6.** EXPRESS Input Generator

| option: | description: |
| --- | --- |
| Design Project: | Select one or more of the predefined (EFED Standard Tier II) scenarios |
| PRZM-Efate: | Define the physical-chemical and environmental fate ("Efate") pesticide properties needed for PRZM. |
| EXAMS-Efate: | Define physical-chemical and "Efate" properties needed for EXAMS. |
| Application: | Choose application date(s), method, rate(s) |

Write:     Write PRZM-EXAMS input files, create (or update) the Master Project File, and add or update a record in the scenario manager data base

All five of these data creation steps should initially be completed in the suggested order (Design, PRZM-Efate, EXAMS-Efate, Application, Write) to guarantee proper creation of the input file set.

Users of EXPRESS should be generally familiar with the use of simulation models for environmental risk assessments. Further information for EXAMS, including detailed model documentation, can be found at http://www.epa.gov/ceampubl/swater/EXAMS/index.htm, and, for PRZM, at http://www.epa.gov/ceampubl/gwater/PRZM3/index.htm. *For authorized Tier II simulations, process implementations and parameter definitions should follow EFED guidelines and reflect the intended uses of the compound. (These guidelines are available on-line at* http://www.epa.gov/oppEFED1/models/water/input_guidance2_28_02.htm*)*

### 4.1 Project Design and Tier II Scenario Selection

To begin scenario definition, click on the **Project Design** menu item (Figure 7). The "Project Design" screen (Figure 7) then presents a pick-list of predefined scenarios. The scenarios are defined by State, crop, soil properties, meteorology, and Major Land Resource Area (MLRA) (SCS 1981). There are approximately 85 EFED standard scenarios currently included within EXPRESS. As additional scenarios are created and certified by EFED, they can be added to the set. This database can only be altered by an authorized database manager (see Chapter 8).

One, many, or all of the currently available scenarios can be selected for inclusion in a project. In addition to scenario selection, the number and transformation product chemistry of chemicals to be simulated is chosen on this screen. Both EXAMS, and PRZM from 3.12.2 onwards, can model the creation and subsequent fate and transport of
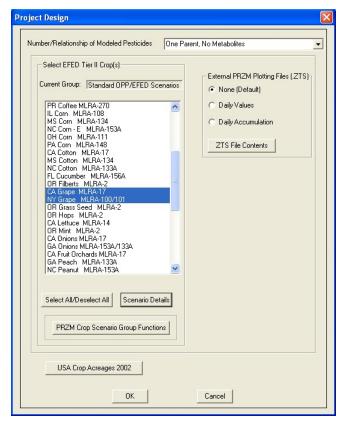


**Figure 7.** Selecting scenarios

13

chemical metabolites and transformation products of the pesticides or toxic chemicals under evaluation. EXPRESS allows for a choice among four possible transformation product chemistries:

1) One Parent, No Metabolites

2) One Parent –> One Metabolite

3) One Parent –> Two Metabolites

4) One Parent –> First Metabolite –> Second Metabolite

The PRZM and EXAMS User Manuals include detailed discussions of metabolite simulation. The EXPRESS input generator does not permit simulation of metabolites in PRZM 3.12 beta (see Chapter 7 for a discussion of PRZM model versions). Because the current (3.12.2) version of PRZM is restricted to three chemical entities, this limitation is also enforced in EXPRESS and EXAMS.

A final option on this screen, the "Scenario Group Functions," allows for the creation or selection of scenario groupings. Two examples of scenario groupings are illustrated in Figure 8, "OP" (organophosphate pesticide) scenarios and "Standard EFED" scenarios. The "Standard EFED" scenarios (Group 1) are selected by default. To create a new scenario group, first select the desired scenarios (from the screen shown in Figure 7), and then press



**Figure 8**. Scenario Group Manager

(mouse-click) the "Scenario Group Functions" button. The scenario group manager then opens (Figure 8). Next, push (click) the "Save the currently selected scenarios to a Group File" button. The "Save Group File" panel (Figure 9) then opens, with space for a file name (required) and for descriptive text and annotation comments for the new group file (strongly recommended).
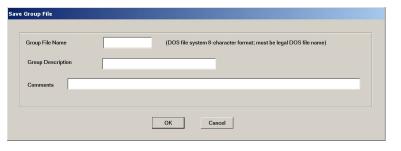


**Figure 9.** Defining a scenario group

## 4.2 PRZM Environmental Fate Parameters

The *PRZM Chemical Parameters* screens include data entry fields for the following chemical properties: molecular weight, solubility, Koc/Kd, vapor pressure, degradation half-life (applied equally to dissolved and sorbed phases), plant uptake factor, foliar half-life, foliar washoff



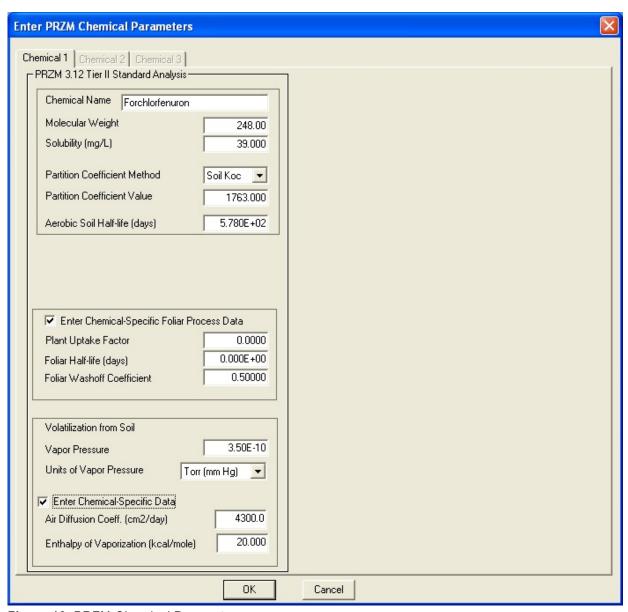**Figure 10.** PRZM Chemical Parameters

coefficient, air diffusion coefficient, and enthalpy of vaporization (Figure 10). When simulating transformation products or metabolites, enter a parameter set for each chemical. Vapor pressure units are specified at the Chemical 1 input pane; vapor pressures for other chemicals must be entered in the units so selected. Enter the percent transformed from the parent to the

transformation product or metabolite as 100 × (mole of product)/(mole of parent); EXPRESS applies the ratio of compound molecular weights prior to entry in the PRZM input files. Chemical dissolved in the soil solution and that sorbed with the soil particulates are parameterized with the same product yield in EXPRESS Tier II simulations. The product yield parameter can be entered as a zero (0) for those cases in which transformation processes are only relevant for the aquatic ecosystems (aquatic product yields are entered on the EXAMS data entry screen).

All compound-specific parameters (parent and metabolites) can be saved in a chemical database provided with EXPRESS. The same chemistry can then be used for additional simulations with alternative soil, crop, and application scenarios. Database maintenance functions include a facility for deleting a single entry (Chapter 8).

### 4.3 EXAMS Environmental Fate Parameters

The *EXAMS Efate Input* screen provides data entry fields for transformation process half-lives; these are converted to chemical dynamics parameters (rate constants) by EXAMS (Figure 11).

Solubility, Koc, and vapor pressure are transferred to EXAMS from the *PRZM Chemical Parameters* data entries (Figure 10). As with PRZM, when simulating transformation products and metabolites the product half-lives must be entered on a separate tab for each secondary chemical. (Although EXAMS can accommodate an arbitrary number of chemicals in a single simulation, the current version of PRZM, and perforce EXPRESS, is limited to three chemicals.) A 0.0 (zero) entry for a half-life is used to indicate that the transformation process is inactive (i.e., not, as a literal interpretation might suggest, that it is immeasurably rapid). Particular care is required with the hydrolysis inputs: at least three non-zero half-lives at three different pH values must be entered (conforming with EPA guidelines), or hydrolysis will not be simulated. (EXPRESS will accept up to 10 pH-half-life observations.) In Figure 11, were the example chemical reacting by a neutral hydrolysis pathway only, the same half-life (e.g., 10 days) would have to be entered for pH 5, 7, and 9: EXPRESS **requires** *entry of all three values for correct calculation of rate constants.* Aerobic and anaerobic metabolism half-lives should be corrected for the contribution due to abiotic hydrolysis prior to entry on these data screens.

In addition to product chemistries, the pathways of formation must also be defined. Transformation product information is communicated to EXAMS by setting an identifying number for each parent and daughter chemical, for each process generating a product, for the reactive form of the parent molecule, and for the process yield. The EXPRESS input parameters are: CHPAR,

the chemical parent number; TPROD, the transformation product number; NPROC, the identifying number of the transformation process generating the TPROD; RFORM, to identify the reactive form of the parent molecule, and YIELD, the (Mole/Mole) transformation process yield from this pathway.



**Figure 11.** EXAMS Efate Input Screen
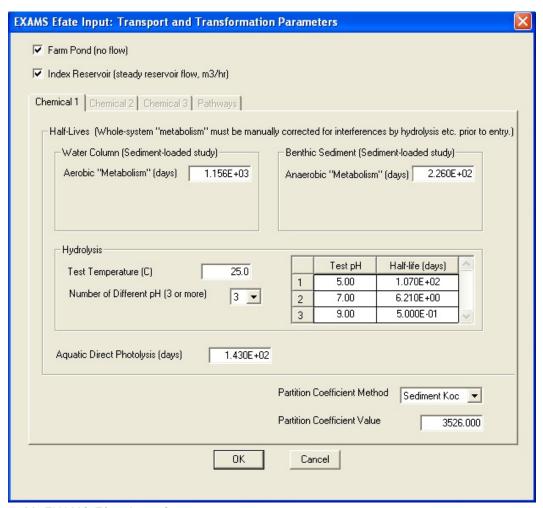
The generating transformation process is specified using the following numerical codes for NPROC:

> 1 = specific acid hydrolysis
>
> 2 = neutral hydrolysis
>
> 3 = specific base hydrolysis
>
> 4 = direct photolysis
>
> 5 = singlet oxygen
>
> 6 = free radical oxidation (e.g., hydroxyl radical)
>
> 7 = water column bacterial biolysis
>
> 8 = benthic sediment bacterial biolysis

9 = reduction

Twenty-eight reactive form numerical codes are available for specifying RFORM, in addition to which total dissolved etc. can be specified using an RFORM code of

29 = all dissolved species

30 = all sediment-sorbed species

31 = all doc-complexed species

32 = all biosorbed species

(The complete list of RFORM specifications is given in Table 1.) In EXPRESS, the process yield must be entered as the simple mole of product per mole reacted (i.e., EXAMS temperature-dependent product yields are not currently supported).

**Table 1**. Product Chemistry "Reactive Forms" for EXAMS

| | Ionic species | Neutral | Cations | | | Anions | | | Total |
|---|---|---|---|---|---|---|---|---|---|
| | Valence | 0 | 1+ | 2+ | 3+ | 1- | 2- | 3- | (all) |
| Forms: | Dissolved | 1 | 5 | 9 | 13 | 17 | 21 | 25 | 29 |
| | Solids-sorbed | 2 | 6 | 10 | 14 | 18 | 22 | 26 | 30 |
| | doc-complexed | 3 | 7 | 11 | 15 | 19 | 23 | 27 | 31 |
| | Biosorbed | 4 | 8 | 12 | 16 | 20 | 24 | 28 | 32 |

For example, if the *CHPAR* parent compound (e.g., parathion) is chemical 1, and the *TPROD* product (e.g., paraoxon) is chemical 2, then a reaction scheme in which direct photolysis of DOC-complexed parathion yields a 50% generation of paraoxon by pathway 1, and hydroxyl radical oxidation of dissolved parathion produces paraoxon in mole-for-mole formation by pathway 2, would be specified in EXPRESS as illustrated in Figure 12.
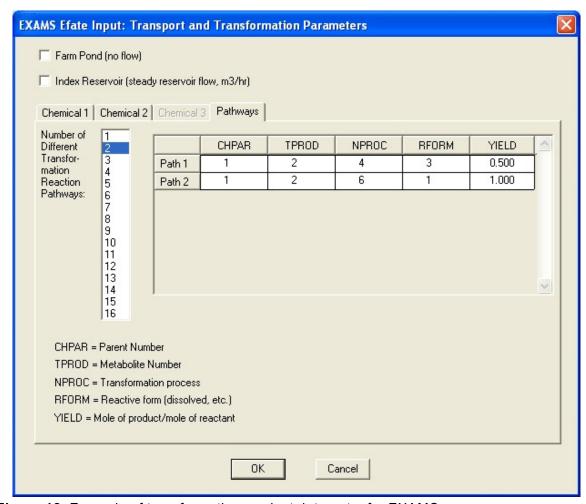
**Figure 12**. Example of transformation product data entry for EXAMS

Section 2.4.1 ("Product Chemistry") of the EXAMS manual (Burns 2000) (also available through the primary EXPRESS screen's "HELP" button) should be consulted for further explanation on entering pathway data.

In addition to product chemistry parameters, the user can also select whether a static pond and/or a steady reservoir flow rate scenario will be simulated. The current default is set for both of these options to be in effect. The static pond does not change volume, nor does it allow for hydrologic export of chemical. Turning the static pond option off (un-checking the box) lets the pond detention time vary (monthly) based on an EXAMS analysis of evaporation and rainfall from the Crop Scenario meteorological file and daily PRZM runoff volumes. The steady flow reservoir scenario uses a period-of-record average daily runoff from the PRZM scenario to calculate the flow. Turning the steady flow reservoir option off will, as with the farm pond scenario, allow EXAMS to calculate a monthly detention time for the reservoir based on meteorology and daily PRZM runoff.

### 4.4 PRZM Application Data for Pesticide Use Patterns

The *Pesticide Application Data* screen contains data entry fields for the number of applications, application timing, application method, application rate, depth of incorporation, and chemical application method (Figure 13). The same values can be applied to all selected scenarios,
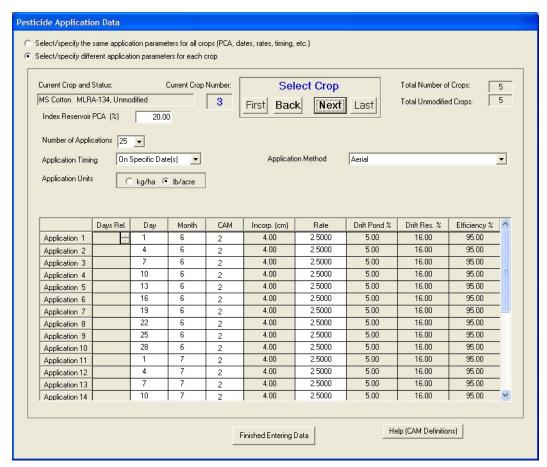


**Figure 13.** Pesticide Application Data Entry Screen

or, as here, specific values can be entered for each of the selected scenarios. To minimize the amount of data entry required, first enter any values that are common among crops, and only then select the option to enter specific values for each crop. At that juncture, the first-entered values will be copied to all additional scenarios, reducing the labor required to enter identical values across the selected scenario set.

For Tier II, the aerial application default drift values have been set at 5% and 16% for the pond and reservoir, respectively. For aerial applications, the default efficiency is 95%. The ground sprayer application default drift values are 1% and 6.4% for pond and reservoir simulations, respectively. The default efficiency value for ground applications is 99%.

Pesticide application dates can either be set absolutely (by calendar date), or relative to crop planting, emergence, maturity, or harvest dates. This feature facilitates rapid configuration of application scenarios for multiple crops. For example, when the pesticide is intended for application 7 days pre-planting, the user can enter -7 days relative to planting and the correct application date for each crop will be calculated from the crop phenology embedded in the crop scenario file.

### 4.5 PRZM-EXAMS Input File Creation

Finally, selecting the **Write** menu option creates all input files needed by PRZM and EXAMS. The current release of EXPRESS includes two PRZM versions when run in OPP mode: PRZM 3.12 beta, and PRZM 3.12.2.  In ORD Mode, the latest version of PRZM (3.12.3) is also available. PRZM 3.12.2, the current regulatory model, is the default selection. Earlier versions of PRZM  contain known bugs and limited features (See PRZM release notes at
 http://www.epa.gov/ceampubl/gwater/PRZM3/prz3reln.htm). Multiple PRZM versions are included within EXPRESS to facilitate comparisons of exposure analysis results across successive versions; PRZM 3.12.3 adds a mass balance reporting function to the suite of Express output graphics.

Once the version of PRZM has been selected, the model input files are created. The information necessary to run PRZM-EXAMS is contained in several input data files:

PRZM
- annotated parameter file incorporating the scenario definition, *.inp
- climate file providing the weather data used, *.dvf
- file with definition of the PRZM run options, *.run

EXAMS
- parameter file including the scenario selection, *.exa
- multiple PRZM to EXAMS transfer files, *.dyr (yr represents year of run)

Each standard scenario is assigned an unique six character name that identifies the USA State and crop. An *R* or *P* is added to this file name to specify whether the input file is a reservoir run or pond run, respectively. All scenario-, chemical-, and application-specific information is also stored in the Master Project File *master.fpj*. In addition, a file of type *.scn is created to support data analysis and data visualization in EXPRESS.

The scenario and parameter definitions combine input data specified by the user in EXPRESS with internal EXPRESS-defined data and parameters (as developed by the OPP/EFED

Water Quality Technical Team). The parameter definitions and values specified by EPA (e.g., in PRZM crop scenarios) and stored internally within EXPRESS cannot be altered by EXPRESS users. EXPRESS also generates some of its input data from user choices within fixed menus of EPA-approved alternatives. All predefined and menu-selected data within model input files produced by EXPRESS can be edited manually to create special scenario definitions. *Under no circumstances, however, should data files created by EXPRESS be modified when producing EPA "Standard Tier II" simulations.*

With the input file set written, the data preparation phase is now complete. Select the **Exit** menu option to return to the main EXPRESS program screen.

## 5.0 Starting and Running the PRZM-EXAMS Simulation

With the input files created, simulations are started by pressing the **lightning bolt** icon (Figure 1). Current versions of PRZM run in a DOS console window. Each successive requested PRZM-EXAMS simulation scrolls in this window. Once simulation runs have been completed, the display screen reverts back to the opening menu (Figure 1), and the graphing options described in Section 6 become available.

## 6.0 Evaluation of the PRZM-EXAMS Simulation

After a completed simulation run, the relevant scenario output data is provided in three PRZM ASCII files ( *.hyd, *.cnc, and *.out), and three EXAMS ASCII files (*.xms, *.yms, and *.zms). These files are analyzed automatically by EXPRESS to generate tables and graphics of the results obtained. For Tier II runs, there is no need to analyze the output files in a different format. The EXPRESS grapher can also, however, export results for each simulated scenario in an ASCII file with an extension of ".tab." These files are created in the current project directory whenever the "Display ... as Text File" option is selected. These files can be used for further data analysis; they include all output data required for Tier II calculations.

EXPRESS generates daily time-series files for each combination of a surface drinking-water reservoir scenario and chemical simulated. These files are deposited in the project folder; they are comma-separated-value (*.csv) formatted files suitable for direct importation into risk assessment models (e.g., dietary exposure models in use by EPA – DEEM/CALENDEX, CARES, and a Lifeline Excel template). An inventory of the produced files is stored in the project directory in file "HED_Files.txt (the name derives from the nominal target audience for these csv files, OPP's "HED" (Health Effects Division).

PRZM Output

*.out = summary of PRZM output. Contains all PRZM output

*.cnc = mean annual soil concentration at depths of 1 meter from the soil surface and at the bottom
of the soil column

*.hyd = annual hydrology summary (total precipitation, runoff, erosion, and evapotranspiration)

*.msb = annual chemical mass balance at depths of 1 meter from the soil surface and at the bottom
of the soil column (total application, runoff flux, decay flux, erosion flux, mass remaining in
soil column, etc.) (ORD mode with PRZM 3.12.3 only)

*.zts = (optional) PRZM times series outputs for closer analysis (using other software)

Note: PRZM 3.12 beta does not create .cnc, .hyd, or .zts files


EXAMS Output

*.xms =        EXAMS standard tabular report file

*.yms =        EXAMS EcoRisk output file containing "instantaneous" and mean 24-hour, 96-hour,
21-day, 60-day, 90-day, and annual average aquatic concentrations of parent and
transformation product chemicals

*.zms =        EXAMS EcoTox output files (daily concentrations of parent and product chemicals)


EXPRESS Output

*.csv =        Comma-separated-value time-series files of dates (as MM/DD/YYY) and associated
exposure concentrations (mg/L), each chemical/scenario in a separate file

HED_Files.txt  Inventory of .csv files generated by an exposure analysis


### 6.1 PRZM-EXAMS Grapher

Start the PRZM-EXAMS grapher by selecting the graph icon on the main EXPRESS screen
(Figure 1) and then selecting the **Standard Tier2** menu item. All EXPRESS graphing functions are
available from the next screen display (Figure 14). Graphical or tabular output is generated by
selecting either the **Display graphs** or **Display tables** radio buttons respectively. Selecting the
**Farm Pond** or **Index Reservoir** radio buttons switches between the pond and reservoir results.
Each created graphic can be printed to any installed printer or exported to a windows metafile by
pressing the **Print** or **Export** buttons located at the bottom of the screen. The **Display ... as Text
File** buttons create ASCII flat files (*.tab) within the project folder; these can be imported into other
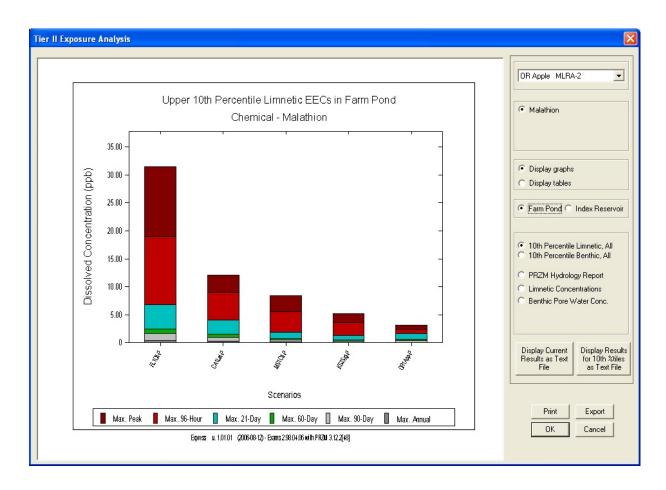software for additional analyses.

**Figure 14**. EXPRESS graphic display

## 7.0 PRZM Versions

EXPRESS includes the obsolete PRZM 3.12 beta, and the current (3.12.2) regulatory release, and the most recent ORD maintenance release (3.12.3 as of 2006-09-30). This facilitates comparisons of results between PRZM versions. In many cases, versions are backwards compatible (i.e., if the input sequences are set up the same, the results will be the same), especially when new model versions are in the main providing new options and simulation capabilities. This is not, however, always the case; e.g., when errors in the code have been discovered and corrected, exact results may not recur unless the corrections have been applied to all versions. In general, EFED prefers that the older codes be maintained in an uncorrected state to provide a baseline for revisions to regulatory analyses. The current version of all programs accessed by EXPRESS are available (Figure 15) by selecting the *Help* button on the main EXPRESS screen (Figure 1). For regulatory submissions, two versions of PRZM 3.12 are included in the shell at

present. PRZM 3.12 beta was released for testing in February, 1998. PRZM 3.12.2 repairs errors and completes implementation of peer-review suggestions received regarding PRZM 3.12 beta, and adds several enhancements as well. A complete description of the several PRZM versions, and the modifications underpinning each, can be found on the CEAM web site at
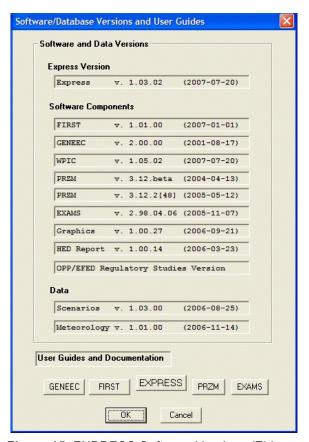http://www.epa.gov/ceampubl/gwater/PRZM3/index.htm and
http://www.epa.gov/ceampubl/gwater/PRZM3/prz3reln.htm, respectively.

Two important changes between the primary (3.12 beta and 3.12.2) PRZM versions in EXPRESS lie in the new ability to enter up to 32 curve numbers in 3.12.2, and correction in 3.12.2 of errors in the parent/metabolite degradation kinetics coded in the older PRZM 3.12 beta. Use of the complete set of available curve numbers in version 3.12.2 sometimes results in small differences in the results obtained. When simulating degradates, versions after PRZM 3.12 beta must be used; these input data are not accessible to version 3.12 beta.

### 8.0 Database and Scenario Management

One of the primary motivations underlying the development of EXPRESS has been realized by creation of the "scenario database": The scenario database contains all the data needed to create PRZM input files, in a fixed form that cannot be cavalierly altered by the analyst community. This ensures that all analysts are using the same base data set, and helps to standardize regulatory analyses and facilitate archiving, public access, and peer review of exposure analysis results. Only an authorized



**Figure 15**. EXPRESS Software Versions (This Figure may not present latest versions or dates)

"scenario manager" can change current scenarios and add or delete scenarios; the database is password-protected. The database as currently constructed can hold up to 200 PRZM scenarios.

In addition, chemical parameters can be entered and stored in a separate database specific to each user. This database includes information used in both PRZM and EXAMS.

### 9.0 Auxiliary Capabilities Included in EXPRESS

In addition to the PRZM and EXAMS Tier II models, EXPRESS includes two Tier I OPP screening models, GENEEC2 and FIRST. GENEEC2 uses the "standard agricultural field-farm pond" scenario that EFED selected for all aquatic exposure assessments. This "standard pond" scenario assumes that ten centimeters of rain fall on a treated, 10-hectare agricultural field, causing pesticide-laden runoff into a one-hectare body of water of 20,000 cubic meters volume, 2.00 meters deep. Although this "standard scenario" was designed to predict pesticide concentrations in a "standard farm pond," it has been shown to be a good predictor of upper level pesticide concentrations in small, but ecologically important, upland streams (Effland et al. 1999; additional detail available on-line at

http://www.epa.gov/oscpmont/sap/meetings/1999/may/pca_sap.pdf).

For Tier I estimations of pesticide concentrations in drinking water, OPP uses a surface water model called FIRST. FIRST is based on an "Index Reservoir" watershed and includes Percent Cropped Area (PCA) factors which account for the percentage of a watershed that is planted with specific crops. The Index Reservoir scenario and the PCA have been built into standard EXPRESS Tier II analyses.

The Index Reservoir is based on a drinking water reservoir in Illinois, Shipman City Lake. This reservoir was selected because it is representative of a number of reservoirs in the central Midwest that are known to be vulnerable to pesticide contamination. It is used similarly to the OPP



Index reservoir: Shipman City Lake

"standard farm pond," except that flow rates through the reservoir are set to reflect site-specific long-term average runoff. Like the standard pond, pesticide loadings to the water body are modeled using local soils and weather data to reflect crop-specific scenarios around the country. These scenarios are intended by OPP to represent sites at roughly the upper 90th percentile of runoff vulnerability for pesticide transport to surface waters.

## 9.1 New Scenarios for Tiers I and II

Following passage of the Food Quality Protection Act (FQPA) by Congress in August of 1996, EFED developed a source water modeling approach (the Tier I FIRST model, and modified agricultural use scenarios for EXPRESS) to supplement that already in place for ecological risk assessment. Recognizing that few people drink water derived from small farm ponds or from small, upland streams, EFED developed an "index agricultural watershed-drinking water [source] reservoir" or "index reservoir" scenario to supplement the "standard field-pond" ecological scenario. In addition, it was noted that most watersheds large enough to support a community drinking water system (CWS) are not entirely planted in only one crop. FIRST and EXPRESS therefore incorporate a method to consider a maximum percent cropped area (PCA) factor to account for this fact.

## 9.2 Index Drinking Water Reservoir

In July, 1998, OPP presented to the FIFRA Science Advisory Panel (SAP) a proposed "index reservoir" scenario to estimate pesticide concentrations in drinking water derived from surface water, supplementing the "field pond" scenario used in its ecological screening models. The concept behind use of a model of an "index" reservoir to screen pesticides was that the chosen reservoir – and its associated characteristics – would become the standard set of conditions by which EPA would judge the potential of a pesticide to contaminate drinking water derived from surface water. The "index" reservoir was selected from a group of actual reservoirs that are the source of drinking water for communities throughout the country. EPA picked from that group a particular reservoir having watershed characteristics associated with a higher potential for pesticide contamination of surface water, and uses those real-world characteristics in its mathematical screening model. Because the "index" reservoir model uses a set of real-world characteristics, it is thought likely to produce more realistic estimates of pesticide concentrations in surface drinking water sources than could a simple assemblage of average watershed properties. Because the "index" reservoir model has characteristics that are associated with a higher potential for pesticide contamination of surface water, the model is also likely to be protective of other drinking water sources less vulnerable to contamination.

The actual reservoir chosen for simulation is a small drinking water reservoir located in Shipman, Illinois. Shipman City Lake is 13 acres in area, 9 feet deep, and has an input drainage watershed area of 427 acres. Its ratio of drainage area to capacity (volume of water in the lake) is approximately 12 m$^{-1}$. As a comparison, the "standard farm pond" currently used has a ratio of 5 m$^{-1}$. Shipman City Lake is one of a number of mid-western potable source water reservoirs that tend to be small and shallow with small input drainage area watersheds, and that frequently have Safe

Drinking Water Act (SDWA) compliance problems with atrazine, a herbicide widely used on corn grown in these watersheds. The Index Drinking Water Reservoir scenario characteristics have been incorporated into the dynamically linked PRZM-EXAMS and FIRST models, and are implemented in conjunction with the percent cropped area adjustment (Effland et al. 1999, available on-line at http://www.epa.gov/oscpmont/sap/meetings/1999/may/pca_sap.pdf). Although estimates of pesticide concentrations in drinking water based on a Midwestern "index drinking water reservoir" may not be wholly representative of residue levels in drinking water sources in other parts of the country, the scenario provides an effective screening tool to determine the need for more refined assessments. The modeling scenarios currently account for region-specific rainfall, soil, and hydrologic/runoff factors. Steps to develop additional scenarios to describe regional reservoirs for more advanced Tiers of modeling have been hampered by the lack of reservoir monitoring data outside of the Midwest that is of sufficient quality and extent to develop such scenarios.

### 9.3 Percent Crop Area (PCA) Adjustments

The PCA is a generic adjustment representing the maximum percent of any watershed that is planted to the crop or crops being modeled and, thus, may potentially be treated with the pesticide in question. PCA factors, generated from Geographic Information System (GIS) overlays of cropping area and watershed delineations, are applied directly to estimates of index reservoir surface water pesticide concentration values from the PRZM-EXAMS and FIRST models. The output concentration estimates generated by these models are multiplied by the maximum decimal fraction of cropped area in any watershed associated with the crop or crops of interest. To be effective as an adjustment to screening model estimates, the PCA should also result in estimated concentrations that are closer to, but not less than, actual observed pesticide concentrations in vulnerable (prone to pesticide-laden runoff) surface drinking water sources. While relaxing the assumption that the entire watershed would be treated at the same time with the pesticide under study, the use of the PCA concept is still regarded as a screening tool because it represents the highest percentage of crop cover of any large watershed in the U.S., and still assumes that the entire **crop** is being treated. Current PCA values and a description of how the values were derived and applied can be found at http://www.epa.gov/oppEFED1/models/water/regional_pca.htm.

### 10.0 Using EXPRESS: Data Preparation and Input Example

Chapter 10 is a worked Tier II example of preparing data and entering them into EXPRESS for Forchlorfenuron. Table 10-1 presents the Efate parameters for Forchlorfenuron and indicates the EXPRESS input generator screen where the values are entered. (An "MRID" (Master Record Identification) Number is a unique cataloging number assigned to an individual pesticide study at

the time of its submission to the Agency.)  (Input parameters based on OPP 2002-02-28 Input

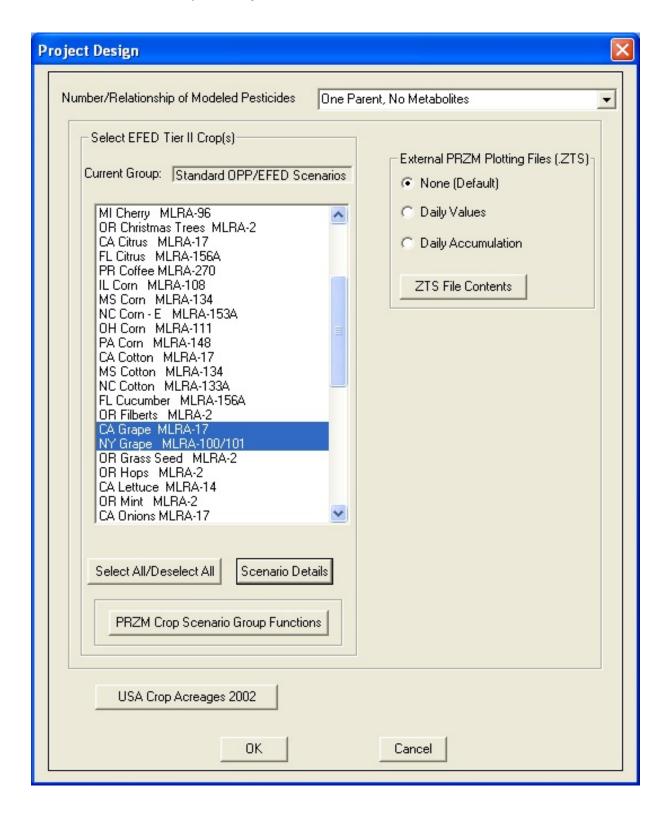Parameter Guidance (http://www.epa.gov/oppEFED1/models/water/input_guidance2_28_02.htm))

**Table 10-1**. **Surface Water Exposure Inputs for Forchlorfenuron**

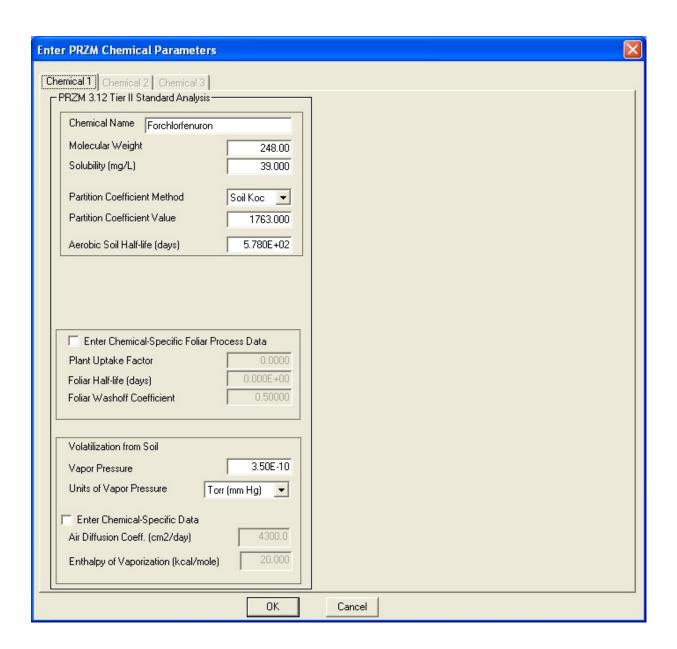| MODEL INPUT VARIABLE | INPUT VALUE | COMMENTS/EXPRESS SCREEN |
|---|---|---|
| Scenario Selection | CA Grape NY Grape | Source: Label; EXPRESS Screen: Project Design California grapes (raisin, wine, and fresh market) NY grapes (wine and fresh market) |
| Application Rate (kg/ha) CA Grape (irrig), MLRA 17 NY Grape, MLRA 100 | 0.025 0.025 | Source: Label EXPRESS Screen: Pesticide Application Data |
| Molecular Weight | 248 | g/mole EXPRESS Screen: PRZM-Efate |
| Vapor pressure | $3.5 \times 10^{-10}$ | Torr EXPRESS Screen: PRZM-Efate |
| Soil $K_{oc}$ (ml/g) | 1763 | Average Koc from 4 soils range of 852-3320. MRIDs 44359516, 45840121 EXPRESS Screen: PRZM-Efate |
| Aerobic Soil Metabolic Half-life (days) parent | 578 | Only aerobic soil metabolism study. Half-life not multiplied by 3 because very long. Based on extractable residues in MRIDs 44359515, 45840119. Half-life based on extractable+ bound was 1,659 days EXPRESS Screen: PRZM-Efate |
| Solubility (mg/L) | 39 | 9-7-00 EUP memo EXPRESS Screen: PRZM-Efate |
| Aquatic Sediment $K_{oc}$ (ml/g) | 3526 | Aquatic sediment Koc entered as 2X terrestrial soil $K_{oc}$ per Exams guidance (Burns 2000, p. 13) EXPRESS Screen: EXAMS-Efate |
| Aerobic Aquatic Metabolic Half-life (days) | 1156 | 2X aerobic soil metabolism half-life (578 days) EXPRESS Screen: EXAMS-Efate |

| MODEL INPUT VARIABLE | INPUT VALUE | COMMENTS/EXPRESS SCREEN |
|---|---|---|
| Anaerobic Aquatic Metabolism half-life (days) | 226 | Anaerobic soil metabolism half-life (MRIDs 44359514, 45840118)<br>EXPRESS Screen: EXAMS-Efate |
| Aquatic Photolysis Half-life (days) | 143 | MRID 44394605<br>EXPRESS Screen: EXAMS-Efate |
| Maximum No. of Applications All outdoor uses | 1 | Label, p. 4<br>EXPRESS Screen: Pesticide Application Data |
| Interval between appl. | N/A | For a single application |
| Application Date(s) | May 15<br>June 15 | All California Grapes<br>NY Grapes (Concord)<br>Based on 2003-12-9 Email from Bernie Schneider of HED to Jim Breithaupt of EFED<br>EXPRESS Screen: Pesticide Application Data |
| Method of application Ground (all uses) | Ground Sprayer | CAM 2 – application to foliage<br>EXPRESS Screen: Pesticide Application Data |
| Incorporation depth All outdoor uses | Default | Can be modified for broadcast applications.<br>EXPRESS Screen: Pesticide Application Data |
| Application Efficiency Ground Sprayer | 0.99 | Per 2000-11-7 Input Parameter Guidance<br>EXPRESS Fixed parameter<br>EXPRESS Screen: Pesticide Application Data |
| Spray Drift (Farm Pond) Ground Sprayer | 0.01 | Per 2000-11-7 Input Parameter Guidance<br>EXPRESS Fixed parameter<br>EXPRESS Screen: Pesticide Application Data |
| Spray Drift (Drinking Water) Ground Sprayer | 0.064 | Per 2000-11-7 Input Parameter Guidance<br>EXPRESS Fixed parameter<br>EXPRESS Screen: Pesticide Application Data |

EXPRESS Example Input Screens

1. EXPRESS Screen: Project Design

2: EXPRESS Screen: PRZM Efate



Enter PRZM Chemical Parameters

Chemical 1 | Chemical 2 | Chemical 3

PRZM 3.12 Tier II Standard Analysis

Chemical Name          Forchlorfenuron
Molecular Weight                    248.00
Solubility (mg/L)                    39.000

Partition Coefficient Method     Soil Koc
Partition Coefficient Value      1763.000

Aerobic Soil Half-life (days)    5.780E+02

☐ Enter Chemical-Specific Foliar Process Data
Plant Uptake Factor                 0.0000
Foliar Half-life (days)          0.000E+00
Foliar Washoff Coefficient         0.50000

Volatilization from Soil

Vapor Pressure                    3.50E-10
Units of Vapor Pressure       Torr (mm Hg)

☐ Enter Chemical-Specific Data
Air Diffusion Coeff. (cm2/day)      4300.0
Enthalpy of Vaporization (kcal/mole)  20.000

OK          Cancel

**EXAMS Efate Input: Transport and Transformation Parameters**

☑ Farm Pond (no flow)

☑ Index Reservoir (steady reservoir flow, m3/hr)

Chemical 1 | Chemical 2 | Chemical 3 | Pathways

Half-Lives (Whole-system "metabolism" must be manually corrected for interferences by hydrolysis etc. prior to entry.)

Water Column (Sediment-loaded study)

Aerobic "Metabolism" (days)　1.156E+03

Benthic Sediment (Sediment-loaded study)

Anaerobic "Metabolism" (days)　2.260E+02

Hydrolysis

Test Temperature (C)　25.0

Number of Different pH (3 or more)　3

| | Test pH | Half-life (days) |
|---|---|---|
| 1 | 5.00 | 0.000E+00 |
| 2 | 7.00 | 0.000E+00 |
| 3 | 9.00 | 0.000E+00 |

Aquatic Direct Photolysis (days)　1.430E+02

Partition Coefficient Method　Sediment Koc

Partition Coefficient Value　3526.000

OK　　Cancel

## 4: EXPRESS screen(s): Pesticide Application Data

## APPENDIX A: Format of Daily Value Meteorological Time-Series Files

| Field | Columns | Description | Units | Type | Format |
|-------|---------|-------------|-------|------|--------|
| 1 | 1 | blank | N/A | Character | 1x |
| 2 | 38389 | Date | mmddyy | Integer | 3i2 |
| 3 | 38580 | Precipitation | cm/day | Real | f10.2 |
| 4 | 18-27 | Pan Evaporation | cm/day | Real | f10.2 |
| 5 | 28-37 | Temperature (mean) | Degrees Centigrade | Real | f10.1 |
| 6 | 38-47 | Wind Speed @ 10 meter | cm/second | Real | f10.1 |
| 7 | 48-57 | Solar Radiation | Langleys/day | Real | f10.1 |
| 8 | 58-63 | FAO Short Grass $Et_0$ | mm/day | Real | f6.1 |
| 9 | 64-73 | Daylight Station Pressure | kiloPascal | Real | f10.1 |
| 10 | 74-77 | Daylight Relative Humidity | Percent | Integer | I4 |
| 11 | 78-80 | Daylight Opaque Sky Cover | Tenths of Sky Covered | Integer | I3 |
| 12 | 81-90 | Daylight Temperature | Degrees Centigrade | Real | f10.1 |
| 13 | 91-96 | Daylight Broadband Aerosol | Optical Depth | Real | f6.3 |
| 14 | 97-102 | Daylight Prevailing Wind Speed at 10 meter height | meter/second | Real | f6.1 |
| 15 | 103-106 | Daylight Prevailing Wind Direction | degrees (N=0, E=90, ...) | Integer | i4 |

Daily values file format:

(1x, 3i2, t8,f10.2, t18,f10.2, t28,f10.1, t38,f10.1, &

t48,f10.1, t58,f6.1, t64,f10.1, t74,i4, t78,i3, &

t81,f10.1, t91,f6.3, t97,f6.1, t103,i4)

Fields 03 - 08 represent daily totals or mean values (Wind Speed and Temperature)

Fields 03 - 07 units preserved from earlier PRZM met files for compatibility

Fields 09 - 15 represent mean values for daylight hours only.

## APPENDIX B: Added Capabilities of ORD Mode

In ORD mode, several additional capabilities are available to the analyst:

1. Terrestrial soil sorption parameters include the octanol-water partition coefficient, $K_{ow}$. For use in PRZM, the soil $K_{oc}$ is calculated as 0.175 $K_{ow}$ and applied to the soil organic carbon content in each soil horizon, as in the following code fragment:

```
do M=1,SSNHORIZ
  select case (KDTYP(J))
    case (1) ! entered soil Koc
      KD(J,M,Zone)=(KDSP(J)*SSOC(M))/100.0
    case (2) ! direct Kd
      KD(J,M,Zone)=KDSP(J)
    case (3) ! Kow (see p. 13 of EXAMS manual (EPA/600/R-00/081))
      KD(J,M,Zone)=(0.175*KDSP(J)*SSOC(M))/100.0
  end select
end do
```

2. The initial default parameters for foliar processes correspond to the ORD-recommended values (Suárez 2005: foliar washoff coefficient FEXTRC=0.10 (p 5.12), plant uptake factor UPTKF=1.0, representing passive movement in the transpiration stream (p. 5-22)). As in OPP mode, these can be altered at the user's discretion.

3. For aquatic chemistry, additional parameters are made available: $Q_{10}$ for aerobic and anaerobic aquatic "metabolism", the temperature of the experiments, and melting point of the chemicals.

4. For a more detailed view of spray drift, AgDrift program outputs tailored to the standard farm pond and index reservoir are displayed. These include several droplet size categorizations for aerial applications and ground sprayers, and orchard/vineyard airblast applications. The protective impact of spray buffers of various widths, separately for the farm pond and the index reservoir, can be evaluated in ORD mode.

5. Available versions of PRZM include 3.12.3, which also provides a mass balance analysis and display by EXPRESS.

## APPENDIX C: References

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