Air Toxics Modeling - Part I: TRIM

Air Toxic Risk Assessment Modeling Tools Symposium
July 15-17, 2003

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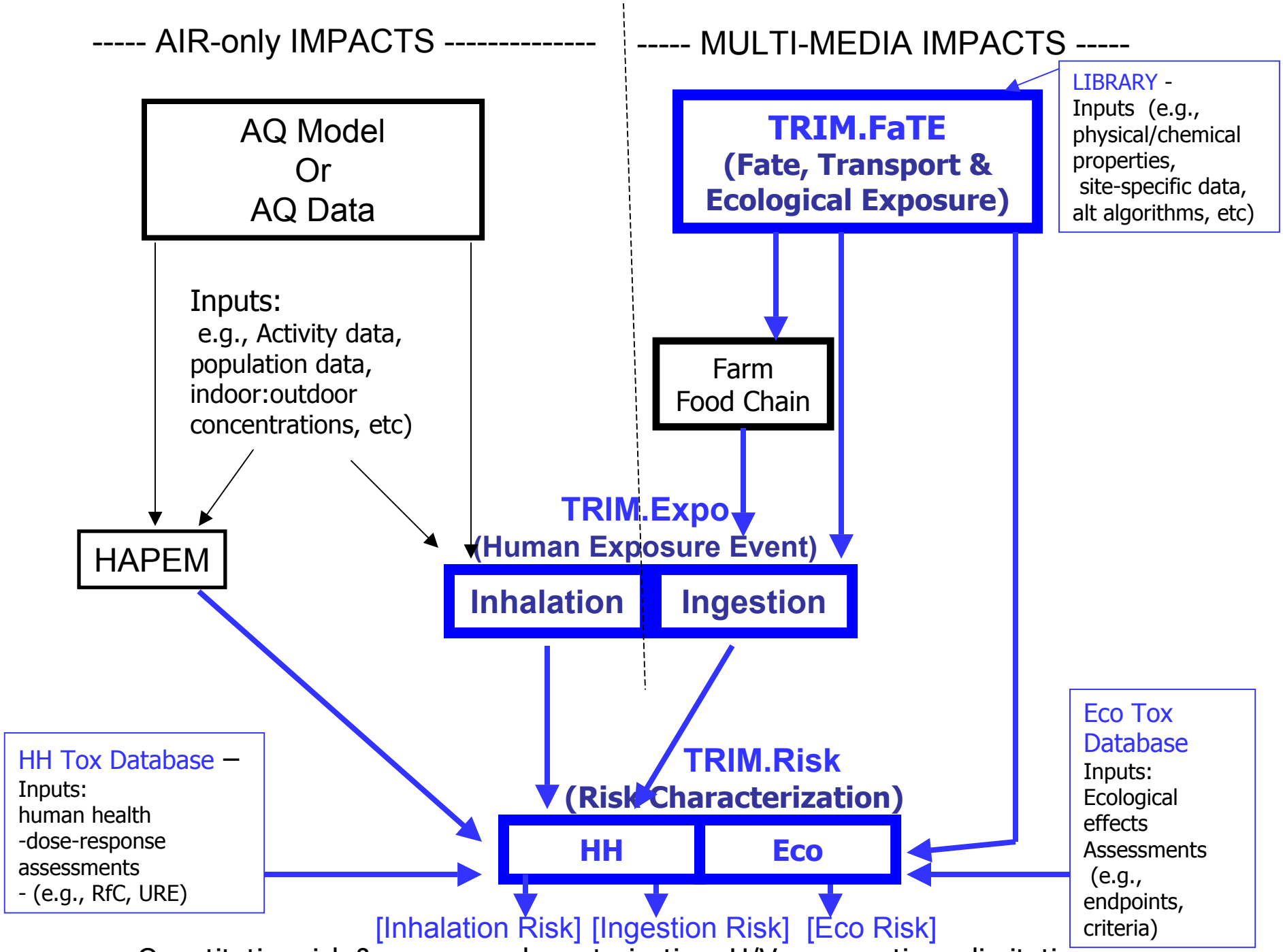
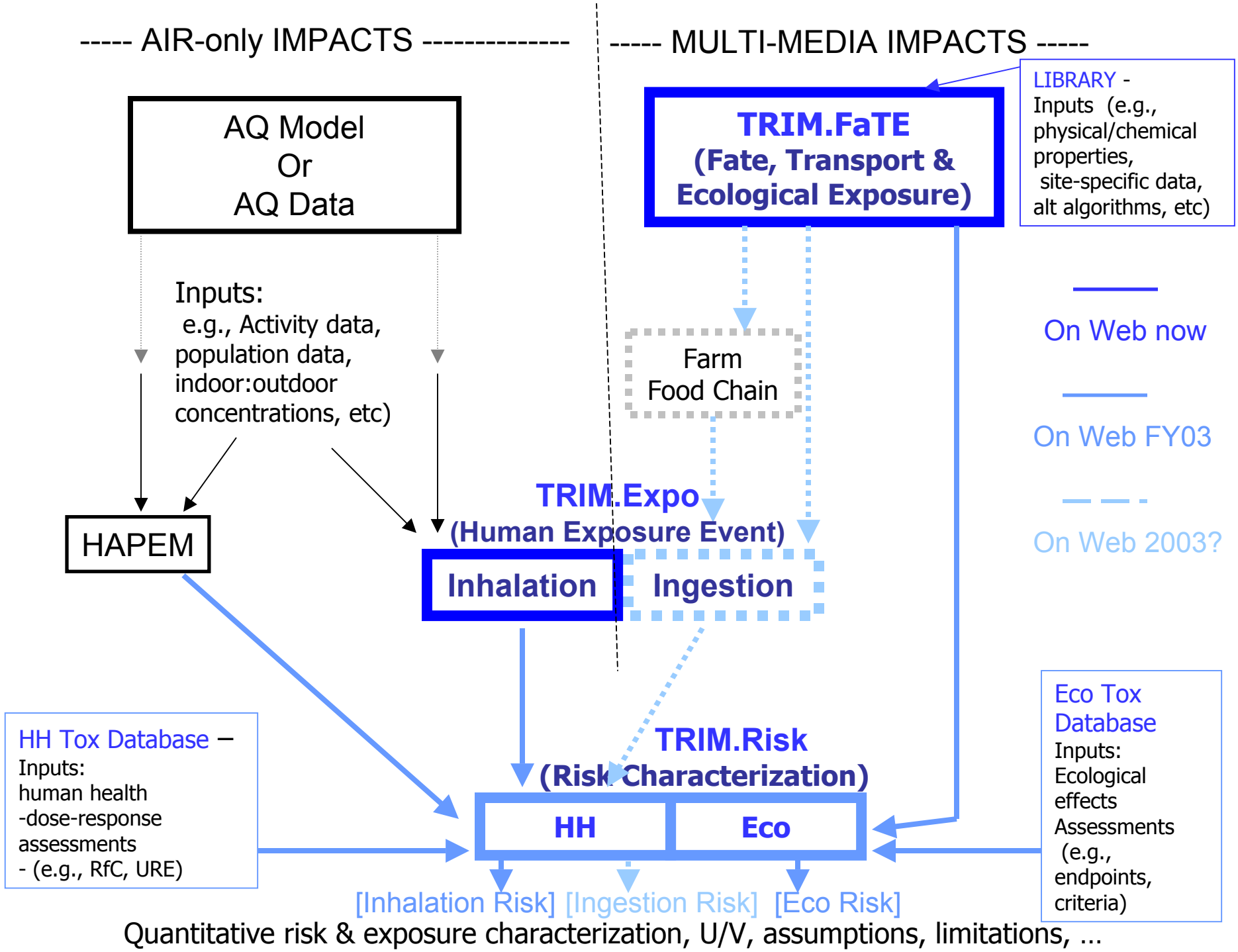
U.S. Environmental Protection Agency

TRIM (FaTE, Expo & Risk) for Air Toxics

1. HH Inhalation Exposure Assessment
   [AQ data + **TRIM.Expo aka APEX**]
2. Multimedia Pollutant Distribution Analysis
   [TRIM.FaTE]

3. HH Inhalation Risk Assessment
   [AQ data + **TRIM.Expo** + TRIM.Risk]
4. Ecological [multimedia] Risk Assessment
   [**TRIM.FaTE** + TRIM.Risk]
5. HH Ingestion Risk Assessment
   [**TRIM.FaTE** +/- FFC + TRIM.Expo + TRIM.Risk]


----- AIR-only IMPACTS ----------
----- MULTI-MEDIA IMPACTS -----
AQ Model
Or
AQ Data
TRIM.FaTE
(Fate, Transport &
Ecological Exposure)
LIBRARY -
Inputs (e.g.,
physical/chemical
properties,
site-specific data,
alt algorithms, etc)
Inputs:
e.g., Activity data,
population data,
indoor:outdoor
concentrations, etc)
Farm
Food Chain
TRIM.Expo
(Human Exposure Event)
HAPEM
Inhalation
Ingestion
HH Tox Database –
Inputs:
human health
-dose-response
assessments
- (e.g., RfC, URE)
TRIM.Risk
(Risk Characterization)
HH
Eco
Eco Tox
Database
Inputs:
Ecological
effects
Assessments
(e.g.,
endpoints,
criteria)
[Inhalation Risk] [Ingestion Risk] [Eco Risk]
Quantitative risk & exposure characterization, U/V, assumptions, limitations, ...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On Web now
On Web FY03
On Web 2003?
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www.epa.gov/ttn/fera

U.S. Environmental Protection Agency

Technology Transfer Network
FERA (Fate, Exposure, and Risk Analysis)

EPA Home > Air & Radiation > TTNWeb - Technology Transfer Network > FERA (Fate, Exposure, and Risk Analysis)

Total Risk Integrated Methodology (TRIM)

- General Information
- TRIM.FaTE
- TRIM.Expo
- TRIM.Risk
- Peer Review and Publications

Multimedia Fate & Transport Modeling

- General
- TRIM.FaTE
- Links to Other Models & Related Information

Human Exposure Modeling

- General
- Databases to Support Exposure Modeling
- Air Pollutants Exposure Model (APEX/ TRIM.Expo Inhalation)
- Hazardous Air Pollutant Exposure Model (HAPEM)
- Human Exposure Model (HEM)
- Links to Other Models & Exposure-Related Information

Risk

- General Agency Information/Policy/Guidance
- Air Toxics Risk Assessment
- Criteria Air Pollutant Risk Assessment
- Links to Other Risk Related Information/Guidelines

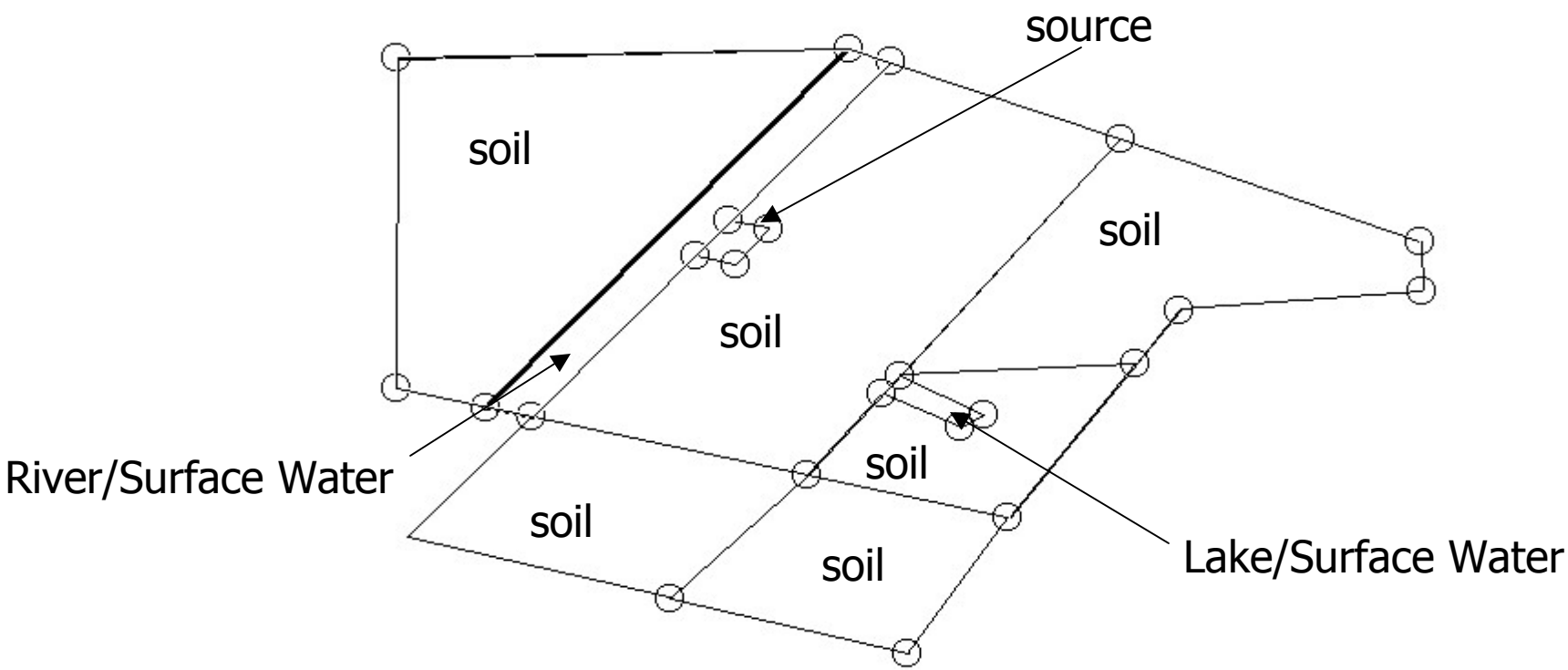
Fate, Exposure & Risk Models Download

TRIM.FaTE - Concepts

TRIM.FaTE Modeling System

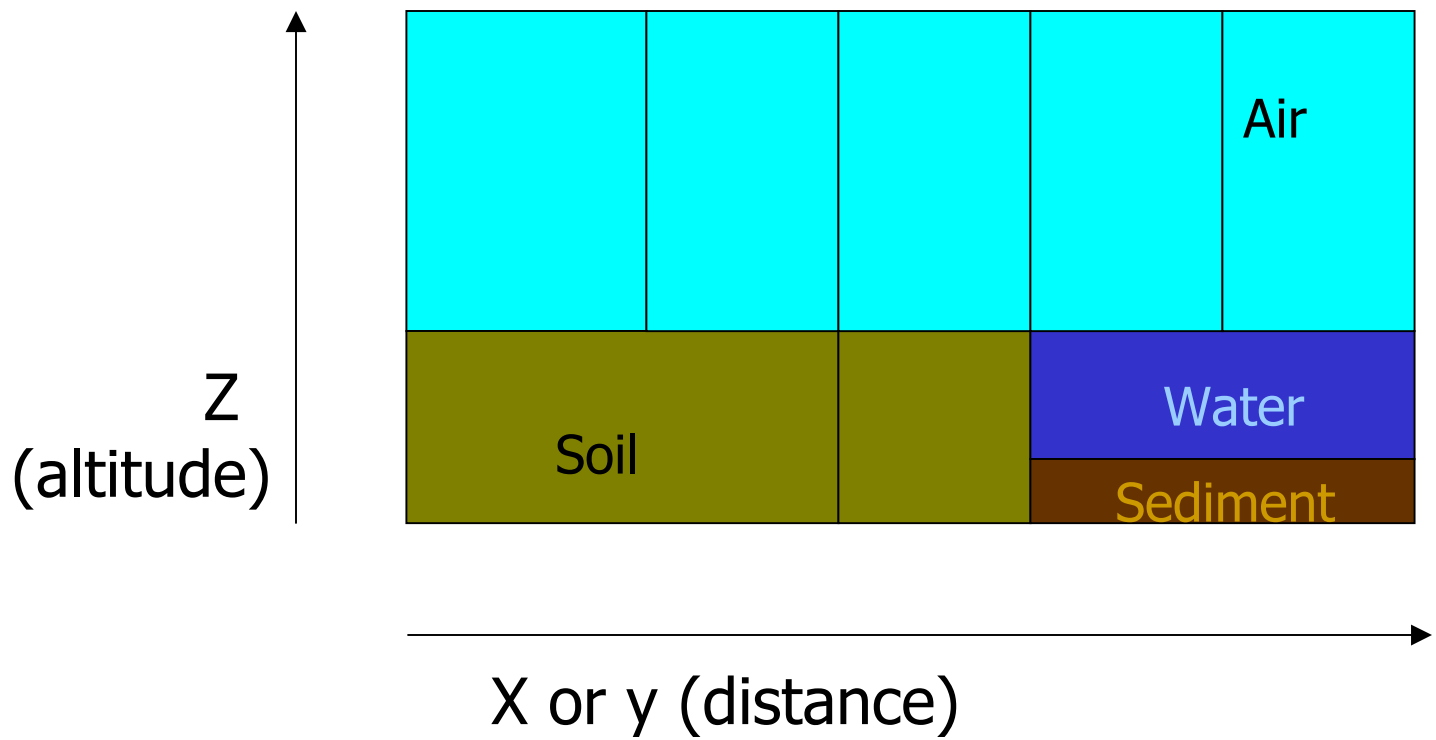
- Parcels, Volume Elements & Compartments
  - Parcels - planar geographical areas used to subdivide the modeling region.
  - Volume elements - bounded 3-dimensional spaces that define the location of $\geq$ 1 compartment.
  - Compartments – Units of environmental media/biota within which it is assumed that chemical is homogeneously distributed.

Parcels (2D)
– Soil & Surface Water Examples

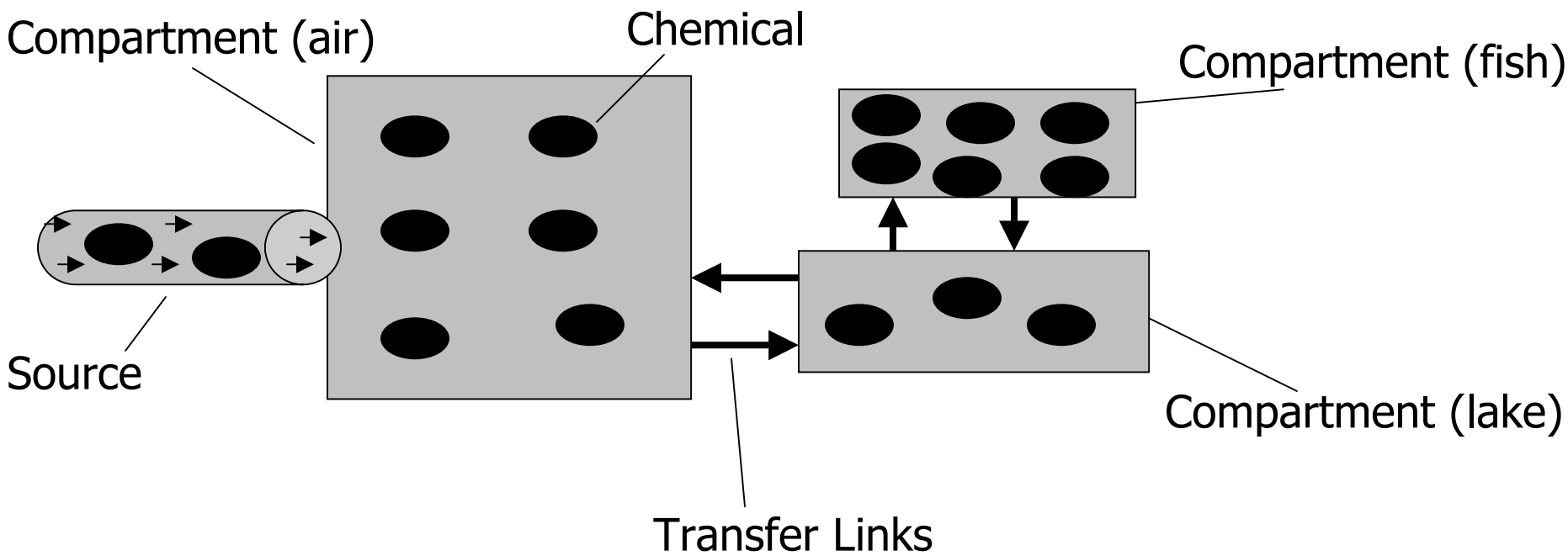


Volume Elements (3D) – air, soil, water, sediment

Simple example



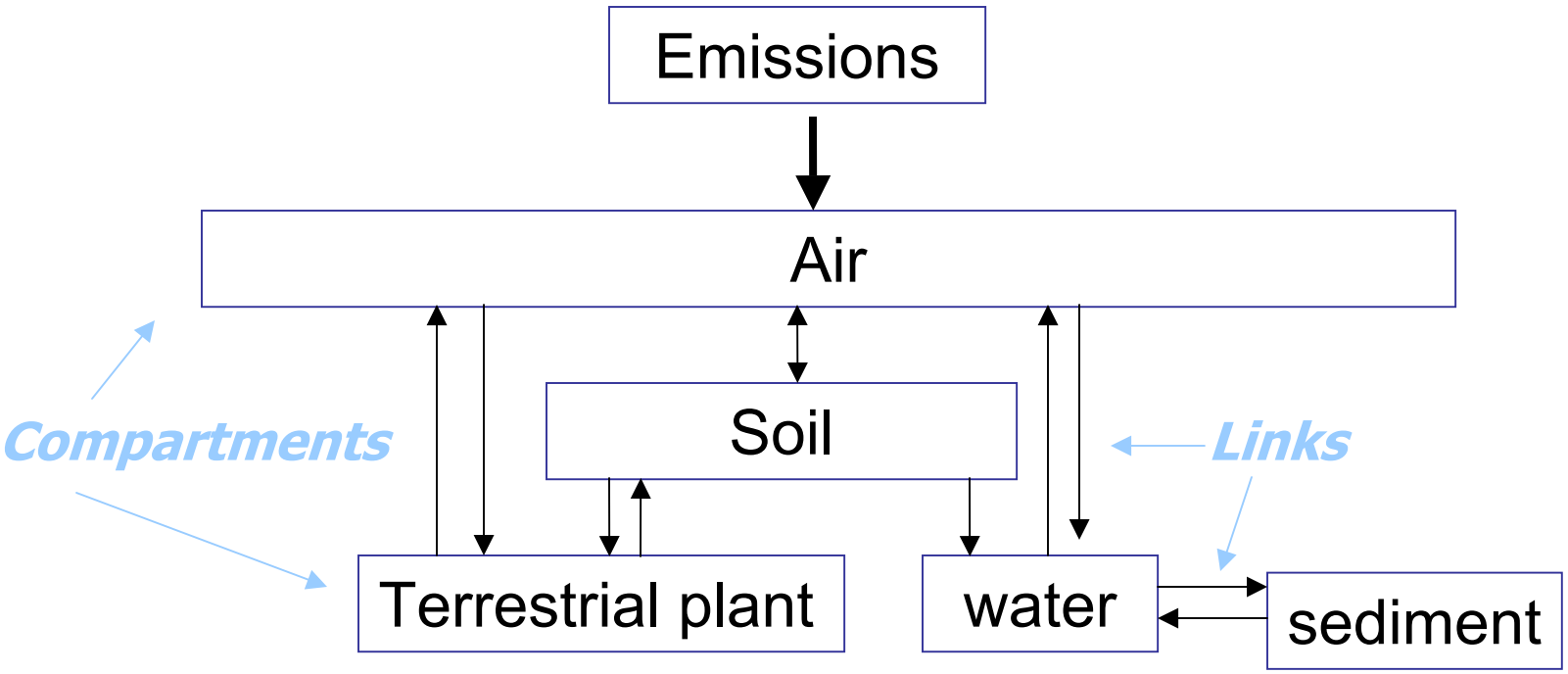
TRIM.FaTE
- Compartments, Links, Chemical, Source



Transfer factors (algorithms) describe pollutant movement via links.

Fully Coupled, Mass Balance Model - Simple Abiotic w. Plants Example

2-way transfer of mass among all linked compartments at each time step



TRIM.FaTE
Performing a Simulation

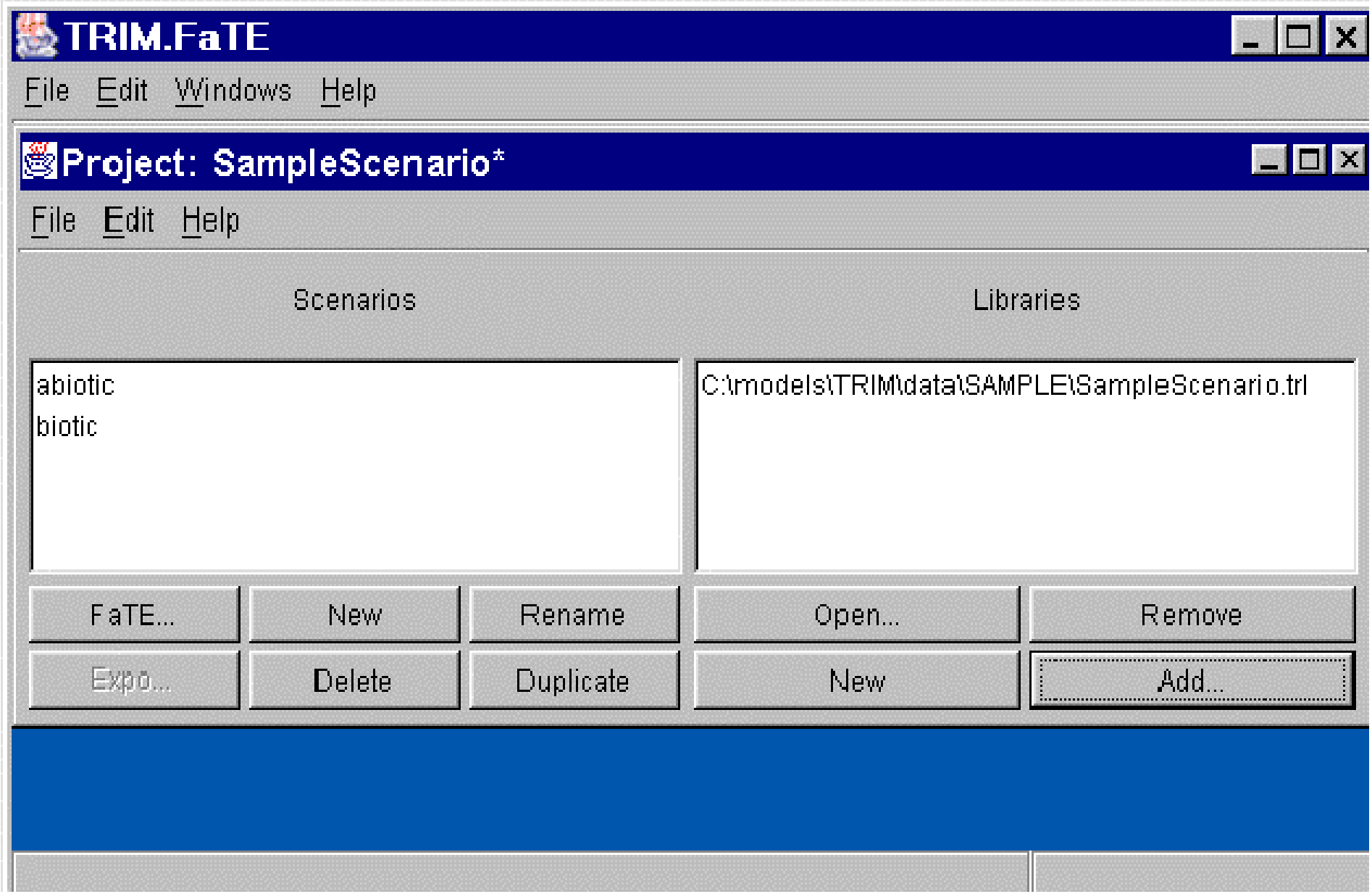
TRIM.FaTE - Computer Framework

- Provides GUI for TRIM.FaTE model
- Defines characteristics of the simulation
  - Time period, geographic region, pollutants, media, biota, emission sources, algorithms to use
- Sets model parameter values (e.g. meteorology, soil characteristics, diets of biota)
- Executes model
- Performs sensitivity and uncertainty analyses
- Analyzes and exports results

TRIM.FaTE
- Computer Framework Concepts

- Project:
  - **Contains Libraries and Scenarios**
- Library:
  - **Contains building blocks to use in model runs (Scenarios)**
- Scenario:
  - **Contains all information needed to do a model run (e.g. time period & details of environmental system to simulate)**
- Libraries and Projects can be saved as files

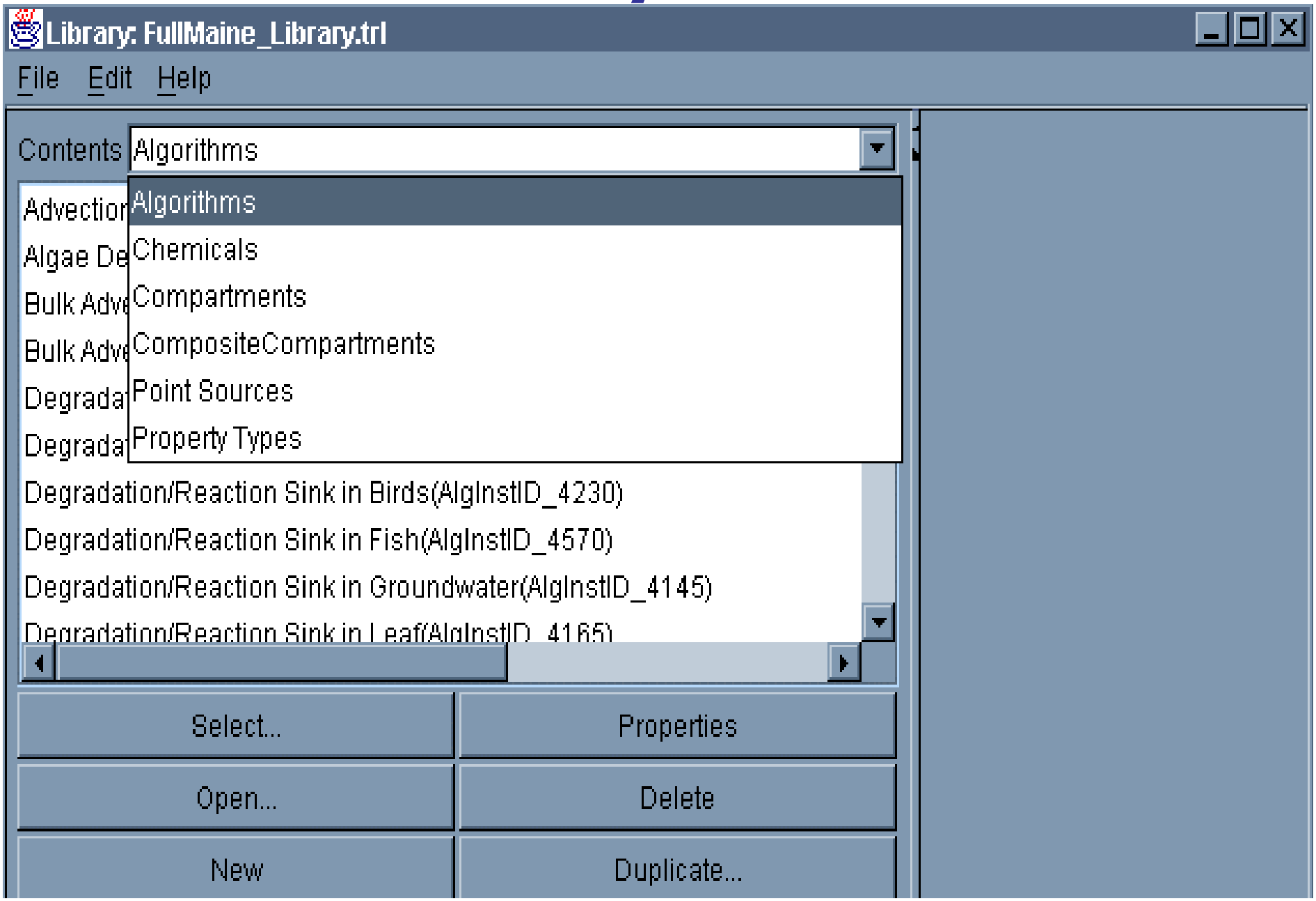
TRIM.FaTE **Project** Window



Library

- Contains information (values, formulas) for Sources, Chemicals, Compartments, and Algorithms
- Is the starting point for a TRIM.FaTE scenario, in which parameter (property) values may be customized

TRIM.FaTE **Library** Window



Scenario

- Combines information from the Library with site-specific & simulation-specific information to create a simulation
- Is what user runs when performing a TRIM.FaTE simulation
- Exists within a Project

TRIM.FaTE **Scenario** Window

FaTE Scenario: SwettsPond-1

File Edit Add Run View Help

Scenario | Sources | Chemicals | Compartments | Links | Algorithms | Analyses

Project: SwettsPond-1.trp

Description:

```
Small Swetts Pond Scenario.
- includes 1 soil and 1 surface water
parcel, plus one 1 air parcel.
```

Store Description Changes

Derived From:

Properties

New | Del | Ref | PType | Form | Show | All | Undo | Redo

#	Property Name	Value	Units	Data
1	AirTemperature_K	D:\Models\TRIM...	K	Real Numb...
2	averageResultsFiles	false		True or Fal...
3	averagingInterval	<Unset>		Text
4	dynSimAbsoluteTolerance	1.0E-12	N/A	Real Numb...
5	dynSimMaxSolverIterations	30000	N/A	Integer
6	dynSimRelativeTolerance	1.0E-10	N/A	Real Numb...
7	elasticityThreshold	0.01	N/A	Real Numb...
8	enableBoundaryContribu...	true		True or Fal...
9	evaluateHTMLProperties...	<Unset>		Date and Ti...
10	exportConcentration	true		True or Fal...
11	exportHTML	false		True or Fal...
12	exportMass	true		True or Fal...

TRIM.FaTE **Scenario** Window

FaTE Scenario: SwettsPond-1

File Edit Add Run View Help

Scenario | Sources | Chemicals | Compartments | Links | Algorithms | Analyses

Outdoor Environment

Links

- Air_SSE3
  - Air in Air_SSE3
    - from / to sel
    - from Surfac
    - from Soil - S
    - from Leaf -
    - from Leaf P
    - to Mallard ir
    - to Commor
    - to Sink in Si
    - to Sink in Si
    - to Sink in Si
    - to Sink in Si
    - to Surface v
    - to Soil - Sur
    - to Leaf - Co
    - to Leaf Part

Select... | Properties | Open... | Show Algs | Delete | Refresh

Algorithms in Links

- Diffusion from Plant Leaf to Air, Hg0, D
- Diffusion from Plant Leaf to Air, MHg, D

Select... | Properties | Open... | Add... | Delete | Add To Lib

Properties for 1 Algorithm Diffusion from Plant Leaf to Air, Hg0, Defau...

New | Del | Ref | PType | Form | Show | All | Undo | Redo

#	Property Name	Chemical	Value
2	chemicalCategory		<Unset>
3	doesTransformChemical		false
4	doesTransportChemical		true
5	enabled		true
6	isDefaultForCategory		true
7	mate		<Unset>
8	receivingChemicalName		Elemental Merc...
9	receivingCompartmentC...		Abiotic | Air | Air ...
10	sendingChemicalName		Elemental Merc...
11	sendingCompartmentCa...		Plant | Leaf
12	transferFactor		<Formula>

Store | Help

```
SendingCompartment.AllowExchange *
(sendinglinkedCompartment[Abiotic | Soil].Area )*
(2*SendingCompartment.LeafAreaIndex *
SendingCompartment.Chemical.TotalCuticularConductan
ce  +
SendingCompartment.Chemical.TotalStomatalConductanc
e) *
(SendingChemical.Z_pureair/SendingCompartment.Chemi
```

Steps to set-up a Simulation

- Add Library to Project
- Set up Scenario spatial layout

(using Volume Element data file)

- Add Sources
- Add Chemicals
- Add Compartments to Volume Elements
  - Customize Property values for site

Steps to set-up a Simulation (continued)

- Link compartments as appropriate
- Implement algorithms on links
- Set any link properties (e.g., runoff/erosion)
- Set scenario properties
  - E.g., simulation and output time steps & simulation options.
- Set all information required by algorithms.
  - Framework identifies missing properties.
  - User can set properties for multiple objects at once.

Verify & Run

FaTE Scenario: SwettsPond-1

File Edit Add Run View Help

Scenario | Sourc

Project: SwettsPo

Description:

Small Swetts
- includes 1
parcel, plus

Store Description Changes

Derived From:

- Verify Scenario
- Run Scenario
- Initialize from previous run
- Sequential Runs
- Sensitivity Analysis
- Monte Carlo Analysis

Links | Algorithms | Analyses

Properties

New | Del | Ref | PType | Form | Show | All | Undo | Redo

#	Property Name	Value	Units	
1	AirTemperature_K	D:\Models\TRIM...	K	R
2	averageResultsFiles	false		Tr
3	averagingInterval	<Unset>		Te
4	dynSimAbsoluteTolerance	1.0E-12	N/A	R
5	dynSimMaxSolverIterations	30000	N/A	In
6	dynSimRelativeTolerance	1.0E-10	N/A	R
7	elasticityThreshold	0.01	N/A	R
8	enableBoundaryContribu...	true		Tr
9	evaluateHTMLProperties...	<Unset>		D
10	exportConcentration	true		Tr
11	exportHTML	false		Tr
12	exportMass	true		Tr

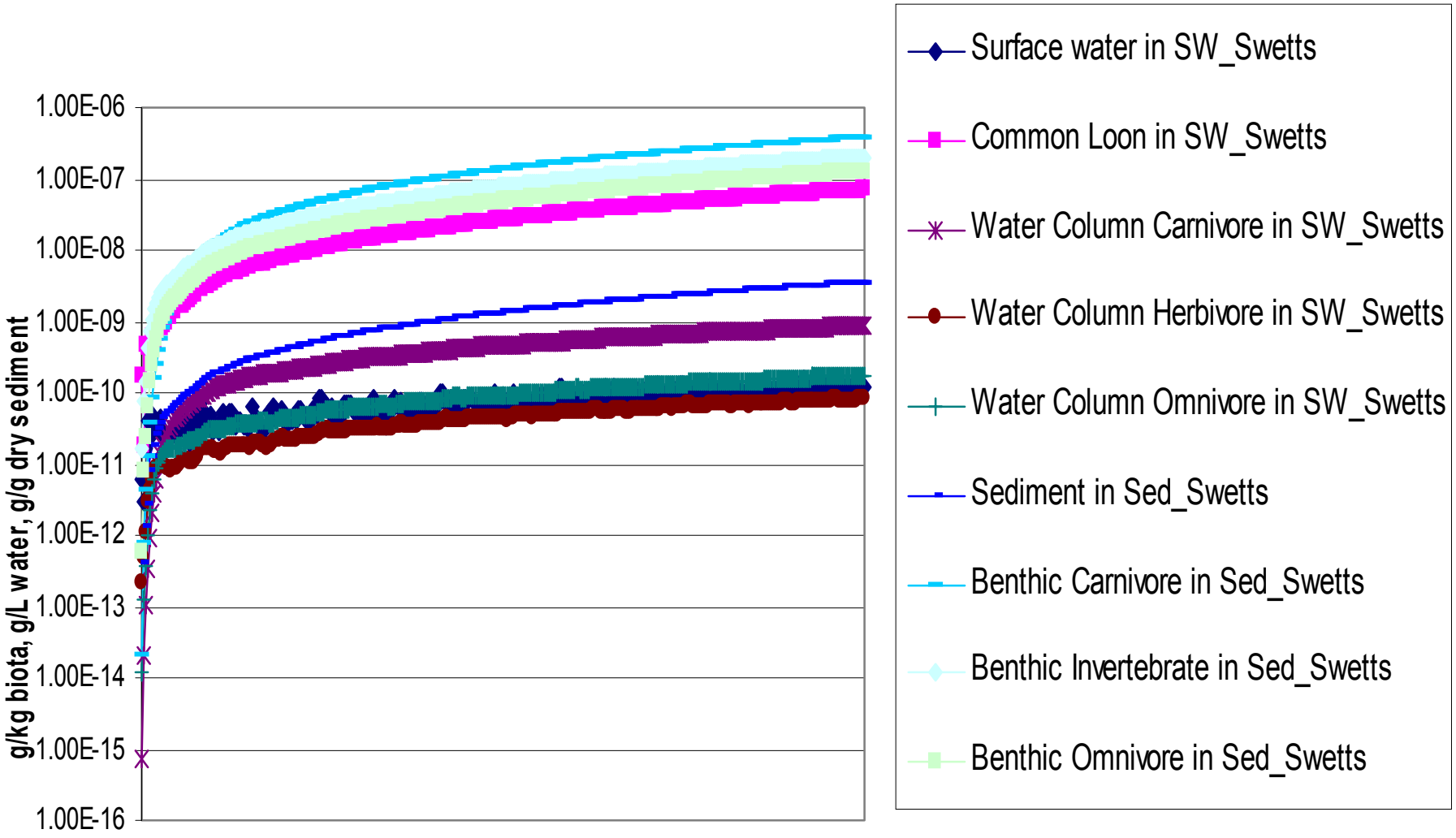
TRIM.FaTE Results

- Moles, Mass, Concentration
  - Instantaneous values
    - at specified frequency during simulation period
  - Averaged values
    - Over specified time periods (e.g., monthly etc)

TRIM.FaTE Results Files

- Output to text files
  - Can be viewed in TRIM.FaTE
    - Table format
    - Chart format
  - Can be imported to many programs for analysis
    - E.g., Excell
- Output to HTML files
  - Can easily confirm all aspects of scenario (compartment property values, active algorithms, links, etc)
- Output to MySQL database
  - Can be queried and analyzed

30 year Simulation with Source (Hg^0 & Hg^{+2}) - Results for total ($MeHg+Hg^0+Hg^{+2}$) as Hg



TRIM.FaTE Helpful Features – for Set-up

- Volume Elements & Parcels
  - Coordinates imported from text file; model flags overlaps
- Compartments
  - Abiotic compartments added automatically w. VEs
  - Sink compartments added automatically at open faces
- Links
  - created automatically with Smart Link
- Algorithms
  - added automatically with links
  - user can enable/disable

TRIM.FaTE Helpful Features –Time-varying Input Values

- Parameter values can be constant or time-varying, e.g.,
  - Meteorological data (e.g., wind speed, temperature, precipitation)
  - Surface water flow values

NOTE: Frequency of time-varying data dictates frequency of some model calculations

- Run time impact

TRIM.FaTE Helpful Features - Importers & Exporters

- Importers - bring information into TRIM.FaTE.
  - Many types of objects (Links, Compartments, etc) can be imported from text files.
  - New types of importers can be easily created.
- Exporters – produce output files
  - ASCII formatted table suitable for import into spreadsheet (Excel)
  - Web pages (HTML Format)
  - New types of exporters can be easily added

TRIM.FaTE Helpful Features - Uncertainty/Variability

- Sensitivity feature
  - Series of runs, each w. variation in value of different parameter
    - Outputs raw and processed results

    (e.g., elasticity/sensitivity scores, etc.)
- Monte Carlo sampling feature
  - Series of runs for which values for selected parameters are drawn from specified distributions

TRIM.FaTE Helpful Features - Steady State Solution

- Short(!) run time
- Useful to test approaches for
  - modeling area design (parcels, volume elements) and
  - biological system (biotic compartments and their characteristics)
- Allows complex sensitivity or Monte Carlo analyses in reasonable run times

TRIM.FaTE Team – current members

- **USEPA's Office of Air Quality Planning & Standards**
  - **Deirdre Murphy, John Langstaff**
- Lawrence Berkeley National Laboratory
  - Tom McKone, Randy Maddalena
- Oak Ridge National Laboratory
  - Rebecca Efroymson, Dan Jones
- University of Tennessee
  - Brad Lyon
- ICF Consulting
  - Baxter Jones, Mark Lee, David Burch, Margaret McVey
- MCNC-Environmental Modeling Center
  - Alison Eyth

TRIM Contacts ...

- USEPA's Office of Air Quality Planning & Standards
  - TRIM.FaTE (and TRIM coordination)
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  - TRIM.Expo-inhalation
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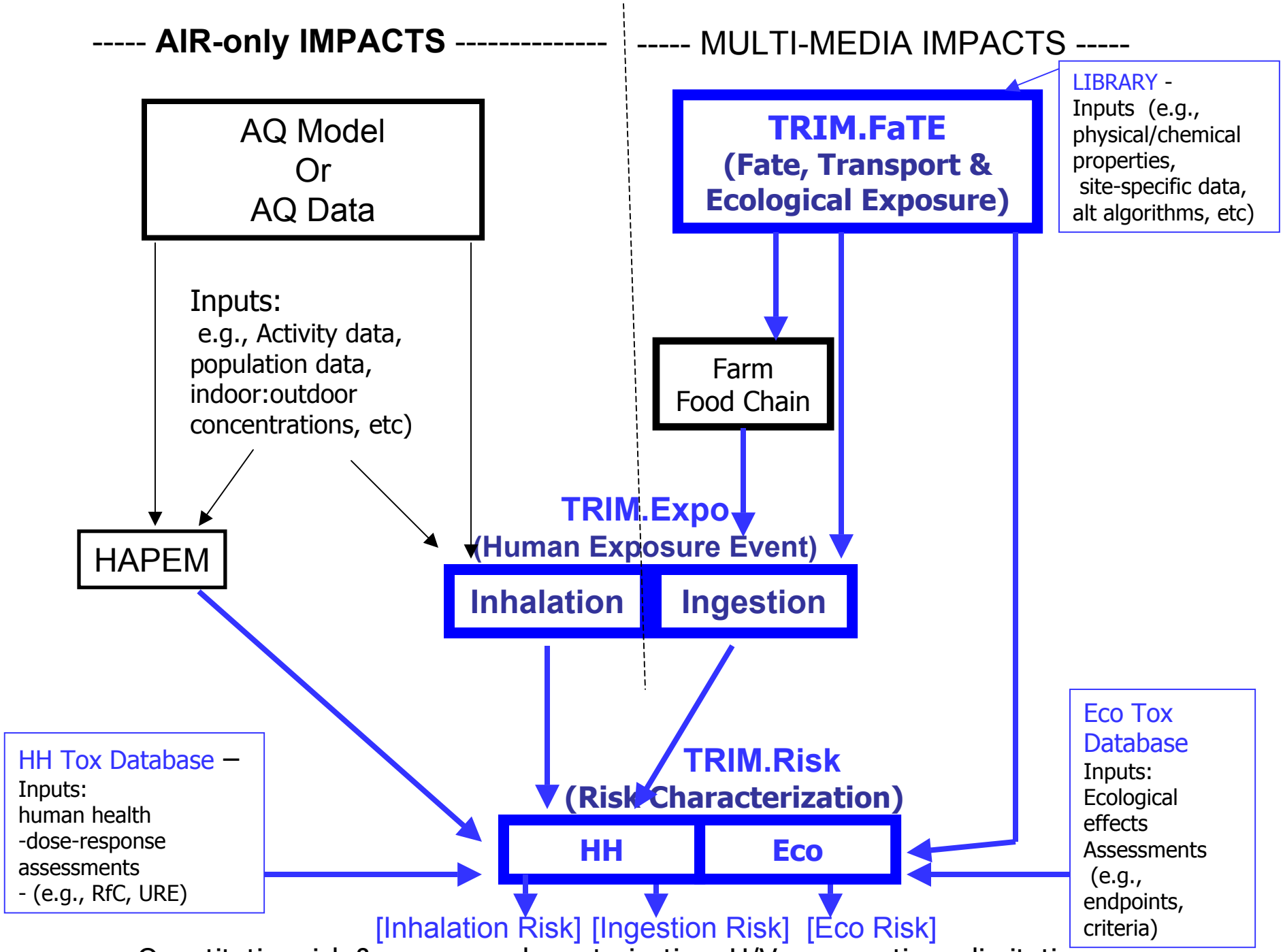
    - Richmond.harvey@epa.gov
    - Langstaff.john@epa.gov
  - TRIM.Expo-ingestion
    - Vasu.amy@epa.gov
  - TRIM.Risk
    - Hollingsworth.terri@epa.gov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Quantitative risk & exposure characterization, U/V, assumptions, limitations, ...

----- AIR-only IMPACTS -----
Current Approaches for HH Exposure Assessment

ISC or Monitoring data
->air concentrations at specific points

HEM
-ISC w. Census data
→air concentration at CB centroid

HAPEM
-ISC w. Census & Activity & Commuting data & annual outputs
→Inhalation exposure concentrations for pop subgroups of interest
[averaging type limitations]

TRIM.Expo (aka APEX)
-ISC/mon w. Census & Activity & Commuting & small time steps & stochastic sampling
-> Inhalation exposure concentrations for pop/individuals of interest, w. distributional info

Both **HAPEM & TRIM.Expo** will **feed TRIM.Risk** to derive inhalation risk estimates

APEX / TRIM.Expo$_{inhalation}$ is being developed to:

- Provide an exposure modeling tool for assessing air pollutants as part of EPA's overall Total Risk Integrated Methodology (TRIM) model framework.
  - TRIM.Expo (inhalation) MIMS (Graphical Users Interface) version
  - Stand alone DOS/Fortran version
  - Available at: http://www.epa.gov/ttn/fera/apex_download.html

- The model is initially intended to:
  - Address inhalation exposures;
  - Be suitable for local, urban, or consolidated metropolitan area scale analyses;
  - Accept as input air quality data based on either monitored or modeled data;
  - Be able to estimate acute or chronic exposures
  - Meet the needs of both the hazardous & criteria air pollutant programs.

A Office of Air Quality Planning & Standards - FERA - Human Exposure Modeling - Air Pollutant - Microsoft Internet Explorer

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http://www.epa.gov/ttn/fera/human_apex.html

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Home

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Human Exposure Modeling - Air Pollutants Exposure Model (APEX/ TRIM.Expo Inhalation)

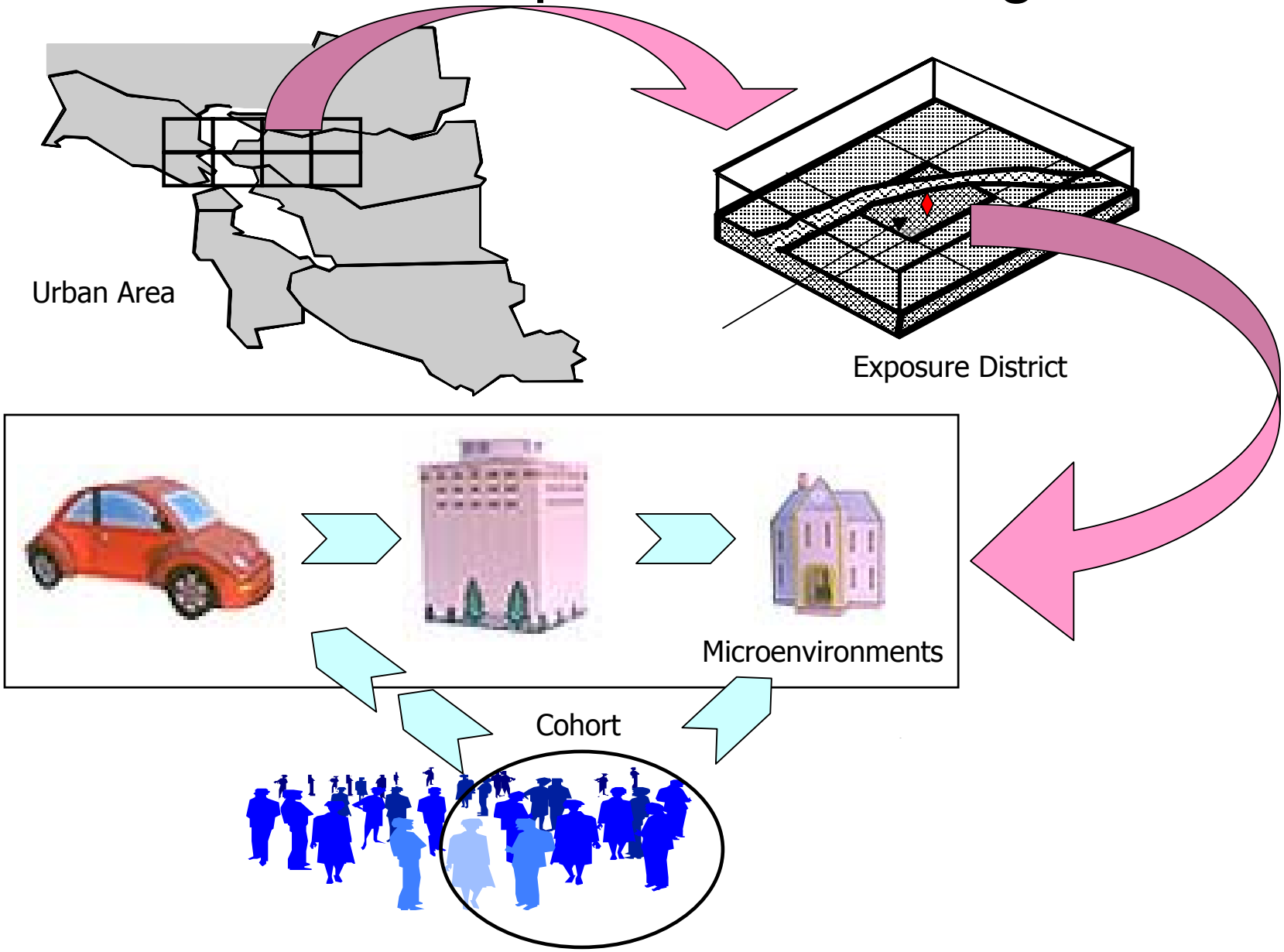
- **General Information.** The Air Pollutants Exposure Model (APEX) is a PC-based model that was derived from the probabilistic NAAQS Exposure Model for carbon monoxide (pNEM/CO). A draft report describing pNEM/CO is available. Reports describing prior OAQPS applications of the pNEM to ozone also are available. APEX serves as the human inhalation exposure model within the Total Risk Integrated Methodology (TRIM) model framework. See TRIM - General Information page for historical information about TRIM and peer review of the TRIM and TRIM.Expo approach. APEX is intended to be applied at the local, urban, or consolidated metropolitan area scale and currently only addresses inhalation exposures. The model simulates the movement of individuals through time and space and their exposure to the given pollutant in various microenvironments (e.g., outdoors, indoors residence, in-vehicle). The user may choose the number and types of microenvironments to be included, select the time period of interest, use either monitored ambient air quality data or values provided from dispersion or other modeling runs, and use either a mass balance approach or an empirical ratio-based (factor) approach to estimate indoor and/or in-vehicle concentrations. OAQPS is releasing the current version of APEX (version 3.2.3) as a beta version to the broader exposure modeling community. We recognize that there are areas where the model may be refined to be more useful and more user-friendly. However, the model provides a useful and informative tool for inhalation exposure modeling. We look forward to feedback from the larger modeling community on model performance and evaluation to help guide further model refinement.

- Download Model

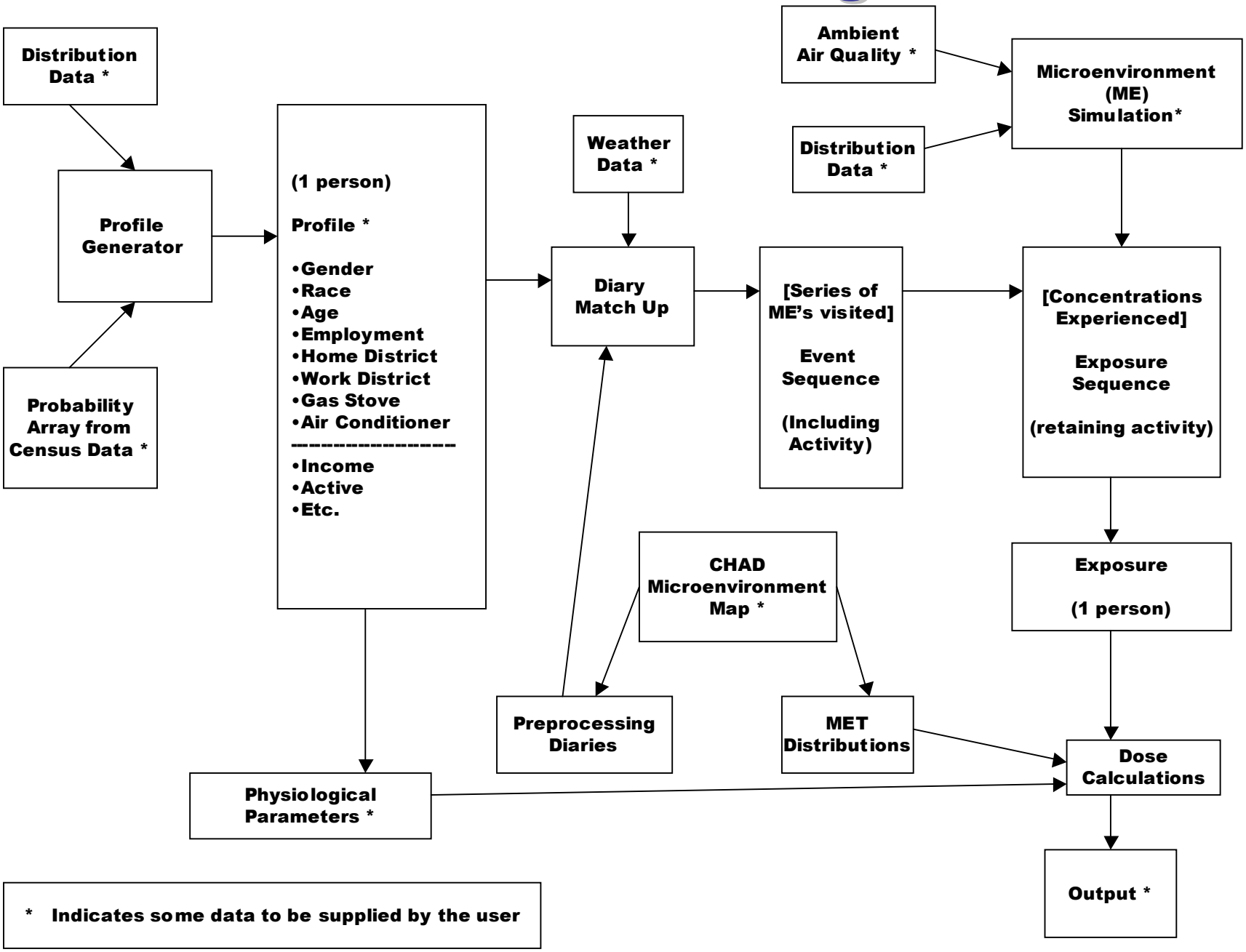
- **User's and Programmer's Manual.** Those planning to use APEX are strongly encouraged to carefully review Volume I, User's Guide. It describes the scientific basis for the APEX model and describes the steps involved in running APEX for both basic and more advance applications. Volume II, Programmer's Guide (available soon) describes the model and computer code in more

Internet

Inhalation Exposure Modeling



APEX 3.2 Flow Diagram



Inputs to APEX 3.0

The parameters file specifies:

- the input and output file names
- various parameter settings for the model run (e.g., simulation start and end dates, numbers of profiles to be run, number of seasons, number of microenvironments, number of districts, altitude, random seed, etc.)

Input data files:

- Air quality: hourly air quality data for all districts
- Temperature: daily 1-hour maxima for each temperature zone in study area
- METS: MET (metabolic activity) distributions from Consolidated Human Activity Data Base (CHAD)
- Physiology: body mass, VO2 max, etc. for each age and gender
- Population: counts by age, gender, race and sector (from census data)
- Distributions: user-defined distributions
- Microenvironments: properties for each microenvironment in the model
- Diary events: the event sequence for all persons in CHAD
- Diary summary: the personal data for all persons in CHAD
- Diary mapping: the location code to microenvironment mapping

P322_Benzene_oth3sources.txt - Notepad

File Edit Format View Help

```
INPUT FILES:
  sectors file      = C:\APEX_CASE_STUDY\Input\population\tp_geo_houston.txt
  districts file    = C:\APEX_CASE_STUDY\input\AirQuality\districts_houston61.txt
  zones file        = C:\APEX_CASE_STUDY\input\temperature\zones_houston.txt
  agegroups file    = C:\APEX_CASE_STUDY\input\employment\tp_minmax.txt
  commuting file    = C:\APEX_CASE_STUDY\input\commute\comm2000_houston.txt
  temperature file  = C:\APEX_CASE_STUDY\input\temperature\temperatures_houston.txt
  air quality file  = C:\APEX_CASE_STUDY\input\AirQuality\benzene_oth3sources\Apexhoustonair61_oth.txt
  metabolic file    = C:\APEX_CASE_STUDY\input\CHAD\CHADMets.txt
  physiology file   = C:\APEX_CASE_STUDY\input\physiology\Physiology.txt
  distribution file = C:\APEX_CASE_STUDY\input\Profile_Functions\Distrib_houston.txt
  microenv. file    = C:\APEX_CASE_STUDY\input\Microenviron\factors\benzene_oth3sources\MP_houston_oth.txt
  diaryevent file   = C:\APEX_CASE_STUDY\input\CHAD\CHADEvents.txt
  diarysum file     = C:\APEX_CASE_STUDY\input\CHAD\CHADQuest.txt
  diarymap file     = C:\APEX_CASE_STUDY\input\Microenviron\mapping\micromap34.txt

POPULATION FILES:
  pop file, Female, White = C:\APEX_CASE_STUDY\input\population\tp_FW_houston.txt
  pop file, Female, Black = C:\APEX_CASE_STUDY\input\population\tp_FB_houston.txt
  pop file, Female, Asian = C:\APEX_CASE_STUDY\input\population\tp_FA_houston.txt
  pop file, Female, NatAm = C:\APEX_CASE_STUDY\input\population\tp_FN_houston.txt
  pop file, Female, Other = C:\APEX_CASE_STUDY\input\population\tp_FO_houston.txt
  pop file, Male,   White = C:\APEX_CASE_STUDY\input\population\tp_MW_houston.txt
  pop file, Male,   Black = C:\APEX_CASE_STUDY\input\population\tp_MB_houston.txt
  pop file, Male,   Asian = C:\APEX_CASE_STUDY\input\population\tp_MA_houston.txt
  pop file, Male,   NatAm = C:\APEX_CASE_STUDY\input\population\tp_MN_houston.txt
  pop file, Male,   Other = C:\APEX_CASE_STUDY\input\population\tp_MO_houston.txt

OUTPUT FILES:
  log file          = C:\APEX_CASE_STUDY\output\benzene_oth3sources\log.txt
  exposure file     = C:\APEX_CASE_STUDY\output\benzene_oth3sources\exp.txt
  dose file         = C:\APEX_CASE_STUDY\output\benzene_oth3sources\dose.txt
  persons file      = C:\APEX_CASE_STUDY\output\benzene_oth3sources\psum.txt
  microsum file     = C:\APEX_CASE_STUDY\output\benzene_oth3sources\msum.txt
  tables file       = C:\APEX_CASE_STUDY\output\benzene_oth3sources\tables.txt
  site file         = C:\APEX_CASE_STUDY\output\benzene_oth3sources\sites.txt

PARAMETER SETTINGS:
  pollutant   = Benzene
  InputUnits  = ug/m3
  OutputUnits = ug/m3
  location    = Houston
  scenario    = test
  #profiles   = 20000
  #micros     = 34
  #sources    = 1
  start_date  = 19960101
  end_date    = 19961231
```

APEX Parameter file

P322_Benzene_oth3sources.txt - Notepad

File Edit Format View Help

APEX Parameter file (part 2)

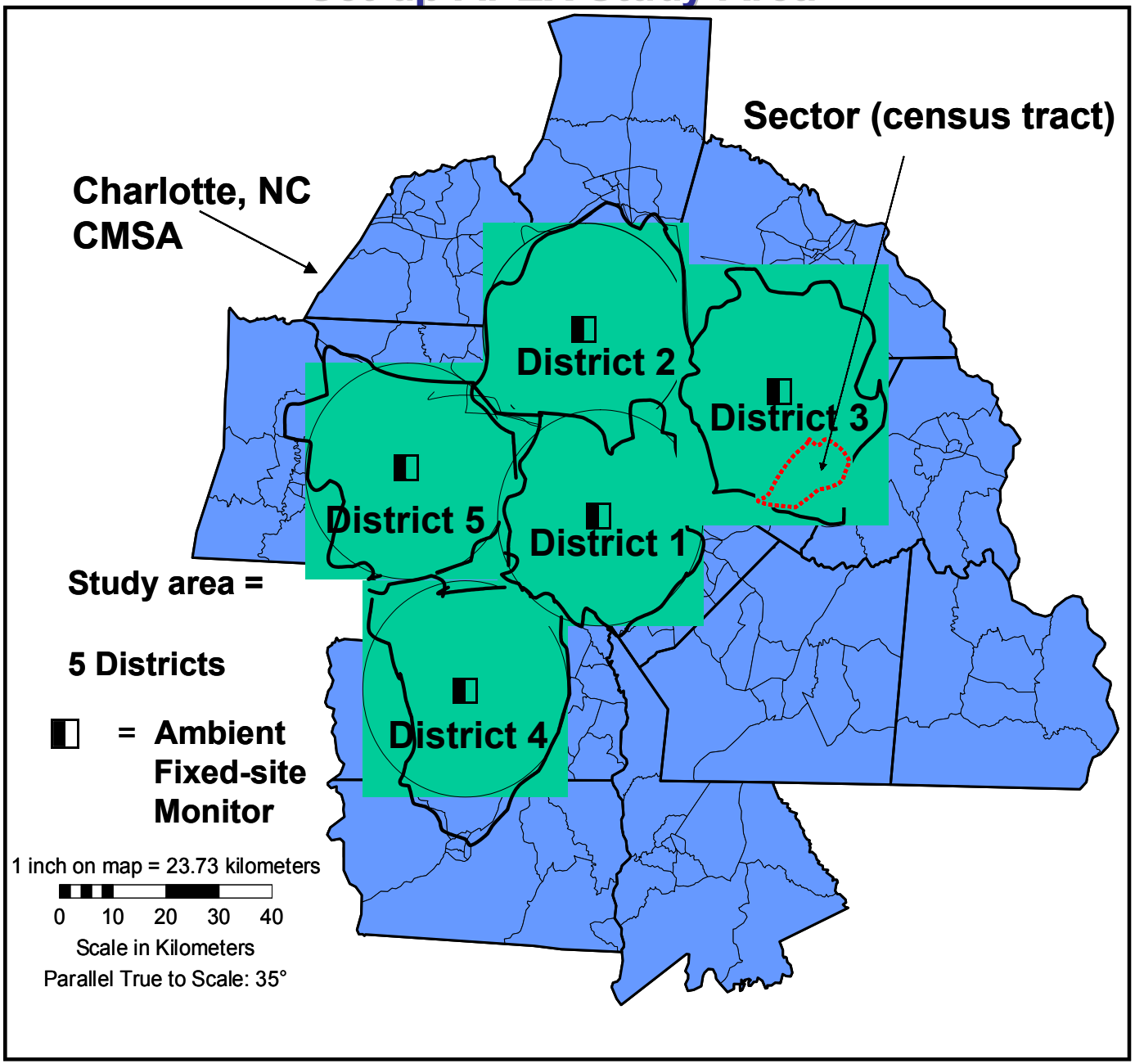
```
PARAMETER SETTINGS:
  pollutant    = Benzene
  InputUnits   = ug/m3
  OutputUnits  = ug/m3
  location     = Houston
  scenario     = test
  #profiles    = 20000
  #micros      = 34
  #sources     = 1
  start_date   = 19960101
  end_date     = 19961231
  Latitude     = 29.7533
  Longitude    = -95.18716
  CityRadius   = 20
  AirRadius    = 0.5
  ZoneRadius   = 300.
  CountyList   = YES
  County       = 48201
  County       = 48201
  Commuting    = YES
  AgeMin       = 0
  AgeMax       = 99
  DSTadjust    = NO
  HourlyOut    = NO
  DoDose       = NO
  rollback     = NO
  RBtarget     =  5.0
  RBbackgnd    =  0.0
  RBmax        = 10.0
  PPMFactor    = 1145.
  MissGender   =  0.1
  MissEmpl     =  0.1
  MissAge      =  0.1
  AgeCutPct    = 25.0
  Age2Probab   =  0.1
  Altitude     = 90
  COHbFact     = 2.5
  COThresh     = 100.
  DebugLevel   = 0
  RandomSeed   = 547862400

OUTPUT TABLE LEVELS:
  Percentiles   = 10, 25, 50, 75, 90, 95, 99
  TimeExp       = 0.5,1.0,1.5,2, 4, 6, 8, 10, 15, 20,30,40,50
  DM1HExp       = 5, 10, 15,20, 30, 40, 50, 75
  DM8HExp       = 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 18, 20, 25
  DAvgExp       = 2, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14, 16, 18, 20
  SAvgExp       = 0.5,0.75, 1, 1.25, 1.5, 1.75, 2, 2.5, 3, 4, 5, 6, 8, 10
  DM1HDose      = 0.5, 1.0, 1.25, 1.5, 1.75, 2.0, 2.25, 2.5, 2.75, 3.0, 4.0, 5.0, 6.0
  DM8HDose      = 0.5, 1.0, 1.25, 1.5, 1.75, 2.0, 2.25, 2.5, 2.75, 3.0, 4.0, 5.0, 6.0
  DMEHDose      = 0.5, 1.0, 1.25, 1.5, 1.75, 2.0, 2.25, 2.5, 2.75, 3.0, 4.0, 5.0, 6.0
  H_EHDose      = 0.5, 1.0, 1.25, 1.5, 1.75, 2.0, 2.25, 2.5, 2.75, 3.0, 4.0, 5.0, 6.0
  DAvgDose      = 0.5, 0.75, 1.0, 1.25, 1.5, 1.75, 2.0, 2.25, 2.5, 2.75, 3.0, 4.0, 5.0
  SAvgDose      = 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.2, 1.4, 1.6, 1.8, 2.0, 2.5
  TimeDose      = 0.5, 1.0, 1.25, 1.5, 1.75, 2.0, 2.25, 2.5, 2.75, 3.0, 4.0, 5.0, 6.0
```

Population, Air Quality, and Temperature Representation in APEX 3.2

- Geographical units for population are **"sectors"** and this version comes with a national file of sectors using the 65,443 census tracts with population data from the 2000 census
- A national commuting database based on 1990 census data is provided which has been mapped onto the 2000 census tracts to provide home-to-work commuting flows
- **"District"** refers to the geographical area represented by a given set of ambient air quality data (either based on a fixed-site monitor or output from an air quality model)
  - User can specify maximum radius distance from center of study area and can specify whether or not to include only sectors (e.g., census tracts) in certain counties
- User can provide temperature category for each **"temperature zone"** within the **"study area"** and zones are created in same fashion as districts

Set-up APEX Study Area



tp_geo_houston.txt - Notepad

File Edit Format View Help

48201100000	29.756478	-95.363281
48201210100	29.767777	-95.351514
48201210200	29.773977	-95.350039
48201210300	29.778227	-95.358484
48201210400	29.785977	-95.359051
48201210500	29.795676	-95.35803
48201210600	29.806026	-95.363014
48201210700	29.806326	-95.353789
48201210800	29.789027	-95.343647
48201210900	29.802876	-95.331738
48201211000	29.797026	-95.333388
48201211100	29.785851	-95.333416
48201211200	29.795176	-95.319413
48201211300	29.777877	-95.327388
48201211400	29.766727	-95.332163
48201211500	29.767352	-95.296818
48201211600	29.782727	-95.311913
48201211700	29.798726	-95.307112
48201211800	29.793776	-95.281145
48201211900	29.783727	-95.298387
48201212000	29.778977	-95.293912
48201212100	29.761127	-95.276445
48201212200	29.754917	-95.300087
48201220100	29.815276	-95.343613
48201220200	29.816626	-95.364489
48201220300	29.823826	-95.366414
48201220400	29.833575	-95.367314
48201220500	29.839175	-95.382691
48201220600	29.843392	-95.366957
48201220700	29.832375	-95.347963
48201220800	29.830175	-95.338998

APEX Sector File

districts_houston61.txt - Notepad

File Edit Format View Help

```
#48201212100  29.76112 -95.27645   19960101   19961231
#48201230900  29.81707 -95.27897   19960101   19961231
#48201231100  29.83677 -95.25692   19960101   19961231
#48201232400  29.82384 -95.19532   19960101   19961231
#48201232500  29.80085 -95.25586   19960101   19961231
#48201232600  29.77837 -95.24390   19960101   19961231
#48201232700  29.77952 -95.21502   19960101   19961231
#48201232800  29.78787 -95.20129   19960101   19961231
#48201232900  29.79972 -95.19659   19960101   19961231
#48201233000  29.79812 -95.17267   19960101   19961231
#48201233100  29.78012 -95.17284   19960101   19961231
#48201233200  29.78017 -95.18892   19960101   19961231
#48201233300  29.75822 -95.20540   19960101   19961231
#48201233400  29.76957 -95.24187   19960101   19961231
#48201233500  29.76332 -95.24027   19960101   19961231
#48201233600  29.74472 -95.25602   19960101   19961231
#48201233700  29.73892 -95.23722   19960101   19961231
#48201252300  29.79932 -95.14999   19960101   19961231
#48201252400  29.78492 -95.14693   19960101   19961231
#48201311100  29.73387 -95.28592   19960101   19961231
#48201311400  29.71867 -95.27707   19960101   19961231
#48201311500  29.70872 -95.28218   19960101   19961231
#48201311600  29.69913 -95.28620   19960101   19961231
#48201320100  29.69397 -95.27917   19960101   19961231
#48201320200  29.69382 -95.27052   19960101   19961231
#48201320300  29.71732 -95.25909   19960101   19961231
#48201320400  29.71381 -95.23800   19960101   19961231
#48201320500  29.69507 -95.24543   19960101   19961231
#48201320600  29.68052 -95.26033   19960101   19961231
#48201320700  29.67392 -95.24697   19960101   19961231
#48201321600  29.67682 -95.21867   19960101   19961231
```

APEX District File

ApexHoustonair61_on.txt - Notepad

File Edit Format View Help

```
Name = #48201212100
Houston TX Modelling Receptor Location #  1
Units = ppm
Start Date = 960101
End Date   = 961231
Lat        =  29.76113
Lon        = -95.27644
 0.00,  0.65,  0.57,  0.45,  0.87,  1.24,  3.46,  3.89,  2.88,  0.00,  1.20,  1.59,  1.89,
 0.29,  0.23,  0.22,  0.17,  0.28,  0.38,  1.00,  1.57,  1.52,  1.14,  1.05,  1.03,  0.96,
 0.25,  0.31,  0.16,  0.29,  0.98,  2.21,  4.76,  6.33,  3.10,  1.45,  1.61,  1.31,  0.54,
 1.53,  1.19,  0.93,  0.00,  0.00,  1.74,  7.25,  6.17,  2.62,  0.59,  0.63,  0.78,  0.37,
 1.68,  0.00,  0.00,  0.00,  0.68,  1.54,  5.81,  5.56,  0.00,  4.00,  4.23,  2.29,  2.83,
 0.60,  0.59,  0.32,  0.23,  0.17,  0.21,  0.56,  0.67,  0.88,  1.07,  1.01,  1.53,  1.35,
 0.70,  0.27,  0.23,  0.23,  0.23,  0.24,  0.41,  0.59,  0.56,  0.69,  0.62,  0.66,  0.97,
 2.30,  0.00,  1.75,  0.00,  0.00,  0.00,  0.00,  0.00,  9.61,  4.75,  2.31,  3.16,  1.25,
 0.00,  0.76,  0.00,  0.00,  0.00,  0.00,  0.00,  0.00,  5.36,  1.60,  0.67,  0.86,  0.78,
 0.00,  0.00,  0.00,  0.00,  0.00,  0.00,  8.87,  0.00,  0.00,  3.54,  2.04,  3.08,  1.06,
 0.60,  0.36,  0.32,  0.38,  0.46,  1.03,  1.57,  1.06,  1.25,  1.04,  0.96,  1.02,  1.11,
 1.21,  0.77,  0.79,  0.81,  1.06,  1.76,  4.41,  9.09,  3.82,  2.75,  1.09,  1.30,  0.65,
 0.00,  0.00,  0.00,  2.25,  1.50,  3.51,  0.00,  0.00,  0.00,  5.42,  2.91,  0.65,  0.39,
 1.61,  1.08,  0.00,  1.85,  0.00,  1.33,  1.95,  0.00,  2.32,  1.40,  0.46,  0.44,  0.60,
 1.06,  0.86,  0.00,  0.00,  2.56,  1.87,  3.24,  4.61,  3.29,  2.40,  1.03,  1.02,  0.49,
 1.30,  0.83,  0.38,  0.33,  0.45,  0.82,  1.54,  3.11,  2.16,  1.09,  1.65,  1.26,  1.56,
 0.37,  0.30,  0.54,  0.27,  0.35,  0.58,  2.42,  3.16,  1.51,  1.34,  1.45,  0.73,  1.28,
 0.24,  0.14,  0.16,  0.23,  0.00,  0.00,  0.00,  1.29,  1.31,  0.76,  1.10,  1.18,  0.64,
 0.64,  0.66,  0.93,  0.98,  1.97,  1.69,  3.38,  7.53,  3.25,  1.46,  1.62,  1.07,  0.94,
 1.89,  1.28,  0.51,  0.53,  0.45,  0.40,  1.00,  1.90,  2.04,  1.89,  1.52,  2.40,  3.04,
 0.00,  0.00,  0.80,  0.44,  0.37,  0.30,  0.43,  0.66,  1.03,  1.22,  1.55,  1.86,  2.09,
 1.06,  0.33,  0.46,  0.36,  0.52,  0.94,  2.78,  3.04,  2.49,  1.49,  0.95,  1.77,  1.33,
 0.29,  0.28,  0.24,  0.21,  0.28,  0.43,  1.04,  1.30,  1.65,  0.98,  0.95,  1.32,  0.90,
 0.60,  0.68,  0.58,  0.55,  0.82,  1.73,  6.74, 18.81,  5.51,  1.86,  2.04,  1.74,  0.94,
 0.00,  0.00,  0.00,  0.00,  0.00,  1.87,  4.97,  5.32,  2.95,  1.58,  1.09,  1.10,  0.87,
 0.59,  0.25,  0.26,  0.38,  0.62,  0.85,  3.31,  4.62,  3.61,  1.71,  1.10,  1.84,  2.23,
 0.77,  1.10,  0.97,  0.90,  0.88,  1.17,  1.87,  3.52,  1.87,  1.53,  1.19,  1.21,  0.84,
 0.00,  0.00,  0.00,  0.00,  0.73,  0.90,  1.16,  2.02,  1.83,  1.12,  1.11,  2.04,  1.95,
 1.15,  1.03,  0.00,  0.38,  0.74,  1.56,  0.00,  5.17,  0.00,  1.38,  2.01,  1.94,  1.18,
 0.26,  0.21,  0.19,  0.30,  0.63,  3.07,  3.12,  3.01,  2.83,  2.12,  0.86,  0.94,  0.51,
 0.27,  0.17,  0.13,  0.11,  0.22,  0.28,  1.08,  1.62,  1.10,  1.07,  1.15,  1.77,  1.25,
 0.49,  0.34,  0.35,  0.29,  0.29,  0.88,  2.10,  3.27,  3.09,  2.70,  2.19,  2.26,  1.93,
 0.47,  0.28,  0.17,  0.27,  0.44,  0.65,  0.85,  1.71,  1.37,  1.17,  1.32,  1.13,  2.00,
```

APEX AQ file

Uses Human Activity Data from CHAD

- Over 22,000 diary days contained in CHAD used by APEX 3.0 (for more info about CHAD see T. McCurdy, G. Glen, L. Smith, and Y. Lakkadi. "The National Exposure Research Laboratory's Consolidated Human Activity Database," Journal of Exposure Analysis and Environmental Epidemiology 10: 566-578 (2000).
- APEX can also use other activity data if provided in same format
- CHAD diary event file provides CHAD ID, start time, duration, activity, and location for a 24-hour period from midnight to midnight
- CHAD questionnaire file provides CHAD ID, day type, gender, age, race, employed outside home, daily max. temperature, occupation, record count (# of events per day)
- Metabolic equivalent (MET) file contains MET distributions for each activity type in the CHAD database; this information is used in APEX to estimate breathing (ventilation) rates
- Can be found at: http://www.epa.gov/chadnet1/

CHADEvents.txt - Notepad

File Edit Format View Help

```
BAL97001A,0000,60,14500,30125,
BAL97001A,0100,60,14500,30125,
BAL97001A,0200,60,14500,30125,
BAL97001A,0300,60,14500,30125,
BAL97001A,0400,60,14500,30125,
BAL97001A,0500,60,14500,30125,
BAL97001A,0600,60,14500,30125,
BAL97001A,0700,30,14500,30125,
BAL97001A,0730,30,14400,30121,
BAL97001A,0800,60,16000,30122,
BAL97001A,0900,60,14500,30125,
BAL97001A,1000,30,14500,30125,
BAL97001A,1030,30,X    ,X    ,
BAL97001A,1100,45,14500,30125,
BAL97001A,1145,15,X    ,X    ,
BAL97001A,1200,60,14500,30125,
BAL97001A,1300,60,14500,30125,
BAL97001A,1400,60,14500,30125,
BAL97001A,1500,60,16000,30122,
BAL97001A,1600,60,14600,30125,
BAL97001A,1700,15,14600,30125,
BAL97001A,1715,45,14400,30123,
BAL97001A,1800,45,14400,30123,
BAL97001A,1845,15,16000,30122,
BAL97001A,1900,60,16000,30122,
BAL97001A,2000,60,17223,30125,
BAL97001A,2100,60,17223,30125,
BAL97001A,2200,60,17223,30125,
BAL97001A,2300,60,17223,30125,
BAL97001B,0000,60,14500,30125,
BAL97001B,0100,60,14500,30125,
BAL97001B,0200,60,14500,30125,
BAL97001B,0300,60,14500,30125,
BAL97001B,0400,60,14500,30125,
BAL97001B,0500,60,14500,30125,
BAL97001B,0600,60,14500,30125,
BAL97001B,0700,60,14500,30125,
```

CHAD Events File

Diary Day

CHADQuest.txt - Notepad

File Edit Format View Help

```
BAL97001A,TUE,F,W,N,77,43,34,X,45,29
BAL97001B,WED,F,W,N,77,51,41,X,135,28
BAL97001C,THU,F,W,N,77,57,47,X,15,30
BAL97001D,FRI,F,W,N,77,45,36,X,0,28
BAL97001E,TUE,F,W,N,77,47,39,X,0,27
BAL97001F,WED,F,W,N,77,36,29,X,0,28
BAL97001G,THU,F,W,N,77,38,29,X,0,26
BAL97001H,FRI,F,W,N,77,43,36,X,0,28
BAL97001I,TUE,F,W,N,77,41,39,X,15,28
BAL97001J,WED,F,W,N,77,54,44,X,15,28
BAL97001K,THU,F,W,N,77,48,40,X,0,30
BAL97001L,FRI,F,W,N,77,42,36,X,30,30
BAL97006A,WED,M,W,N,80,51,41,X,0,31
BAL97006B,THU,M,W,N,80,57,47,X,60,36
BAL97006C,FRI,M,W,N,80,45,36,X,75,31
BAL97006D,TUE,M,W,N,80,47,39,X,15,33
BAL97006E,WED,M,W,N,80,36,29,X,30,31
BAL97006F,THU,M,W,N,80,38,29,X,210,34
BAL97006G,FRI,M,W,N,80,43,36,X,165,30
BAL97006H,TUE,M,W,N,80,41,39,X,45,31
BAL97006I,WED,M,W,N,80,54,44,X,60,34
BAL97006J,THU,M,W,N,80,48,40,X,15,31
BAL97008A,TUE,F,W,N,88,43,34,X,0,31
BAL97008B,WED,F,W,N,88,51,41,X,60,27
BAL97008C,THU,F,W,N,88,57,47,X,345,33
BAL97008D,FRI,F,W,N,88,45,36,X,90,28
BAL97008E,TUE,F,W,N,88,47,39,X,30,29
BAL97008F,WED,F,W,N,88,36,29,X,90,26
BAL97008G,TUE,F,W,N,88,41,39,X,270,32
BAL97008H,WED,F,W,N,88,54,44,X,150,31
BAL97008I,THU,F,W,N,88,48,40,X,465,35
```

CHAD Diary Questionnaire

APEX Creates Event Sequence for Each Simulated Individual for Study Period

- The Profile Generator reads data from a probability array based on 2000 population census data and adds other variables from the user-defined distributions to create set of profiles

- User-defined distributions include:
  - Diary pools: assigns both CHAD diaries and calendar days to pools based on temperature (# of temperature categories and cut points) and day type (i.e., weekend or weekday)
  - Season/Months: assigns a season to each calendar month
  - Employed Age: determines the probability of employment based on age
  - Work Sector: assigns a work sector to each profile based on home sector and employment status
  - Has AC: probability of a person (profile) having air conditioning

- Profile Module groups the profiles into pools of CHAD diaries, then uses a set of rules to determine the diary selection probability

- Profile Module then picks diaries at random based on pool and diary probabilities, for each day in the simulation for each target personal profile to create event sequence for study period

Flexible Approach for Simulating Microenvironmental Concentrations

- User defines number of microenvironments (ME) (up to 127)
- Each ME can also be tagged as: at home, at work, or other
- User provides input file that maps CHAD location codes into set of ME's chosen (e.g., kitchen, living room, dining room location code in CHAD might all be assigned as "indoor residential" ME)
- For each ME user decides between two model types: **factors** or **mass balance**
- **Factors type** - user must provide distributions for following factors:
  - *Proximity factor*: a multiplicative factor that represents relationship between air at nearest ambient monitoring site and air in immediate vicinity of ME
  - *Penetration factor*: multiplicative factor less than or equal to one
  - *Sources*: no limit on number of sources specified
- **Mass Balance type** – user must provide distributions for following inputs:
  - *Proximity factor* (same as above)
  - *Penetration factor*: (same as above)
  - *Sources*: can be expressed as additive concentration (as above) or as emission rates (if specified as emission rates, then distributions of volumes for ME required)
  - *Air exchange rate* (AER): distributions expressed in air changes per hour
  - *Decay rate for pollutant*: set to zero for nonreactive pollutants like CO

Outputs from APEX 3.2

- Output files (All in ASCII (text) format):
  - Log file: provides a report of highlights as the job progresses. Useful for debugging if the job stops abnormally and documenting input files and parameter settings used for a run.
  - Profile summary: summary of each personal profile in the simulation, including age, gender, home & work sectors, air quality district for home & work
  - ME summary: summary for each ME for each person. Variables include number of minutes spent by each profile in the ME, & mean and maximum concentration in ME
  - Hourly exposure: contains hour-by-hour time series of exposure for each profile
  - Hourly dose: contains hour-by-hour times series of dose (%COHb in blood) for each profile (model currently addresses dose estimates only for CO)
  - Site Mapping File: provides mapping between sectors and districts
  - Output Tables: contains a series of summary tables for the model run

psum.txt - Notepad

File Edit Format View Help

Person	HSect	WSect	HDis	WDis	Zone	DGRP	Age	Gender	Race	Empl	Stove	Pilot	ACHom	ACCar	Height	Weight	Hemoglob
1	59	59	59	59	1	11	68	Female	White	NoWrk	NoGas	NoPlt	HasAC	HasAC	64.686	149.106	13.744
2	10	10	10	10	1	1	10	Male	White	NoWrk	Gas	NoPlt	HasAC	HasAC	70.499	109.937	15.112
3	9	1	9	1	1	9	54	Female	Black	Works	Gas	Pilot	HasAC	HasAC	63.402	138.516	14.553
4	45	45	45	45	1	1	1	Female	Other	NoWrk	NoGas	NoPlt	HasAC	NoAC	60.177	26.342	17.740
5	17	17	17	17	1	1	12	Male	Other	NoWrk	NoGas	NoPlt	HasAC	NoAC	67.379	92.788	16.653
6	9	9	9	9	1	1	5	Male	White	NoWrk	Gas	Pilot	HasAC	HasAC	65.404	47.764	16.170
7	58	58	58	58	1	11	96	Female	White	NoWrk	Gas	NoPlt	HasAC	NoAC	64.581	123.784	15.124
8	11	11	11	11	1	1	3	Male	White	NoWrk	NoGas	NoPlt	HasAC	HasAC	57.904	34.395	17.529
9	18	40	18	40	1	7	38	Female	White	Works	NoGas	NoPlt	HasAC	HasAC	65.939	162.729	13.043
10	54	54	54	54	1	1	9	Female	White	NoWrk	NoGas	NoPlt	HasAC	HasAC	65.864	80.077	15.684

psum.txt - Notepad

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Weight	Hemoglob	Diffday	BloodVol	HemFac	Endgn1	Endgn2	#Events	AvgExp	AvgDose	MaxExp	MaxDose
49.106	13.744	22.176	3982.07	0.000000	0.011680	0.007309	13282	0.3147E+01	0.0000E+00	0.4199E+02	0.0000E+00
09.937	15.112	39.430	4232.07	0.000000	0.006412	0.006412	15085	0.6021E+01	0.0000E+00	0.5870E+02	0.0000E+00
38.516	14.553	23.072	3720.34	0.000000	0.004013	0.002511	14344	0.5330E+01	0.0000E+00	0.2007E+03	0.0000E+00
26.342	17.740	27.373	1895.30	0.000000	0.011499	0.007195	14435	0.3662E+01	0.0000E+00	0.5365E+02	0.0000E+00
92.788	16.653	37.840	3636.67	0.000000	0.008875	0.008875	15132	0.3011E+01	0.0000E+00	0.4659E+02	0.0000E+00
47.764	16.170	38.751	2692.85	0.000000	0.004793	0.004793	14222	0.5067E+01	0.0000E+00	0.4506E+02	0.0000E+00
23.784	15.124	18.897	3603.46	0.000000	0.010977	0.006869	12374	0.7765E+01	0.0000E+00	0.5820E+02	0.0000E+00
34.395	17.529	36.507	1880.74	0.000000	0.007205	0.007205	13853	0.4082E+01	0.0000E+00	0.5408E+02	0.0000E+00
62.729	13.043	26.322	4289.64	0.000000	0.008888	0.005562	14592	0.3501E+01	0.0000E+00	0.4949E+02	0.0000E+00
80.077	15.684	29.615	3268.49	0.000000	0.006052	0.003787	14687	0.3432E+01	0.0000E+00	0.1081E+03	0.0000E+00

CHAD Summary Output File

tables.txt - Notepad

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25.0 %ile :	366.000	362.000	67.000	14.000	4.000	2.000	1.000	0.000	0.000
50.0 %ile :	366.000	365.000	154.000	32.000	10.000	4.000	2.000	1.000	1.000
75.0 %ile :	366.000	366.000	341.000	217.000	77.000	17.000	7.000	3.000	2.000
90.0 %ile :	366.000	366.000	363.000	346.000	266.000	136.000	36.000	8.000	4.000
95.0 %ile :	366.000	366.000	365.000	358.000	319.000	210.000	84.000	16.000	6.000
99.0 %ile :	366.000	366.000	366.000	365.000	356.000	316.000	208.990	75.000	15.000
Maximum :	366.000	366.000	366.000	366.000	366.000	363.000	351.000	328.000	280.000
Mean (%) :	100.000	98.975	50.645	29.237	18.137	9.658	3.893	1.258	0.451
Min (%) :	100.000	56.557	0.273	0.000	0.000	0.000	0.000	0.000	0.000
Max (%) :	100.000	100.000	100.000	100.000	100.000	99.180	95.902	89.617	76.503
Counts(Sim):	0.732E+07	0.724E+07	0.371E+07	0.214E+07	0.133E+07	0.707E+06	0.285E+06	0.921E+05	0.330E+05
#Meet (Sim):	20000	20000	20000	19972	19527	17839	15399	12869	10322

Exposure: Persons at or above each Overall Average Exposure level (ug/m3), for N = 20000 Profiles. Area Populatior

Level:	0.000	0.500	1.000	1.250	1.500	1.750	2.000	2.500	3.000
Counts(Pop):	0.182E+06	0.182E+06	0.182E+06	0.182E+06	0.182E+06	0.182E+06	0.182E+06	0.181E+06	0.172E+06
#Meet (Pop):	181866	181866	181866	181866	181866	181866	181866	181420	171518
%Meet (Pop):	100.000	100.000	100.000	100.000	100.000	100.000	100.000	99.755	94.310
Counts(Sim):	0.200E+05	0.200E+05	0.200E+05	0.200E+05	0.200E+05	0.200E+05	0.200E+05	0.200E+05	0.189E+05
#Meet (Sim):	20000	20000	20000	20000	20000	20000	20000	19951	18862

CHAD Output Tables File

Principal Limitations and Caveats

- Provides modeling framework that is **heavily dependent** on user provided inputs (e.g., ambient air quality, distributions for mass balance or factors approach, assignment of CHAD location codes to microenvironment types, etc.), thus, exposure estimates only as good as the quality of the inputs to the model
- Uncertainty about season-long exposure event sequence because APEX 3.2 creates seasonal or year long sequence for a simulated individual by sampling human activity data from more than one subject
- Currently does not capture very well human activities that are correlated and which can impact microenvironmental concentrations (e.g, cigarette smoking leading to individual opening window which impacts AER that affects amount of outdoor air penetrating to residence)
- APEX 3.2 currently does not characterize separately uncertainty and variability
- Initial model testing and evaluation continue