Predicting Chemical Properties and Fate Using the Estimation Programs Interface (EPI) Suite™ of Models

Bob Boethling

International Science Forum on Computational Toxicology, RTP, North Carolina

23 May 2007

U.S. Environmental Protection Agency
Office of Pollution Prevention and Toxics
Washington, DC 20460

Office of Prevention, Pesticides, and Toxic Substances

- Develops national strategies for toxic substances control and promotes pollution prevention and the public's right to know about chemical risk
- Office of Pesticide Programs (OPP)
- Office of Pollution Prevention and Toxics (OPPT)
- Office of Science Coordination and Policy (OSCP)

Office of Pollution Prevention and Toxics

- Pre-manufacture review of new industrial chemicals
- Testing, assessment, and risk reduction of existing industrial chemicals
- Management of “national chemicals” (e.g. PCBs)
- International chemical issues (e.g. POPs)
- Pollution prevention advocacy
- Partnership programs, e.g. HPVC Challenge, Green Suppliers Network, DfE and Green Chemistry

Estimation Programs Interface (EPI Suite™)

- Estimates physical/chemical properties and environmental fate and transport
- Runs estimation programs sequentially with chemical structure as only input
- Includes PHYSPROP, a database of measured properties for >40,000 chemicals
- Considered a screening-level tool; not applicable to all substances
- Intended for use only in absence of measured values

Things to Look for in Estimation Software

(1) How comprehensive is the methodology?

(2) How accurate are the methods?

(3) Have the methods been validated?

(4) Have the methods been published / peer-reviewed?

(5) Is the software easy to use?

(6) Does it

- (a) Run structures batchwise?
- (b) Provide adequate help information?

Chemical Property and Fate Programs in EPI Suite™

P/Chem Property Programs

AEROWIN	sorption to atmospheric particulates (φ)
BCFWIN	bioconcentration factor
HENRYWIN	Henry's law constant; air-water partition coefficient
KOAWIN	octanol-air partition coefficient
KOWWIN	octanol-water partition coefficient
MPBPWIN	melting point, boiling point, vapor pressure
PCKOCWIN	soil organic carbon sorption coefficient
WSKOWWIN	water solubility from log Kow
WATERNT	water solubility from fragments

Chemical Property and Fate Programs in EPI Suite™

Environmental Fate Programs

degradation processes

AOPWIN	atmospheric oxidation
BIOWIN	biodegradability
BioHCWIN	biodegradability of hydrocarbons
HYDROWIN	aqueous hydrolysis

multimedia fate

STPWIN	removal in activated sludge treatment
LEVEL III	transport/distribution by fugacity model
WVOLWIN	volatilization from water

A Brief History of EPI

- 1980
  - "Lyman" published—the original handbook of estimation methods—Lyman, Rheel and Rosenblatt
  - Hand calculators widely used
  - Only mainframe computers available
- Early 1980s
  - Personal computers become common in EPA offices, but not yet 1 for every person
  - Lyman methods encoded in a DOS program called "CHEMEST"
- About 1986
  - First fragment-based biodegradation models developed—now called BIOWIN1 &2

A Brief History of EPI, cont.

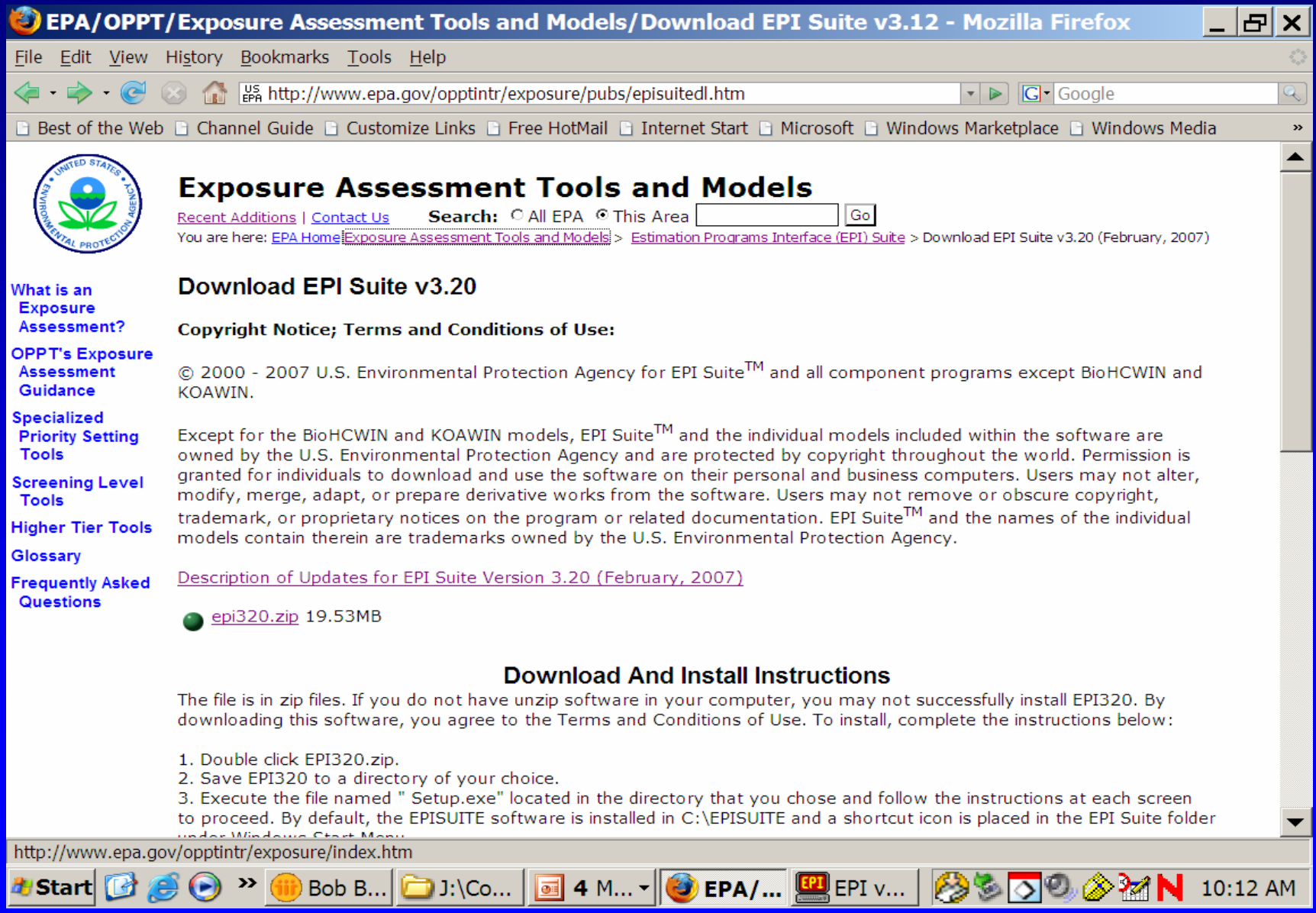
- About 1990/1991
  - Sabljic's molecular connectivity-based Koc method enhanced and encoded in a DOS program
  - Atmospheric Oxidation Program (AOP) and Henry program (now HENRYWIN) developed
- Early 1990s
  - BIOWIN "expert survey" models developed—now called BIOWIN3 and 4
  - EPA asked, "Why not unite the growing collection of methods in a 'shell program' for easier use?"
  - The shell program is named EPI—the Estimation Programs Interface—and first appears in DOS format

A Brief History of EPI, cont.

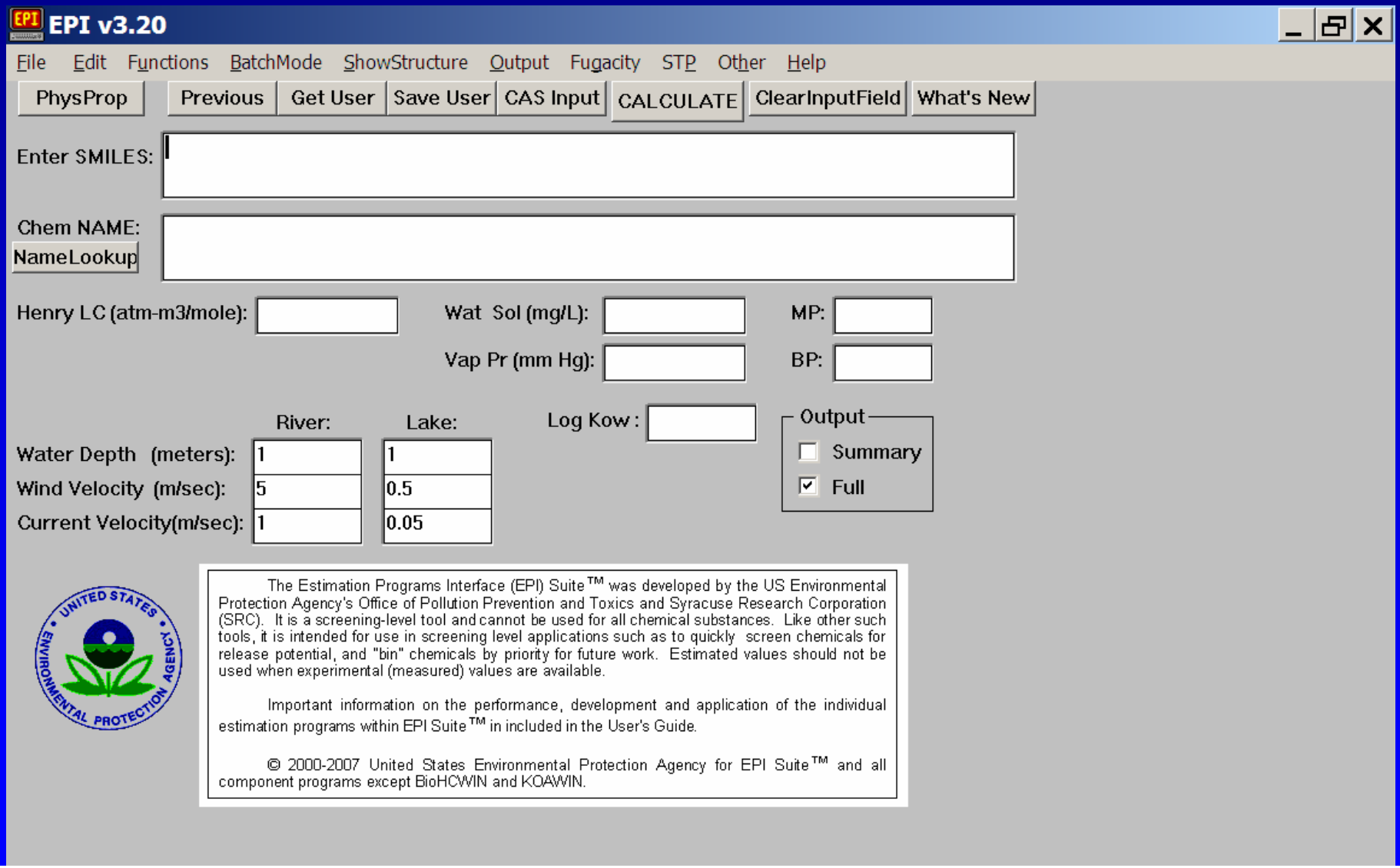
- Mid 1990s
  - More new models: MPBPWIN, KOWWIN, WSKOWWIN
  - SRC sees the future and converts EPI (DOS) on its own to EPIWIN
- Late 1990s
  - BCFWIN; fugacity models (STP and EQC); more
- 2000 to present
  - Many user interface and convenience features added. Several new models
  - EPIWIN copyright purchased by EPA. EPA renamed it EPI Suite and has ***sole ownership***

→ EPI Suite is a result of an ***evolutionary process***, not a grand plan

EPI Suite™ Download Page



EPI Suite™ v3.20 Input Screen (Feb 2007)



EPI Suite™ Chemical Structure Entry

- Runs from SMILES representation of chemical structure
- SMILES can be entered directly or using a chemical's CAS number
- Chemicals can be run batchwise
- Accepts MDL Mol files (generated by Isis Base/Draw)

EPI Suite™ Core Property Estimation Programs

- MPBPWIN
  - Estimates properties at 25 C; if run as a standalone, VP can be estimated for any temperature of interest
  - Various methods used, including Joback, Stein and Brown, Antoine, others
- KOWWIN
  - If run as a standalone, can provide an estimate using the “experimental value adjusted” (analog) method
- WSKOWWIN
- WATERNT
  - If run as a standalone, can provide an estimate using the “experimental value adjusted” method

EPI Suite™ Property Estimation Programs, cont.

- HENRYWIN
  - Henry's Law constant from bond/group contribution methods (improved Hine-Mookerjee)
  - If run as a standalone, can estimate H_c as a function of temperature, and using the "experimental value adjusted" method
- BCFWIN
  - Metabolism not considered
- PCKOCWIN
  - Organic carbon partition coefficient from molecular connectivity

EPI Suite™ Transformation (Degradation) Programs

- AOPWIN
  - Rate constants for hydroxyl radical and ozone oxidation in the atmosphere
- BIOWIN
  - Biodegradability using seven predictive models
  - Semi-quantitative rates from two models, likelihood of fast degradation from the other five
- HYDROWIN
  - Hydrolysis rate constants for acid- and base-catalyzed reactions, but only for a small number of classes
  - Neutral hydrolysis rate not estimated

EPI Suite™ Modeling Programs

(1) Rate of volatilization from water

EPI adaptation of model from Lyman Handbook

Results: volatilization half-lives for model river & lake

(2) Sewage treatment plant model

EPI adaptation of Mackay's Toronto (STP) Model

Results: percent removal (air, biodegradation, sludge)

(3) Level III fugacity model

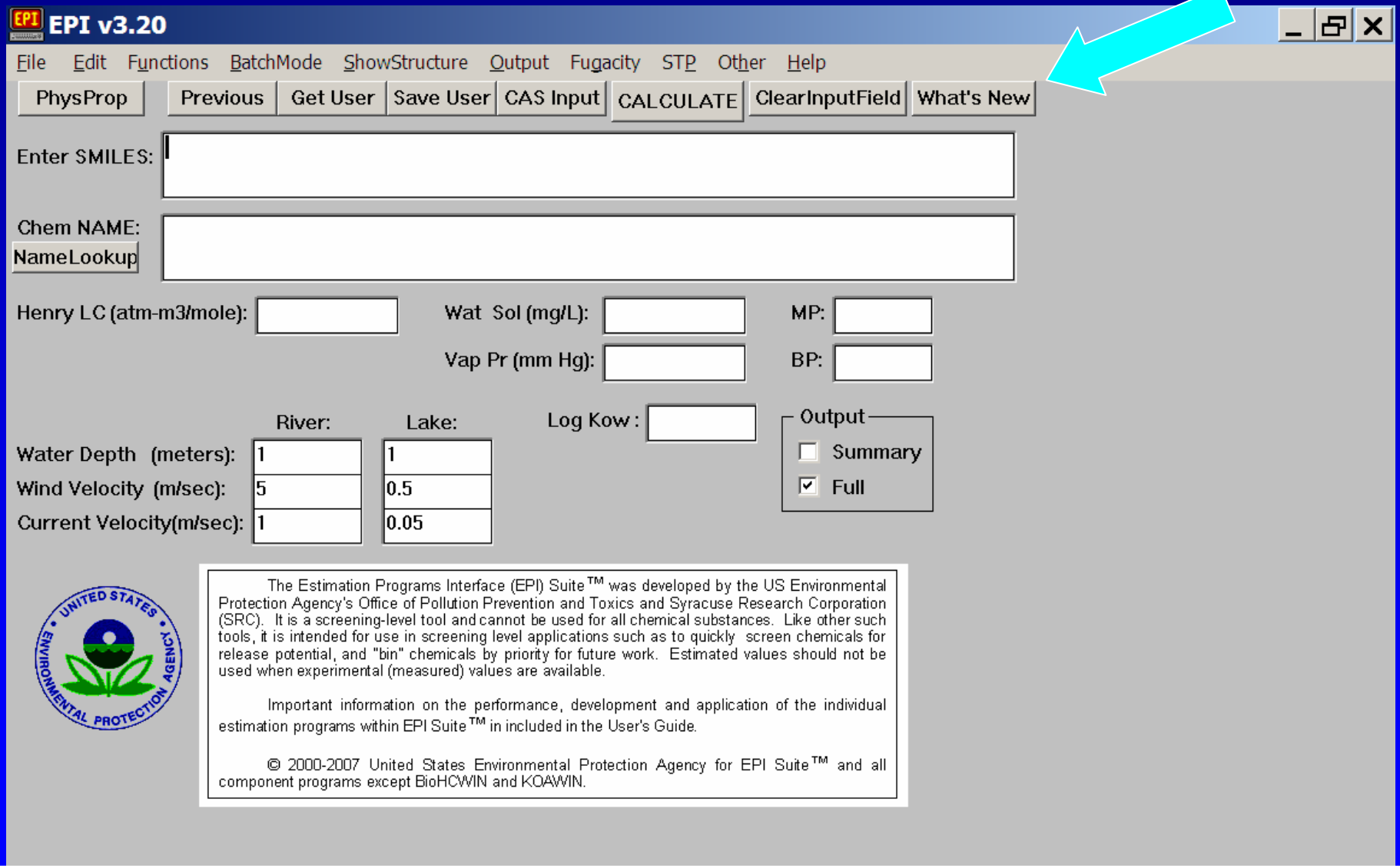
EPI adaptation of Mackay's EQC Model

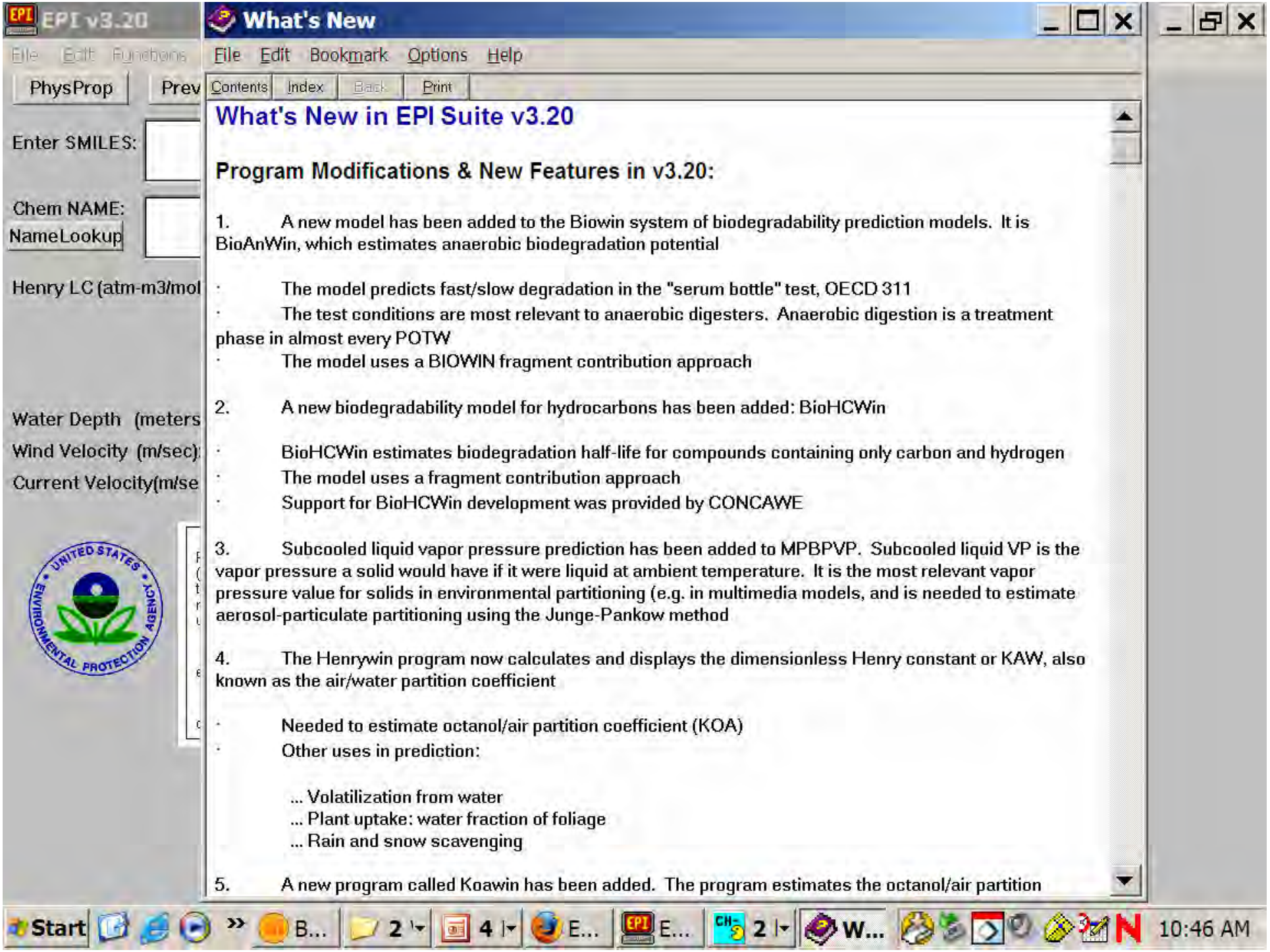
Results: overall persistence; mass distribution in air, water, soil, sediment

EPI Suite™: New Properties and Methods in v3.20

- Subcooled liquid vapor pressure—to MPBPWIN
- Air/water partition coefficient (dimensionless Henry constant, K_{AW})—to HENRYWIN
- Octanol/air partition coefficient (K_{OA})—new model KOAWIN
- Fraction of airborne substance in particulates (φ), by 3 methods—new model AEROWIN
- Methanogenic anaerobic biodegradation potential—to BIOWIN as "BIOWIN7"
- Biodegradation half-life of hydrocarbons—new model BioHCWIN

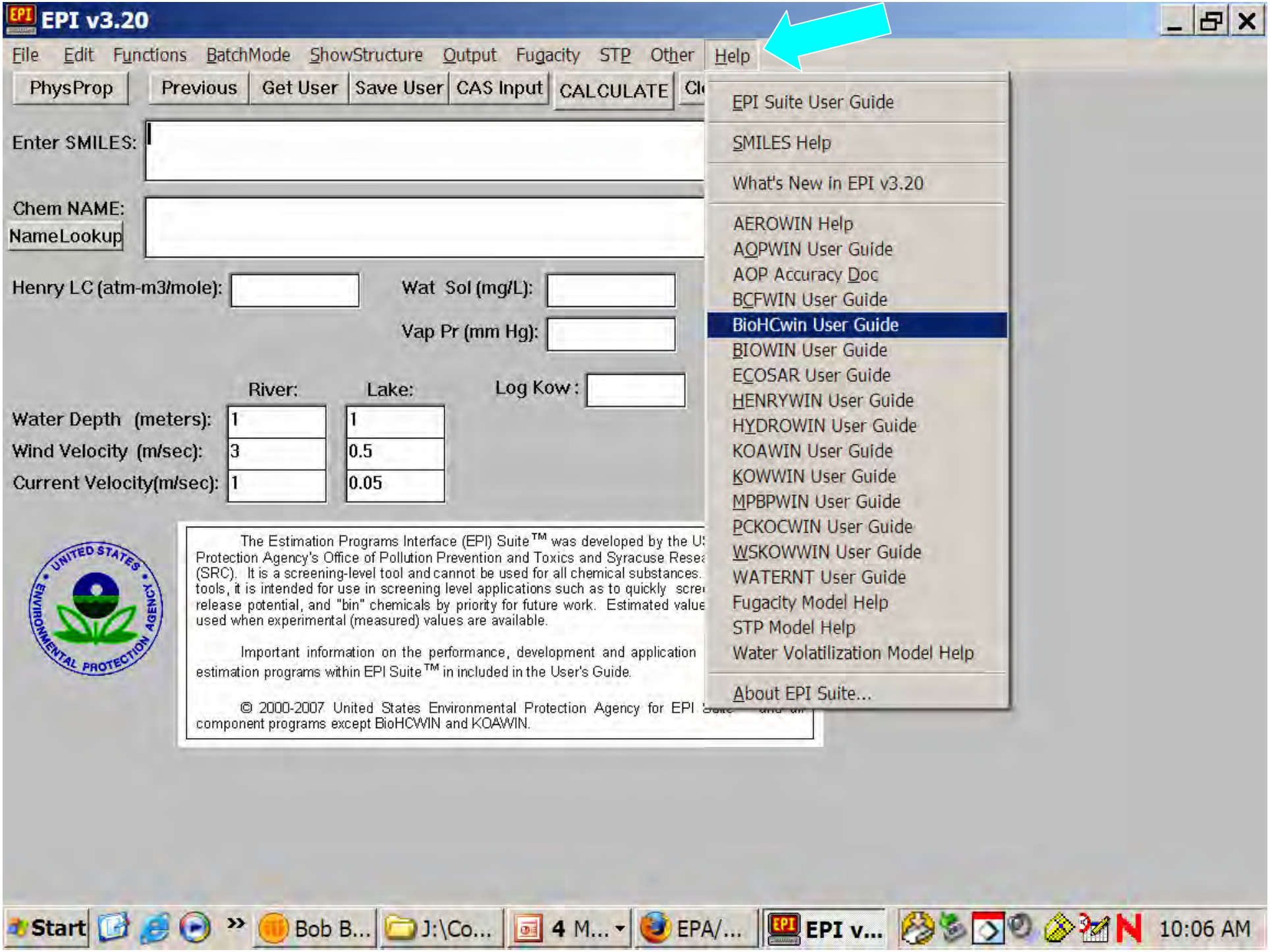
EPI Suite™ v3.20 Input Screen (Feb 2007)

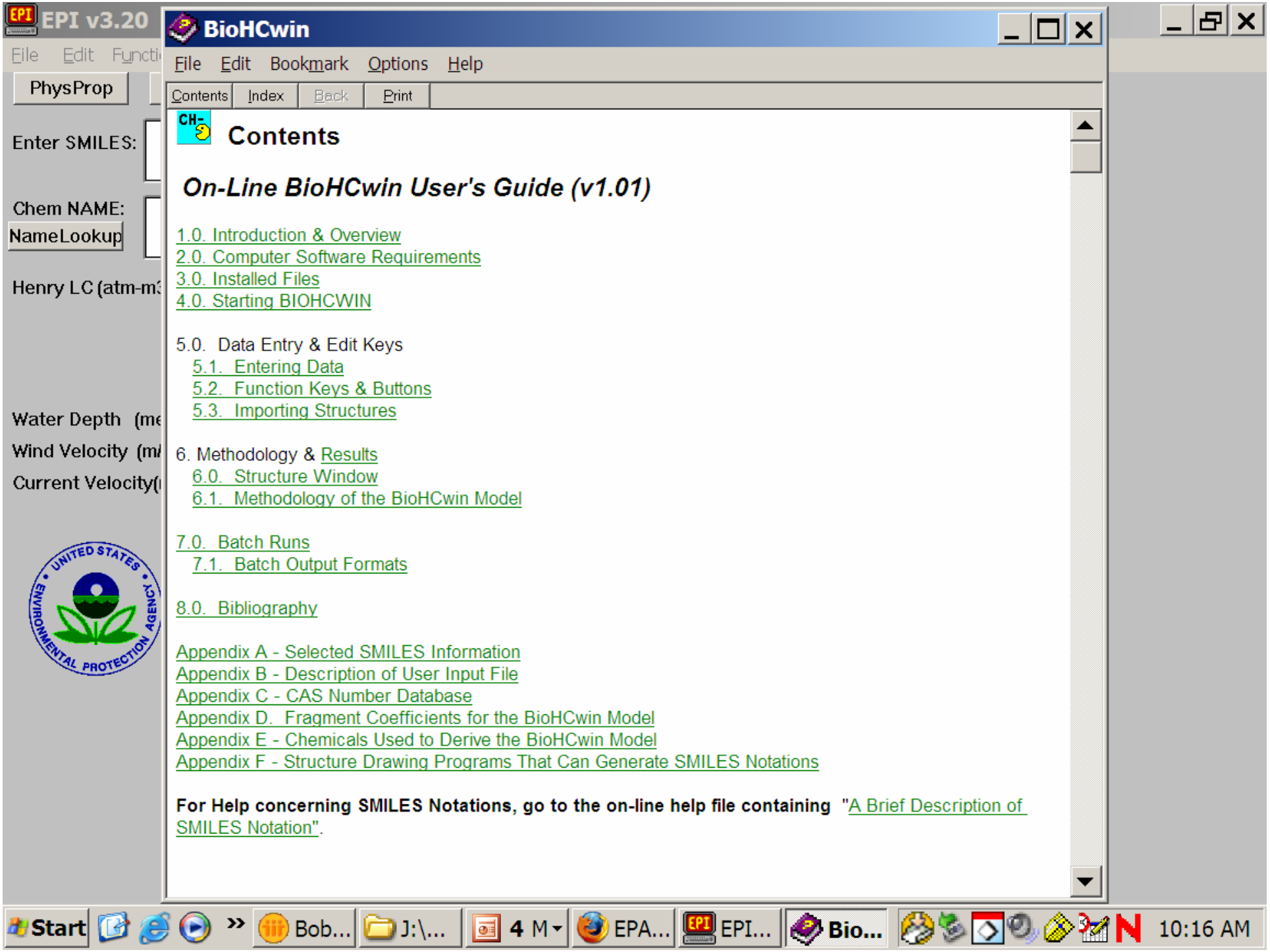



EPI v3.20
File Edit Functions
PhysProp
Prev
Enter SMILES:
Chem NAME:
NameLookup
Henry LC (atm-m3/mol
Water Depth (meters
Wind Velocity (m/sec)
Current Velocity(m/se
What's New
File Edit Bookmark Options Help
Contents Index Back Print
What's New in EPI Suite v3.20
Program Modifications & New Features in v3.20:
1. A new model has been added to the Biowin system of biodegradability prediction models. It is BioAnWin, which estimates anaerobic biodegradation potential
· The model predicts fast/slow degradation in the "serum bottle" test, OECD 311
· The test conditions are most relevant to anaerobic digesters. Anaerobic digestion is a treatment phase in almost every POTW
· The model uses a BIOWIN fragment contribution approach
2. A new biodegradability model for hydrocarbons has been added: BioHCWin
· BioHCWin estimates biodegradation half-life for compounds containing only carbon and hydrogen
· The model uses a fragment contribution approach
· Support for BioHCWin development was provided by CONCAWE
3. Subcooled liquid vapor pressure prediction has been added to MPBPVP. Subcooled liquid VP is the vapor pressure a solid would have if it were liquid at ambient temperature. It is the most relevant vapor pressure value for solids in environmental partitioning (e.g. in multimedia models, and is needed to estimate aerosol-particulate partitioning using the Junge-Pankow method
4. The Henrywin program now calculates and displays the dimensionless Henry constant or KAW, also known as the air/water partition coefficient
· Needed to estimate octanol/air partition coefficient (KOA)
· Other uses in prediction:
... Volatilization from water
... Plant uptake: water fraction of foliage
... Rain and snow scavenging
5. A new program called Koawin has been added. The program estimates the octanol/air partition
Start
10:46 AM

EPI Suite™: Method Details, Accuracy, Validation

- Method details
  - Estimation methods for chemical properties and degradation are based on standard regression techniques
  - Most use correction factors
  - Method details are summarized online in the Help files
  - Full reference citations are also given so that users can examine methods in more detail, if they desire


EPI v3.20
File Edit Functions BatchMode ShowStructure Output Fugacity STP Other Help
PhysProp Previous Get User Save User CAS Input CALCULATE
Enter SMILES:
Chem NAME:
NameLookup
Henry LC (atm-m3/mole):
Wat Sol (mg/L):
Vap Pr (mm Hg):
Log Kow:
River: Lake:
Water Depth (meters): 1 1
Wind Velocity (m/sec): 3 0.5
Current Velocity(m/sec): 1 0.05
The Estimation Programs Interface (EPI) Suite™ was developed by the U
Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Rese
(SRC). It is a screening-level tool and cannot be used for all chemical substances.
tools, it is intended for use in screening level applications such as to quickly scre
release potential, and "bin" chemicals by priority for future work. Estimated value
used when experimental (measured) values are available.
Important information on the performance, development and application
estimation programs within EPI Suite™ in included in the User's Guide.
© 2000-2007 United States Environmental Protection Agency for EPI
component programs except BioHCWIN and KOAWIN.
EPI Suite User Guide
SMILES Help
What's New in EPI v3.20
AEROWIN Help
AOPWIN User Guide
AOP Accuracy Doc
BCFWIN User Guide
BioHCwin User Guide
BIOWIN User Guide
ECOSAR User Guide
HENRYWIN User Guide
HYDROWIN User Guide
KOAWIN User Guide
KOWWIN User Guide
MPBPWIN User Guide
PCKOCWIN User Guide
WSKOWWIN User Guide
WATERNT User Guide
Fugacity Model Help
STP Model Help
Water Volatilization Model Help
About EPI Suite...
Start
Bob B...
J:\Co...
4 M...
EPA/...
EPI v...
10:06 AM


EPI v3.20
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Chem NAME:
NameLookup
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Wind Velocity (m/
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UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
BioHCwin
File Edit Bookmark Options Help
Contents Index Back Print
Contents
On-Line BioHCwin User's Guide (v1.01)
1.0. Introduction & Overview
2.0. Computer Software Requirements
3.0. Installed Files
4.0. Starting BIOHCWIN
5.0. Data Entry & Edit Keys
5.1. Entering Data
5.2. Function Keys & Buttons
5.3. Importing Structures
6. Methodology & Results
6.0. Structure Window
6.1. Methodology of the BioHCwin Model
7.0. Batch Runs
7.1. Batch Output Formats
8.0. Bibliography
Appendix A - Selected SMILES Information
Appendix B - Description of User Input File
Appendix C - CAS Number Database
Appendix D. Fragment Coefficients for the BioHCwin Model
Appendix E - Chemicals Used to Derive the BioHCwin Model
Appendix F - Structure Drawing Programs That Can Generate SMILES Notations
For Help concerning SMILES Notations, go to the on-line help file containing "A Brief Description of SMILES Notation".
Start
Bob...
J:\...
4 M
EPA...
EPI...
Bio...
10:16 AM

EPI Suite™: Method Details, Accuracy, Validation

- Method details
- Accuracy
  - EPA considers the accuracy acceptable for a screening-level tool
  - Information on method error is summarized online in the Help files
  - Full reference citations are also given so that users can examine the statistics in more detail, if they desire

KOWWIN Program - log K_{ow} (log P)

Methodology - Atom/Fragment Contributions:

170 Fragments

290 Correction Factors

Log Kow used by:

- **BCFWIN**
- **DERMWIN**
- **ECOSAR**
- **WSKOWWIN**

Statistical Accuracy:

	number	Corr(r^2)	Std Dev	Mean Error
Total	13229	0.954	0.436	0.316
Training	2467	0.981	0.219	0.162
Validation	10762	0.943	0.473	0.354

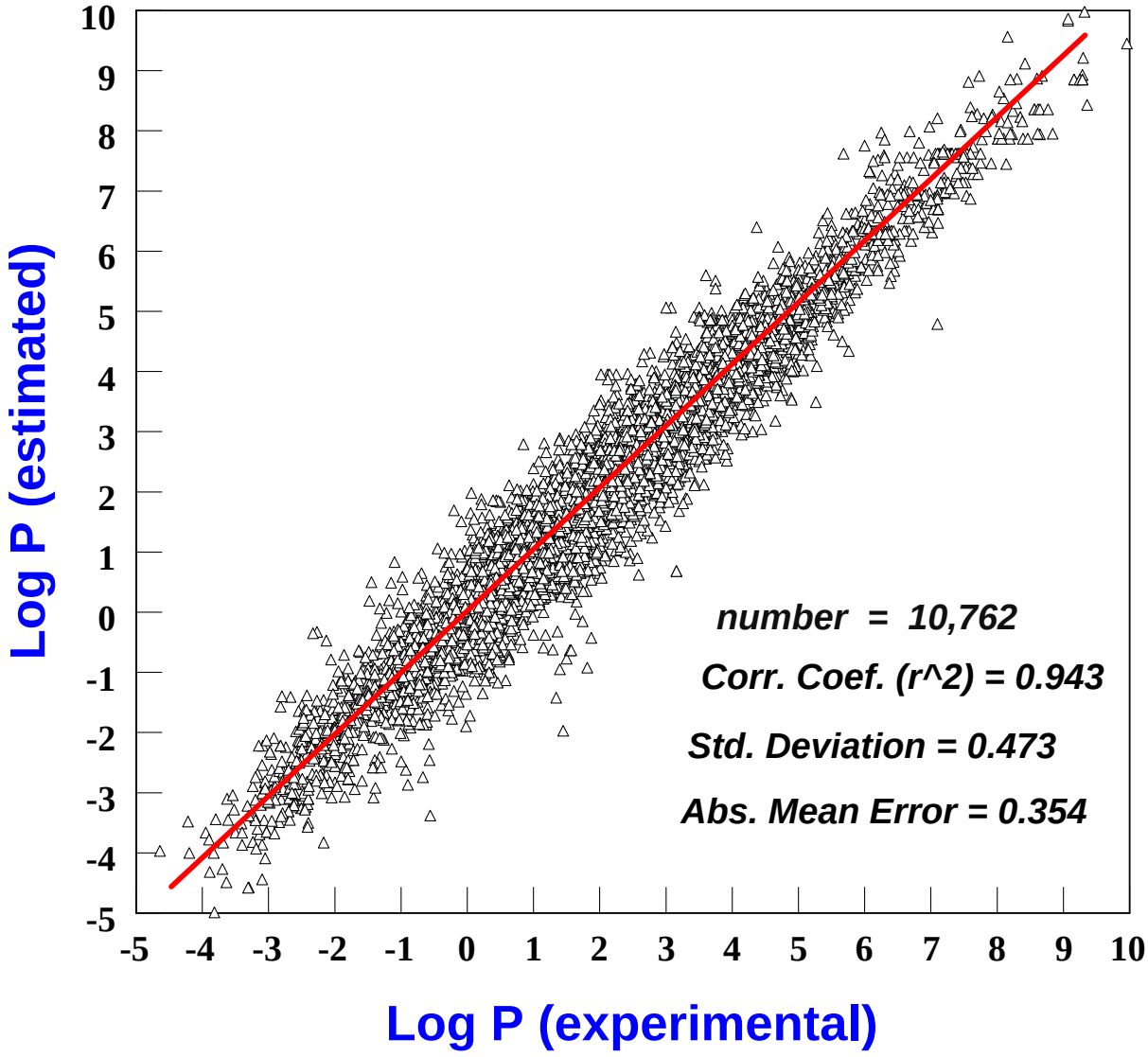
KOWWIN includes the experimental database of 13,229 recommended log P values

Journal Article Description: J. Pharm. Sci. 84(1): 83-92 (1995)

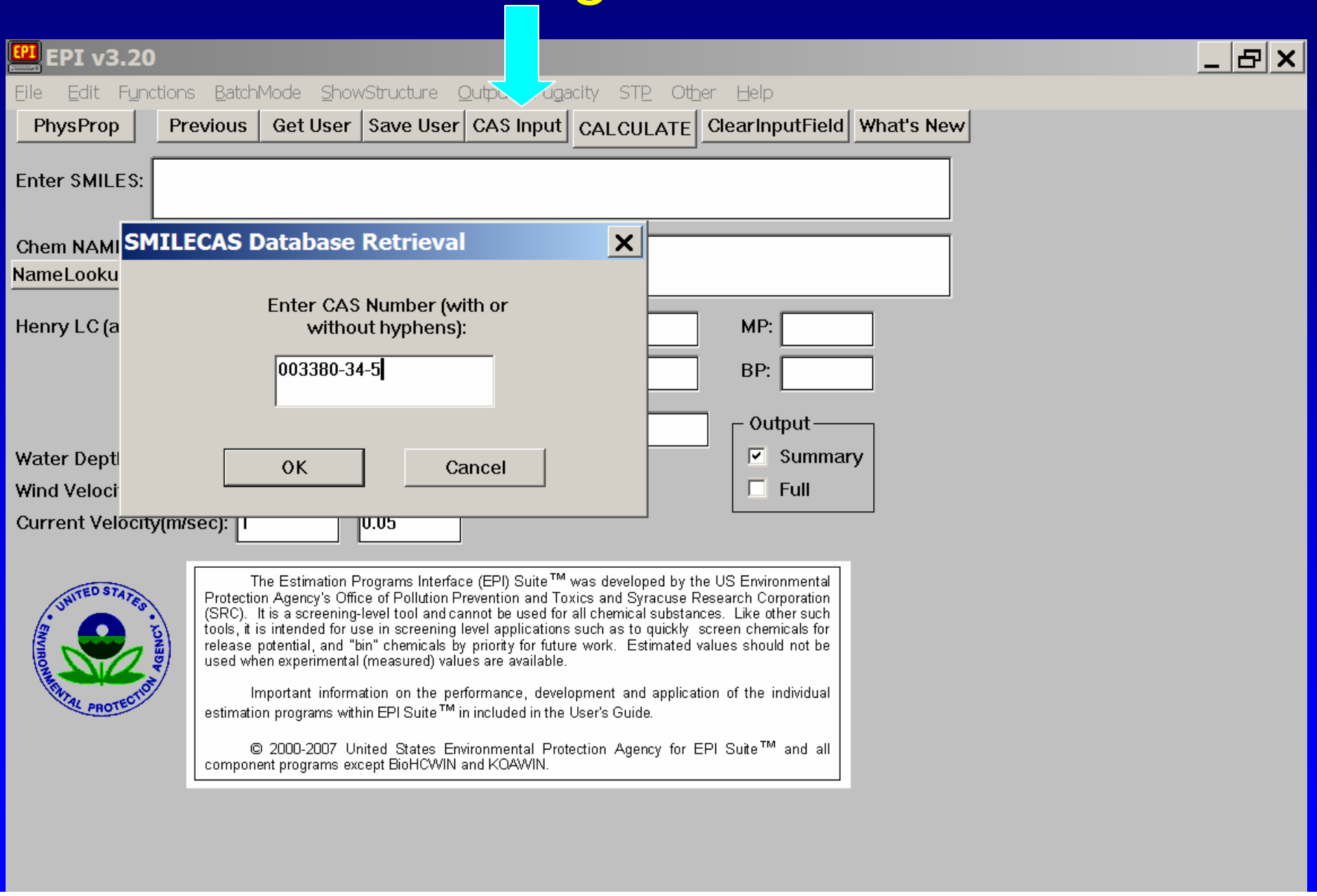
EPI Suite™: Method Details, Accuracy, Validation

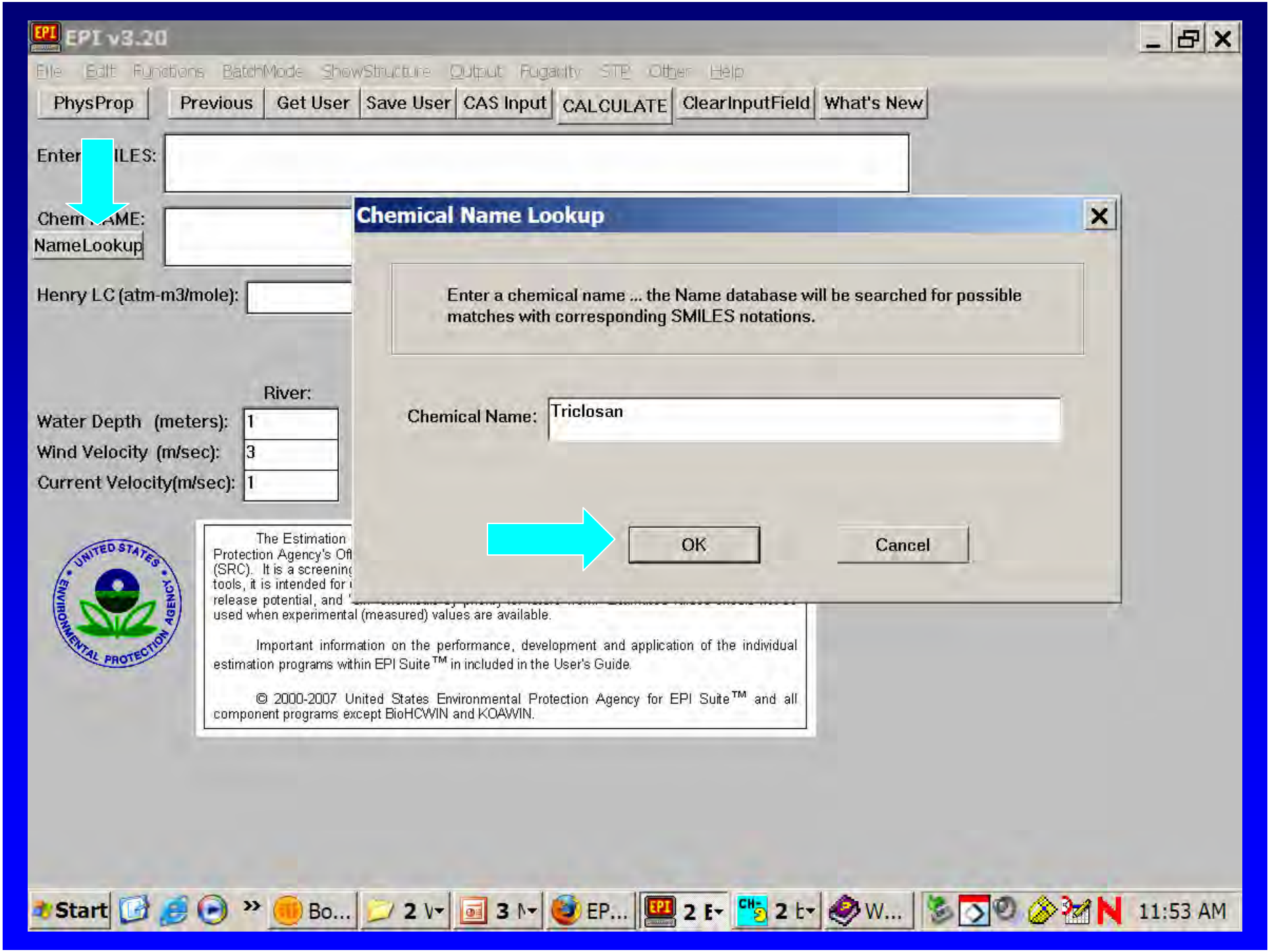
- Method details
- Accuracy
- Validation
  - Most methods have been validated using independent (external) validation sets
  - Information on validation is summarized online in the Help files
  - Full reference citations are also given so that users can examine the statistics in more detail, if they desire

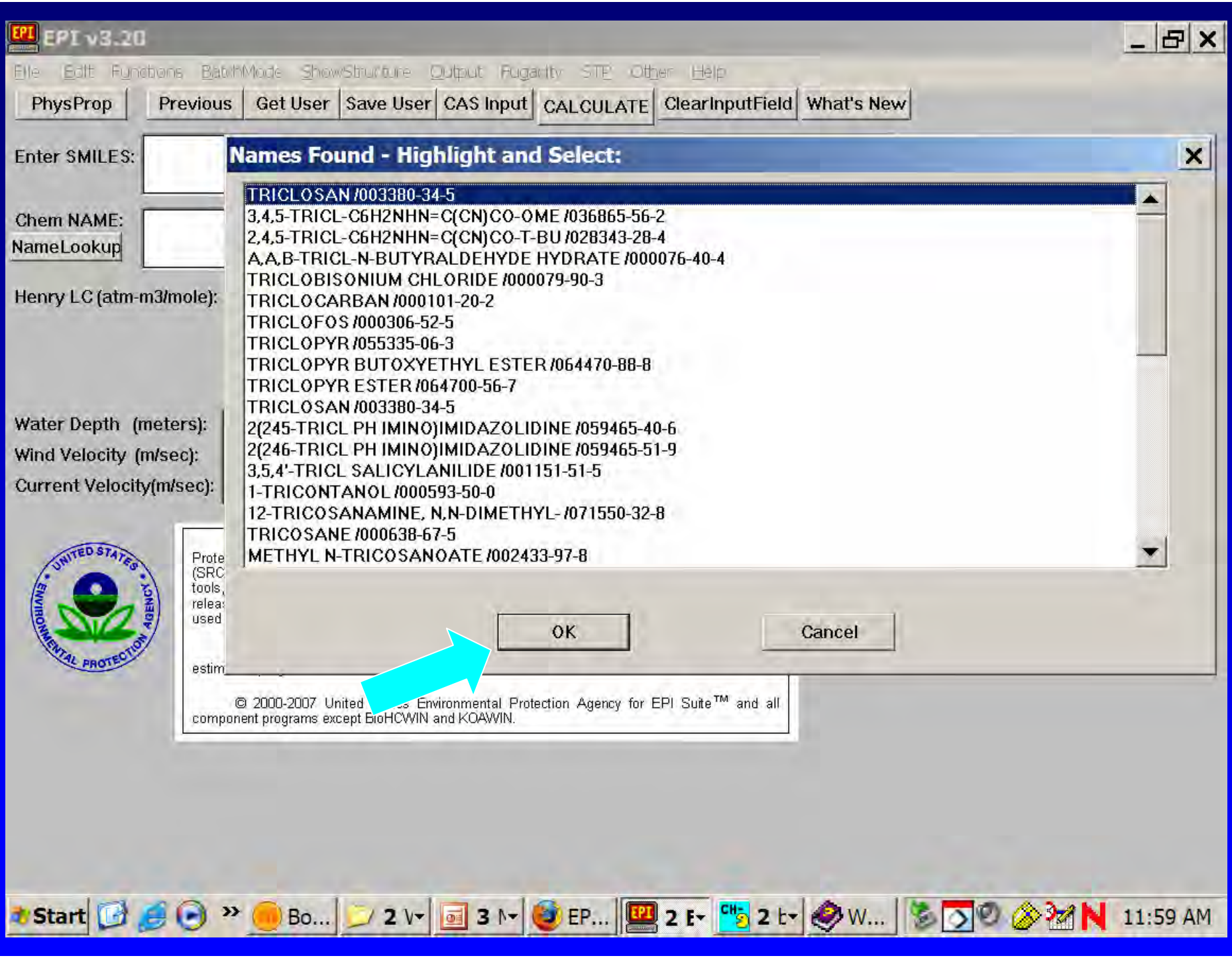
KOWWIN:
Validation Data Set



Running EPI Suite™




EPI v3.20
File Edit Functions BatchMode ShowStructure Output Fugacity STP Other Help
PhysProp
Previous
Get User
Save User
CAS Input
CALCULATE
ClearInputField
What's New
Enter SMILES:
Chem NAME:
NameLookup
Henry LC (atm-m3/mole):
River:
Water Depth (meters): 1
Wind Velocity (m/sec): 3
Current Velocity(m/sec): 1
Chemical Name Lookup
Enter a chemical name ... the Name database will be searched for possible matches with corresponding SMILES notations.
Chemical Name: Triclosan
OK
Cancel
The Estimation
Protection Agency's Off
(SRC). It is a screening
tools, it is intended for
release potential, and
used when experimental (measured) values are available.
Important information on the performance, development and application of the individual estimation programs within EPI Suite™ in included in the User's Guide.
© 2000-2007 United States Environmental Protection Agency for EPI Suite™ and all component programs except BioHCWIN and KOAWIN.
Start
11:53 AM


EPI v3.20
File Edit Functions BatchMode ShowStructure Output Fugacity STP Other Help
PhysProp
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Get User
Save User
CAS Input
CALCULATE
ClearInputField
What's New
Enter SMILES:
Chem NAME:
NameLookup
Henry LC (atm-m3/mole):
Water Depth (meters):
Wind Velocity (m/sec):
Current Velocity(m/sec):
Names Found - Highlight and Select:
TRICLOSAN /003380-34-5
3,4,5-TRICL-C6H2NHN=C(CN)CO-OME /036865-56-2
2,4,5-TRICL-C6H2NHN=C(CN)CO-T-BU /028343-28-4
A,A,B-TRICL-N-BUTYRALDEHYDE HYDRATE /000076-40-4
TRICLOBISONIUM CHLORIDE /000079-90-3
TRICLOCARBAN /000101-20-2
TRICLOFOS /000306-52-5
TRICLOPYR /055335-06-3
TRICLOPYR BUTOXYETHYL ESTER /064470-88-8
TRICLOPYR ESTER /064700-56-7
TRICLOSAN /003380-34-5
2(245-TRICL PH IMINO)IMIDAZOLIDINE /059465-40-6
2(246-TRICL PH IMINO)IMIDAZOLIDINE /059465-51-9
3,5,4'-TRICL SALICYLANILIDE /001151-51-5
1-TRICONTANOL /000593-50-0
12-TRICOSANAMINE, N,N-DIMETHYL- /071550-32-8
TRICOSANE /000638-67-5
METHYL N-TRICOSANOATE /002433-97-8
OK
Cancel
© 2000-2007 United States Environmental Protection Agency for EPI Suite™ and all component programs except BioHCWIN and KOAWIN.
Start
11:59 AM

EPI v3.20

File Edit Functions BatchMode ShowStructure Output Fugacity STP Other Help

PhysProp | Previous | Get User | Save User | CAS Input | CALCULATE | ClearInputField | What's New

Enter SMILES: O(c(c(O)cc(c1)Cl)c1)c(c(cc(c2)Cl)Cl)c2

003380-34-5

Chem NAME: Phenol, 5-chloro-2-(2,4-dichlorophenoxy)-

NameLookup

Henry LC (atm-m3/mole):

Wat Sol (mg/L):

Vap Pr (mm Hg):

Log Kow

	River:	Lake:
Water Depth (meters):	1	1
Wind Velocity (m/sec):	3	0.5
Current Velocity(m/sec):	1	0.05

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Protection Agency's Office of Pollution Prevention and Toxic
(SRC). It is a screening-level tool and cannot be used for all
tools, it is intended for use in screening level applications su
release potential, and "bin" chemicals by priority for future v
used when experimental (measured) values are available.

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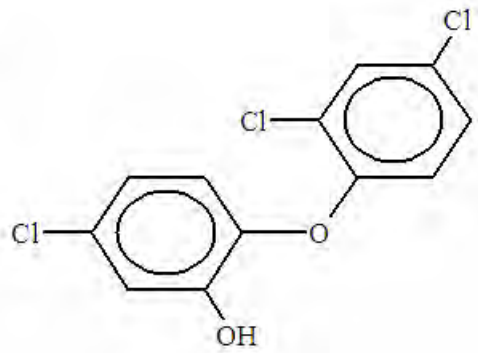
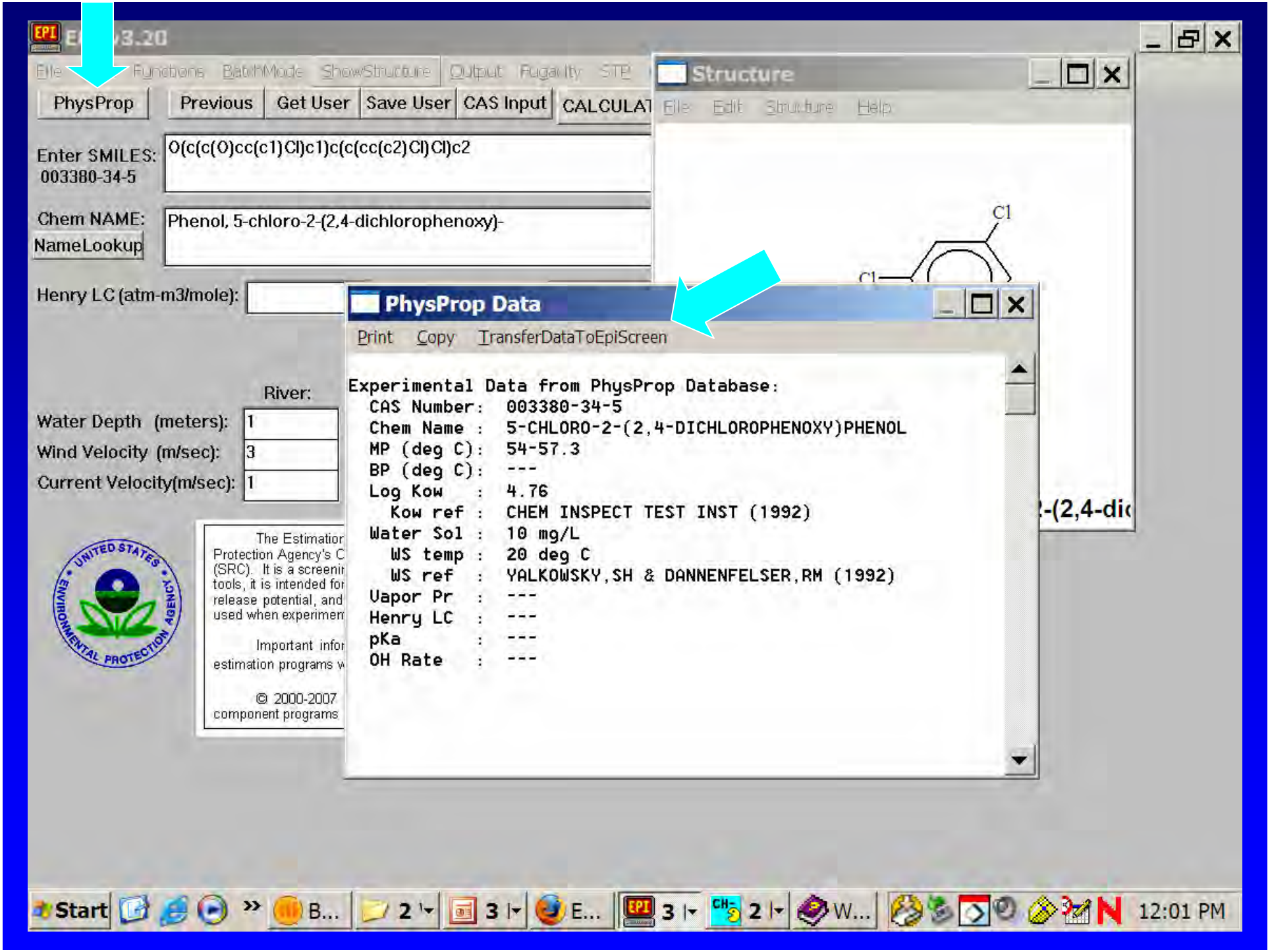
Structure

File Edit Structure Help



MolWt: 289.55 C12 H7 CL3 O2
003380-34-5 Phenol, 5-chloro-2-(2,4-dic

Start Bo... 2 V 3 M EP... 2 E 2 b W... 11:50 AM


File Functions BatchMode ShowStructure Output Fugacity STP
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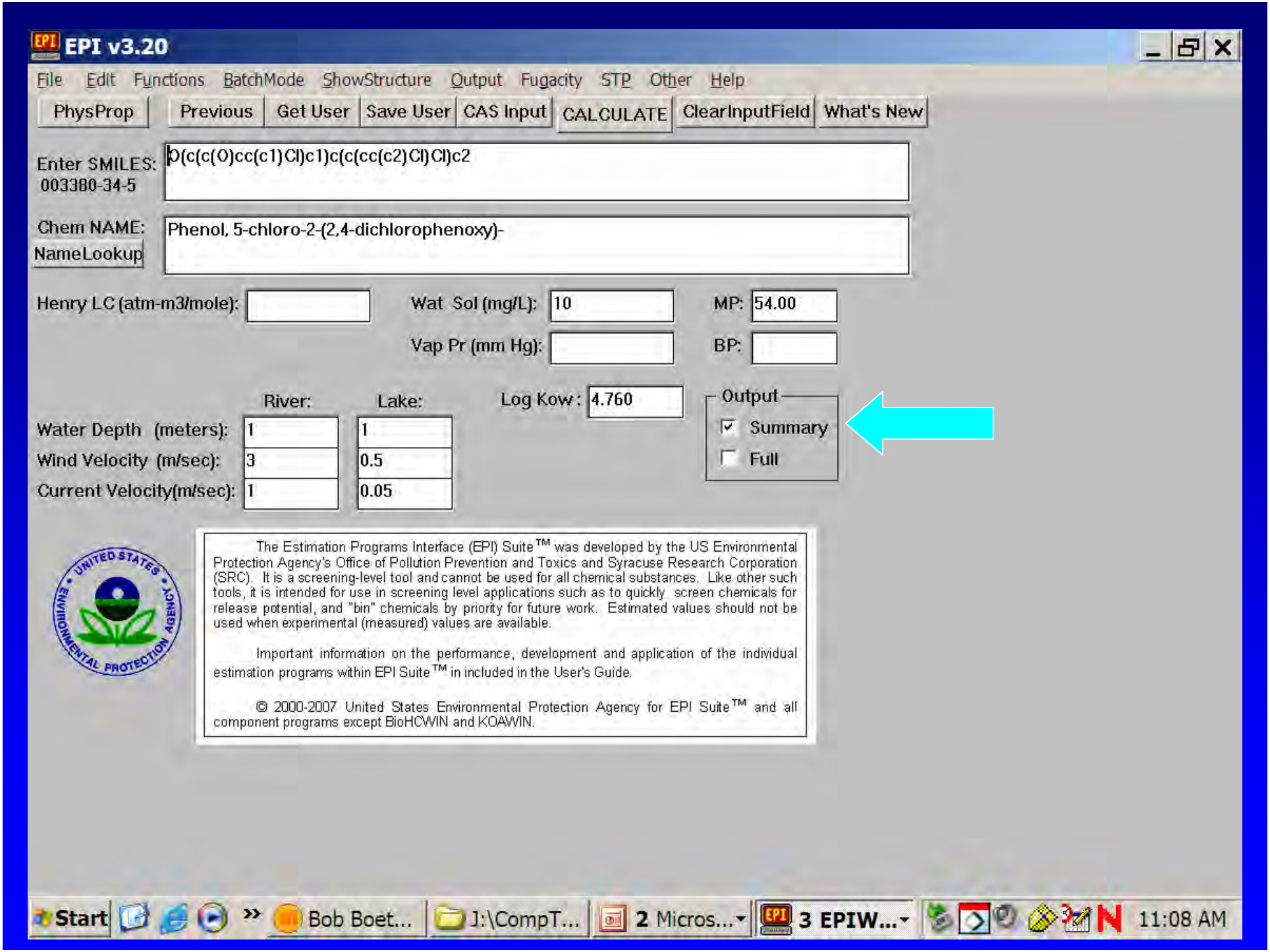
Get User
Save User
CAS Input
CALCULAT
Enter SMILES:
003380-34-5
O(c(c(O)cc(c1)Cl)c1)c(c(cc(c2)Cl)Cl)c2
Chem NAME:
NameLookup
Phenol, 5-chloro-2-(2,4-dichlorophenoxy)-
Henry LC (atm-m3/mole):
River:
Water Depth (meters):
1
Wind Velocity (m/sec):
3
Current Velocity(m/sec):
1
Structure
File Edit Structure Help
Cl
Cl
PhysProp Data
Print Copy TransferDataToEpiScreen
Experimental Data from PhysProp Database:
CAS Number: 003380-34-5
Chem Name : 5-CHLORO-2-(2,4-DICHLOROPHENOXY)PHENOL
MP (deg C): 54-57.3
BP (deg C): ---
Log Kow : 4.76
Kow ref : CHEM INSPECT TEST INST (1992)
Water Sol : 10 mg/L
WS temp : 20 deg C
WS ref : YALKOWSKY,SH & DANNENFELSER,RM (1992)
Vapor Pr : ---
Henry LC : ---
pKa : ---
OH Rate : ---
Start
12:01 PM


EPI v3.20
File Edit Functions BatchMode ShowStructure Output Fugacity STP Other Help
PhysProp Previous Get User Save User CAS Input CALCULATE ClearInputField What's New
Enter SMILES:
003380-34-5
O(c(c(O)cc(c1)Cl)c1)c(c(cc(c2)Cl)Cl)c2
Chem NAME:
NameLookup
Phenol, 5-chloro-2-(2,4-dichlorophenoxy)-
Henry LC (atm-m3/mole):
Wat Sol (mg/L): 10
MP: 54.00
Vap Pr (mm Hg):
BP:
River: Lake:
Log Kow : 4.760
Output
Summary
Full
Water Depth (meters): 1 1
Wind Velocity (m/sec): 3 0.5
Current Velocity(m/sec): 1 0.05
The Estimation Programs Interface (EPI) Suite™ was developed by the US Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). It is a screening-level tool and cannot be used for all chemical substances. Like other such tools, it is intended for use in screening level applications such as to quickly screen chemicals for release potential, and "bin" chemicals by priority for future work. Estimated values should not be used when experimental (measured) values are available.
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Start
Bob Boet...
J:\CompT...
2 Micros...
3 EPIW...
11:08 AM

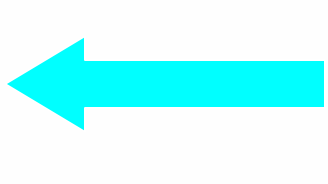
EPI Results

Print EPA_upload Save Results Copy Help

```
SMILES : O(c(c(O)cc(c1)CL)c1)c(c(cc(c2)CL)CL)c2
CHEM   : Phenol, 5-chloro-2-(2,4-dichlorophenoxy)-
CAS NUM: 003380-34-5
MOL FOR: C12 H7 CL3 O2
MOL WT : 289.55
----------------------------- EPI SUMMARY (v3.20) -------------------------
 Physical Property Inputs:
    Water Solubility (mg/L):   10
    Vapor Pressure (mm Hg) :   ------
    Henry LC (atm-m3/mole) :   ------
    Log Kow (octanol-water):   4.76
    Boiling Point (deg C)  :   ------
    Melting Point (deg C)  :   54.00

 Log Octanol-Water Partition Coef (SRC):
    Log Kow (KOWWIN v1.67 estimate) =  4.66
    Log Kow (Exper. database match) =  4.76
       Exper. Ref:  Chem Inspect Test Inst (1992)

 Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1.42):
    Boiling Pt (deg C):  373.62  (Adapted Stein & Brown method)
    Melting Pt (deg C):  136.79  (Mean or Weighted MP)
    VP(mm Hg,25 deg C):  4.65E-006  (Modified Grain method)
    MP  (exp database):  54-57.3 deg C
    Subcooled liquid VP: 8.61E-006 mm Hg (25 deg C, Mod-Grain method)
```



Full KOWWIN Output for Triclosan

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	12	Aromatic Carbon	0.2940	3.5280
Frag	3	-CL [chlorine, aromatic attach]	0.6445	1.9335
Frag	1	-OH [hydroxy, aromatic attach]	-0.4802	-0.4802
Frag	1	-O- [aliphatic O, two aromatic attach]	0.2923	0.2923
Factor	1	Ortho-sub on di-aromatic ether (non-cyl)	-0.8396	-0.8396
Const		Equation Constant		0.2290

Log Kow = 4.6630

EPI 2006 enhancements: octanol/air partition coefficient (K_{OA}) via KOAWIN model

- K_{OA} = Conc. in *n*-Octanol / Conc. in Air

  Importance (uses in prediction):

  - Soil - Air partitioning
  - Vegetation - Air partitioning
  - Aerosol - Particulate partitioning
  - Bioaccumulation by terrestrial biota
  - Long-range transport potential (LRTP)

EPI 2006 enhancements: fraction of airborne substance on particles (φ), via AEROWIN

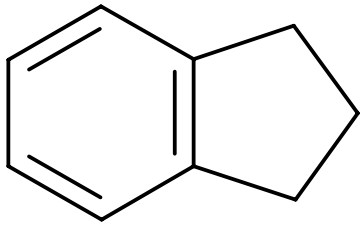
- Distribution of an airborne chemical between particulate and gas phases is a key factor controlling photooxidation and deposition
- Fraction of chemical in the particulate phase (φ) is highly dependent upon VP
- Reactivity of particle-bound chemicals is poorly understood. It is generally assumed, but not always true, that bound chemical is unreactive

Summary Output for AEROWIN and AOPWIN: Triclosan

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 0.00115 Pa (8.61E-006 mm Hg)
Log Koa (Koawin est): 11.450
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 0.00261
Octanol/air (Koa) model: 0.0692
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 0.0862
Mackay model : 0.173
Octanol/air (Koa) model: 0.847

Atmospheric Oxidation (25 deg C) [AOPWIN v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 16.1147 E-12 cm3/molecule-sec
Half-Life = 0.664 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life = 7.965 Hrs
Ozone Reaction:
No Ozone Reaction Estimation
Reaction With Nitrate Radicals May Be Important!
Fraction sorbed to airborne particulates (phi): 0.13 (Junge,Mackay)
Note: the sorbed fraction may be resistant to atmospheric oxidation

BioHCWIN v1.01
Sample Results: Indane



TYPE	NUM	LOG Hydrocarbon FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Aromatic-CH2	0.1774	0.3548
Frag	4	Aromatic-H	0.0419	0.1678
Frag	1	-CH2- [cyclic]	0.0888	0.0888
Frag	1	Number of fused acyclic rings	0.5817	0.5817
Frag	1	Number of fused 6-carbon aromatic rings	0.0887	0.0887
Frag	1	Indane	-1.3080	-1.3080
Const	*	Equation Constant		0.4898
RESULT		LOG BioHC Half-Life (days)		0.4635
RESULT		BioHC Half-Life (days)		2.907

Other EPI Suite™ Programs

ECOSAR

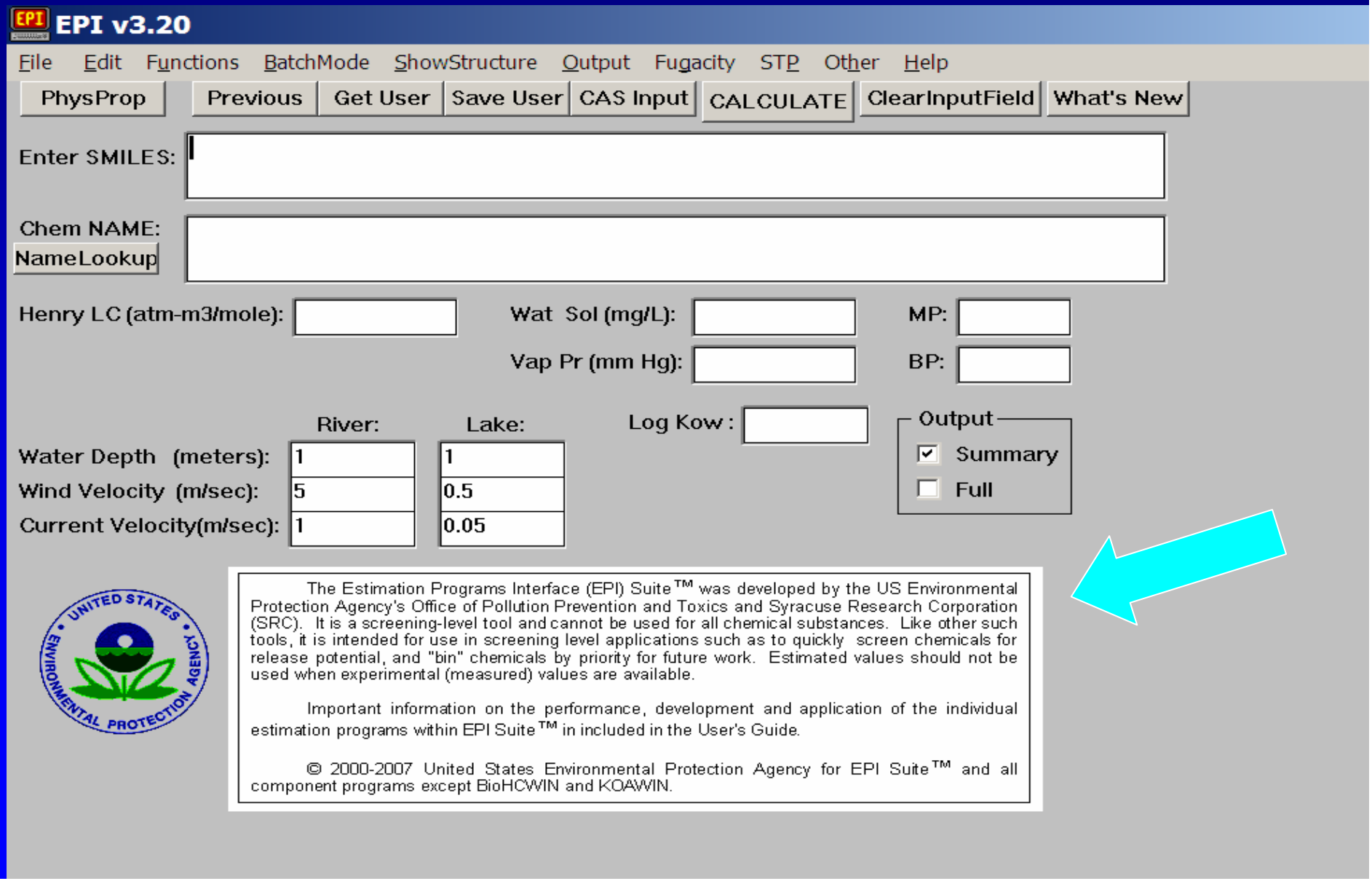
- Discussed in Tala Henry's poster
- Library of QSARs for predicting aquatic toxicity and an Expert System for selecting the appropriate QSAR
- Runs automatically as integral part of EPI Suite™; also available by free download at: www.epa.gov/oppt/newchems/tools/21ecosar.htm

Dermwin v1.43

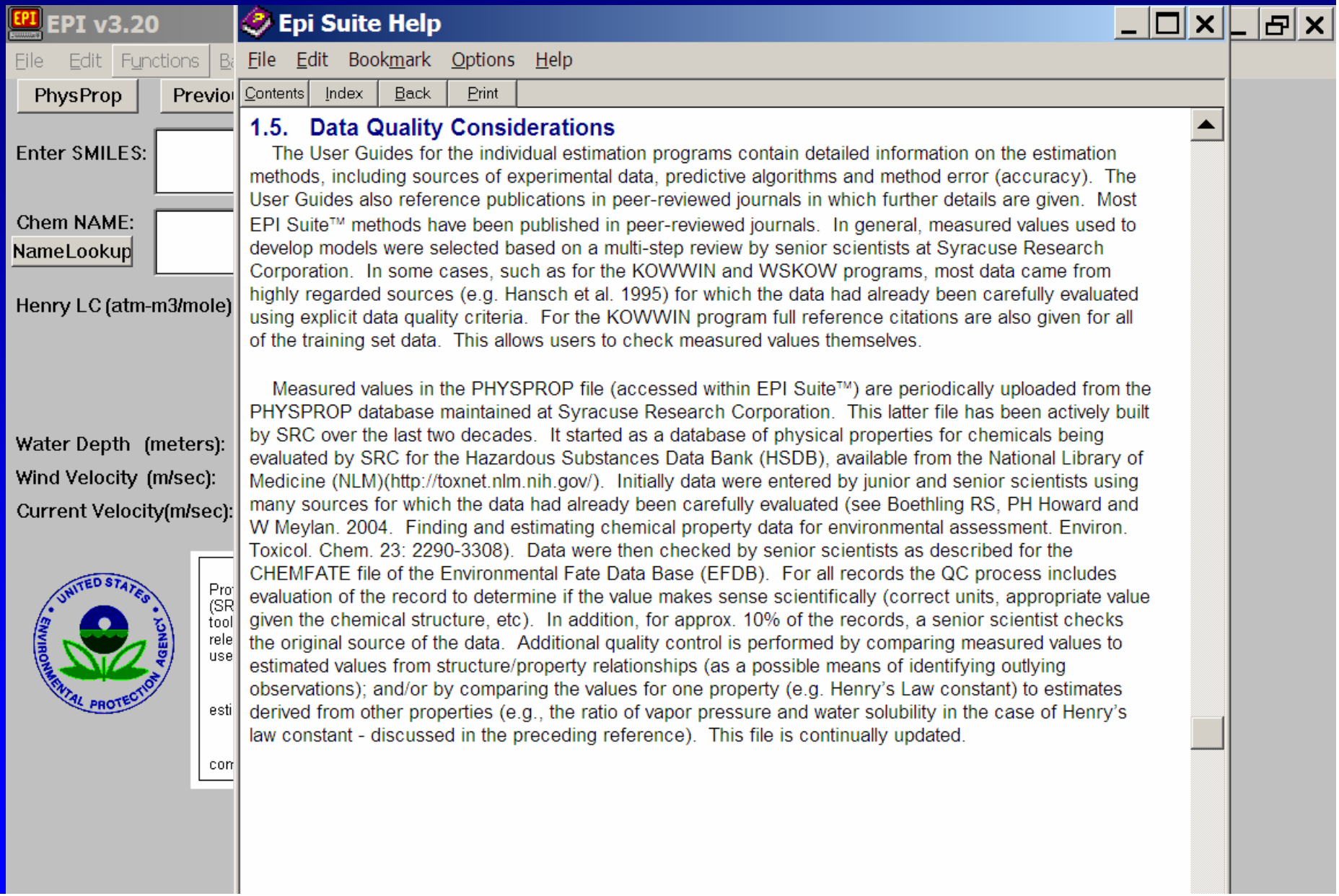
-- Dermal permeability coefficient from log Kow (KOWWIN)

-- Runs only from EPI Suite™ subdirectory, not data entry screen

EPI Suite™: Appropriate Use



EPI Suite™: Data Quality



2005/6 Science Advisory Board (SAB) Review of EPI Suite™

- The charge: evaluate

  -- The supporting science for comprehensiveness, accuracy, validation

  -- Functionality: program documentation, user interface, etc

  -- Whether EPI Suite™ is being used appropriately

- The SAB concluded that

  -- EPI Suite™ is based on sound science and is user friendly, transparent, cost effective

  --Accuracy is sufficient to support regulatory screening

  --Numerous changes can be made to enhance scope, accuracy, ease of use

- December 2006 "Quality Review Draft" available at www.epa.gov/sab/panels/epi_suite_review_panel.htm

EPI Suite™ Enhancements 2007/2008

- Existing programs: update
  - PCKOCWIN; HYDROWIN
- Add new properties and models
  - Bioaccumulation factor (BAF) and "Apparent K_m" (fish metabolism) model to BCFWIN; add pK_a
- Model accuracy issues
  - Domain; uncertainty; confidence interval; validation
- Transparency issues
  - Help files; international units; temperature dependence; complex mixtures
- Functionality—many SAB suggestions
  - Example: add ability to launch individual programs from main EPI screen

For More Information

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- Internet
  - Latest version (v3.20) dated Feb 2007
  - *FREE* download at
    http://www.epa.gov/opptintr/exposure/pubs/episuite.htm