

## **User's Manual**

### **Swimmer Exposure Assessment Model (SWIMODEL) Version 3.0**

U.S. Environmental Protection Agency  
Office of Pesticide Programs  
Antimicrobials Division

November 2003

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## 1.0 INTRODUCTION

The exposure equations used in the Swimmer Exposure Model (SWIMODEL) were originally conceived by the U.S. Environmental Protection Agency (U.S. EPA) Office of Pesticide Programs (OPP) Antimicrobials Division (AD). These equations are used to develop screening exposure estimates tailored to swimmers exposed to pool chemicals and breakdown products in indoor pools and spas (Dang, 1996). This model is a modification of a study used by Beech (1980) for estimating exposure to trihalomethanes (THMs) in swimming pools. The model uses well-accepted screening exposure assessment equations to calculate swimmers' total exposure expressed as a mass-based intake value (mg/event), or lifetime average daily dose (mg/kg/day). SWIMODEL focuses on potential chemical intakes only, it does not take into account metabolism or excretion of the chemical of concern.

Versar, Inc. was requested by EPA to computerize the SWIMODEL building on the equations of EPA. The software includes a number of useful default values (e.g., body weights and surface area values for children and adults, and physico-chemical data for several common trihalomethane pool water contaminants, etc.) The user also has the option of inserting his/her own data values for other chemical compounds of interest.

The user may generate exposure estimates for either of the three exposure routes in the "abridged" calculation (i.e., oral, inhalation and dermal) or for six exposure routes in the "full" calculation (i.e., oral, dermal, inhalation, buccal/sublingual, nasal/orbital, and aural routes). In addition, a user may calculate an exposure estimate based on any single or combination of exposure routes.

If the user selects one of the chemicals carried in the SWIMODEL pick-list, only a water concentration value is required to calculate an exposure estimate. SWIMODEL can estimate an air concentration from the water concentration data point using one of two basic methods, Henry's Law or Raoult's Law. However, for best results, it is recommended that an empirically derived ambient indoor air data point be obtained.

Should the user define a chemical of concern that is not on the SWIMODEL pick-list, data inputs required are:

- Concentration of the chemical of concern found in water ( $C_w$ );
- Permeability coefficient of the chemical of concern ( $K_p$ ); and
- Octanol/water partition coefficient of the chemical of concern ( $K_{ow}$ ) (required for the aural exposure route).

For inhalation route exposure, required data inputs are:

- Ambient vapor concentration value that is empirically measured ( $C_{vp}$ );
- Molecular weight of the chemical of concern (MW);
- Vapor pressure of the chemical of concern at a relevant temperature ( $V_p$ );
- Solubility of the chemical of concern in water at a relevant temperature (Sol); and
- Henry's law constant for the chemical of concern (H).

## 1.1 Limitations and Caveats

- SWIMODEL focuses on chemical intakes only. It does not account for metabolism or excretion of the chemical of concern.
- SWIMODEL uses the following absorption factors for each route of exposure:
  - *Ingestion:* 100% absorption of ingested chemical is assumed
  - *Dermal:* Chemical-specific dermal  $K_p$  is used
  - *Inhalation:* 100% absorption of inhaled chemical is assumed
  - *Buccal/Sublingual:* 1% absorption is generally assumed (may be adjusted)
  - *Orbital/Nasal:* Assumed by default to be equivalent to Buccal/Sublingual exposure
  - *Aural:* Chemical-specific dermal  $K_p$  and  $K_{ow}$  are used
- Dermal exposure estimates are predicated on a one compartment model of the skin. The rate-limiting step is penetration of the stratum corneum. The model uses Fick's Law of Diffusion to calculate a general exposure value, without regard for differences in the skin permeability of specific body parts.
- Dermal permeability values for organic and inorganic chemicals are estimated based on the equation recommended in the EPA Dermal Exposure Assessment : Principles and Applications (EPA, 1992), non-steady state values based on the molecular weight and the log  $K_{ow}$  partitioning coefficient (i.e., lipophilicity).
- The effects of exercise on chemical intake can be adjusted for the inhalation exposure route only in SWIMODEL.
- SWIMODEL does not account for the effect of ambient temperature on intake.

## 1.2 When to Use the SWIMODEL

SWIMODEL can be used to estimate exposure when the following circumstances exist:

- Dosimeter estimation techniques are not appropriate.
- Information on hydrolysis, degradation, and photolysis of the parent compound in water is available, but not required.
- Basic physico-chemical properties of the compound (i.e., molecular weight, vapor pressure, solubility, permeability coefficient, octanol/water partition coefficient) are known.
- The solubility of compound in water is known.
- The expected mean and maximum water concentrations of the chemical of concern in a swimming pool at the maximum label use rate is known.
- The compound demonstrates the following potential to be absorbed into the body:

- *Inhalation*      The chemical must be volatile and should not be directly reactive with tissues (e.g., chlorine is not an appropriate candidate for the SWIMODEL).
- *Dermal*            Skin absorption is favored by chemicals with low molecular weight and a high  $K_{ow}$ .
- *Ingestion*        There should be evidence of gastrointestinal absorption after ingestion.

Gas phase concentrations are based on an ideal gas model and Raoult's law. However, for chloroform, Raoult's Law was found to underestimate, and Henry's Law to overestimate, measured ambient air concentrations.

### 1.3 When Not to Use the SWIMODEL

SWIMODEL should not be used to estimate exposure when the following circumstances exist:

- The exposure assessment is for outdoor inhalation exposure. The SWIMODEL inhalation exposure route is only applicable to indoor exposure assessment calculations.
- Information is not available to indicate that absorption for a given exposure route is possible. Use of any of the equations for a given route of exposure must be based on knowledge or professional judgement that absorption by that route is possible. Otherwise, exposure estimates will be too conservative.
- It is inappropriate to use  $C_w$  values to estimate  $C_{vp}$  values (using Henry's Law or Raoult's Law, for example) for input to the inhalation exposure equation when:
  - the chemical in question is NOT volatile, or
  - the chemical is an acutely-toxic irritant or reactive gas (e.g., chlorine).

### 1.4 Installation

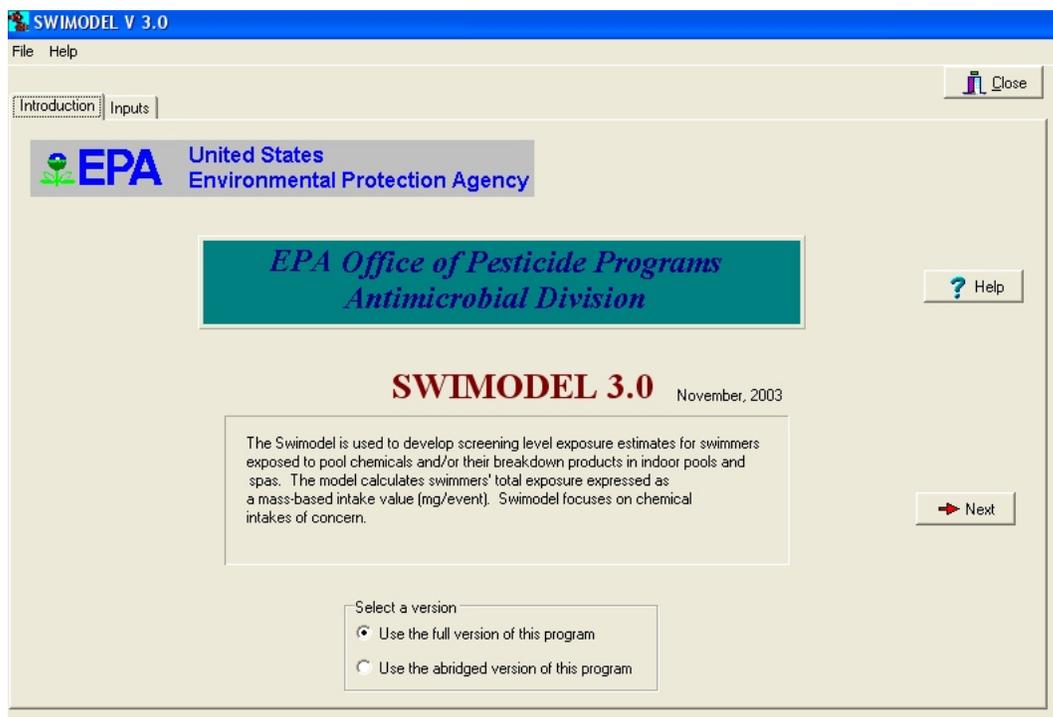
SWIMODEL has the following system requirements:

- At least 13 MB of free disk space (24 MB if downloading the installation file);
- 32 MB of RAM;
- Windows XP, 2000, 98, 95, or NT operating system; and
- 800 x 600 screen resolution.

To install SWIMODEL, download the swiminst.exe file from the EPA web site and run the installation program. Follow the instructions on the screen to complete the installation. The installation program will create an icon on the desktop and a program folder on the Programs list in the Start menu.

## 2.0 SWIMODEL INTRODUCTION

The SWIMODEL **Introduction** screen is depicted below (Figure 2-1).



**Figure 2-1. SWIMODEL Introduction Screen**

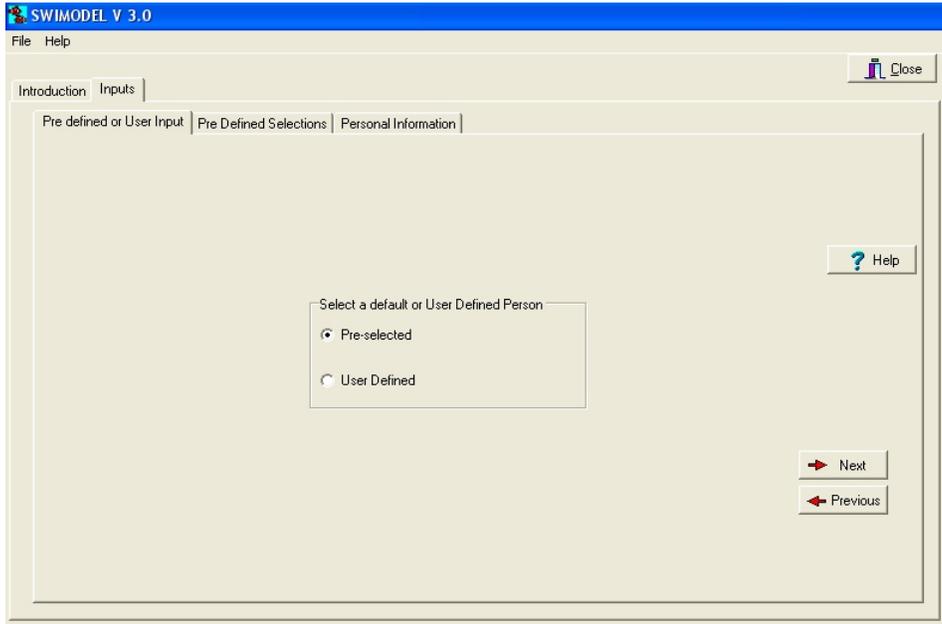
This screen allows the user to select either the full or abridged version of the program. The full version of the program allows for one to generate exposure estimates for all exposure routes. The user also has the option of disabling selected exposure routes.

The abridged version allows generation of exposure estimates for three exposure routes: oral, inhalation and dermal exposure routes. As with the full version, any of the exposure routes can be disabled when calculations are performed.

Once a selection has been made, click the “**Next**” button located on the lower right side of the screen. This button will display the **Personal Information** screen.

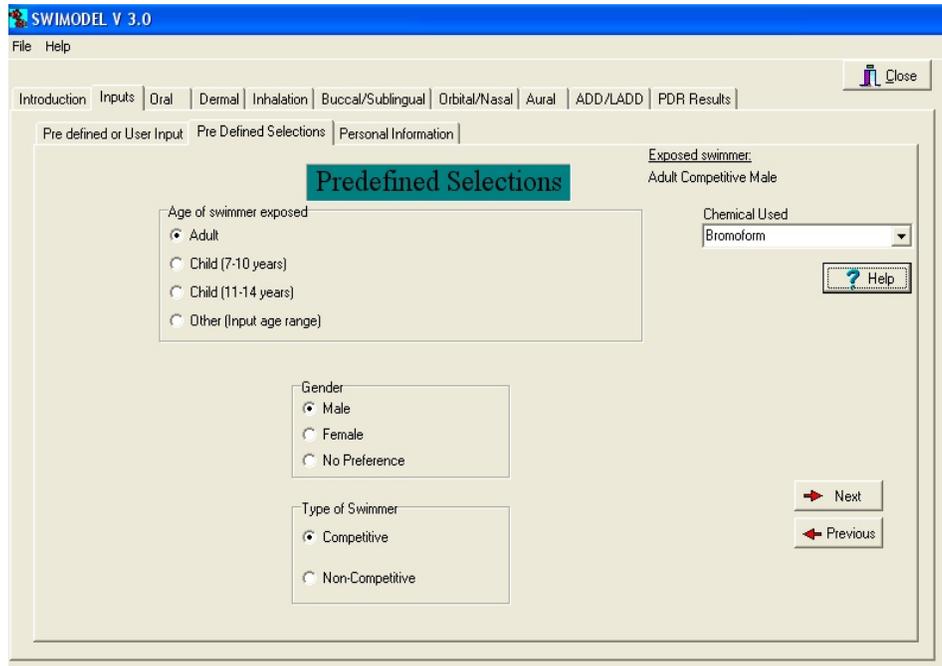
### 3.0 PERSONAL INFORMATION

Depicted below is the first tab of the **Inputs** screen (Figure 3-1). This tab allows the assessor to select a pre-defined swimmer or create a user defined swimmer for the exposure scenario. If a pre-defined swimmer is selected, then select the “**Next**” button to continue to the **Pre Defined Selections** screen.



**Figure 3-1. Inputs Screen**

Figure 3-2 below represents the **Pre Defined Selections** tab.

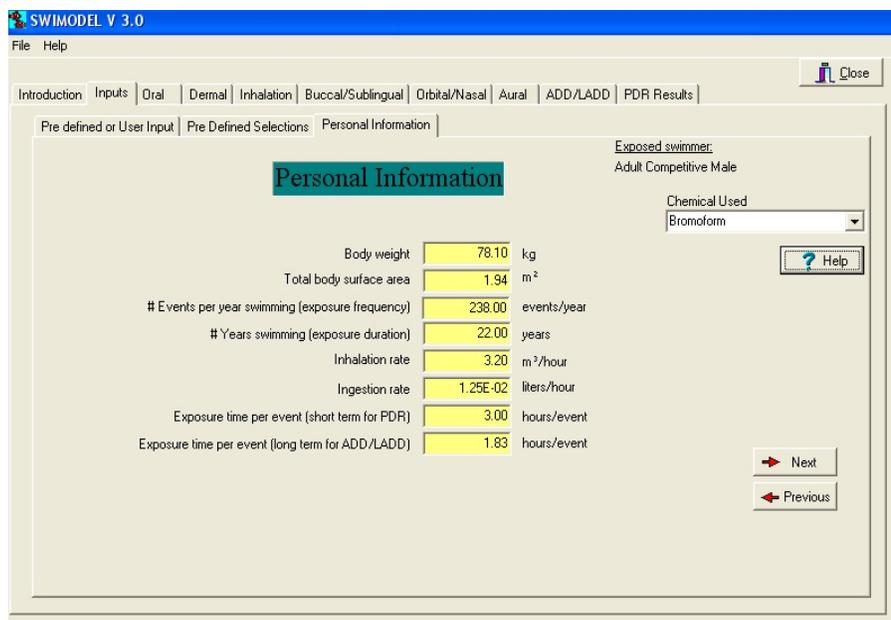


**Figure 3-2. Pre defined Selections Screen**

In this screen, the assessor can select the age, gender, and competitive level of the swimmer. There are eight pre-defined swimmers in SWIMODEL:

- Adult competitive male,
- Adult competitive female,
- Younger competitive child (7-10 years old),
- Older competitive child (11-14 years old),
- Adult non-competitive male,
- Adult non-competitive female,
- Younger non-competitive child (7-10 years old), and
- Older non-competitive child (11-14 years old).

Selection of the type of pre-defined swimmer is accomplished by choosing the desired combination of age, gender, and type of swimmer shown on the **Pre defined Selections** screen. If the assessor wishes to input an age range, the last radio button in the “Age of swimmer exposed” box should be selected and the lower and upper ends of the age range should be input. When using this selection, the assessor can make adjustments to assumption regarding each year of the swimmer's exposure (discussed in detail later in this section). Once the selections have been made, press the “**Next**” button. This will



**Figure 3-3. Personal Information Screen**

bring up the **Personal Information** screen shown in Figure 3-3, below.

The **Personal Information** screen shows the default values for physical parameters (e.g., skin surface area, body weight) and exposure times assumed for the selected swimmer (note - this appearance of this screen is different when individual ages for a custom age range are selected). These default values appear in yellow fields, which indicate that the user can modify the data and override the recommended values shown (note - data shown in blue fields cannot be changed). Default values for the input parameters shown on the **Personal Information** screen are presented in Tables 3-1 through 3-6, below.

Table 3-1, below, lists the pre-defined skin surface areas and body weights for each of the pre-defined swimmers.

**Table 3-1. Default surface areas and body weights for pre-defined swimmers.**

Age (years)	Surface Area (m <sup>2</sup> )	Reference	Body Weight (kg)	Reference
Younger child (7-10 years)	1.04	Average of male and female 50 <sup>th</sup> percentiles for ages 7<8, 8<9, 9<10, and 10<11 from Tables 6-6 & 6-7 of EFH.	30.2	Average of 7, 8, 9, 10 year old girls & boys, Table 7-3 of EFH.
Older child (11-14 years)	1.42	Average of male and female 50 <sup>th</sup> percentiles for ages 11<12, 12<13, 13<14, and 14<15 from Tables 6-6 & 6-7 of EFH.	48.2	Average of 11, 12, 13, 14 year old girls & boys, Table 7-3 of EFH.
Adult male	1.94	50 <sup>th</sup> percentile value from Table 6-4 of EFH.	78.1	Average of 18-75 years, Table 7-2 of EFH.
Adult female	1.69	50 <sup>th</sup> percentile value from Table 6-4 of EFH.	65.4	Average of 18-75 years, Table 7-2 of EFH.
Adult <sup>a</sup>	1.82	Average of 50 <sup>th</sup> percentile values from Table 6-4 of EFH.	71.8	Average of 18-75 years, Table 7-2 of EFH

EFH = Exposure Factors Handbook (U.S. EPA, 1997).

a No gender preference selected.

Recommended values for the number of events per year of swimming for each pre-defined swimmer are presented in Table 3-2. The values for competitive swimmers are based on estimates reported in a study sponsored by the American Chemistry Council and entitled “An Analysis of the Training Patterns and Practices of Competitive Swimmers” (2002). The subject report provides information on a relatively recent survey that was conducted among coaches of amateur and collegiate swim teams to elicit data on swimming habits that might be useful in refining the exposure assumptions used in EPA’s SWIMODEL. A total of 45 geographically distributed amateur swim team coaches and 45 collegiate swim team coaches were interviewed to gather data on 4 groups of competitive swimmers:

- Young Children (Amateur- 7-10 years old),
- Youth (Amateur- 11-14 years old),
- Adult (Amateur- Masters level), and
- Adult (Collegiate level).

Information on exposure frequency was estimated based on the fraction of the year that teams practiced. For example, for young children, ages 7 to 10 years old, the exposure frequency was determined as follows:

$$\text{Exposure frequency}_{\text{children, 7-10}} = \frac{2.5 \text{ hrs practice}}{\text{week}} \times \frac{6 \text{ months/year}}{12 \text{ months/year}} \times \frac{52 \text{ weeks}}{\text{year}}$$

For non-competitive swimmers, the exposure frequencies were based on data in EPA's Exposure Factors Handbook (U.S. EPA, 1997) summarizing the number of times survey respondents went swimming in a month in a freshwater swimming pool.

**Table 3-2. Default exposure frequencies (swimming events per year) for pre-defined swimmers.**

Age	Competitive		Non-competitive	
	Events/yr	Reference	Events/yr	Reference
7-10 years	65	Mean ACC recommendation <sup>a</sup> .	120	90 <sup>th</sup> percentile rate from Table 15-65 of EFH <sup>b</sup> .
11-14 years	189	Mean ACC recommendation <sup>c</sup> .	120	90 <sup>th</sup> percentile rate from Table 15-65 of EFH <sup>b</sup> .
Adult male	238	Mean ACC value for collegiate swimmers <sup>d</sup> .	120	90 <sup>th</sup> percentile rate from Table 15-65 of EFH <sup>b</sup> .
Adult female	238	Mean ACC value for collegiate swimmers <sup>d</sup> .	120	90 <sup>th</sup> percentile rate from Table 15-65 of EFH <sup>b</sup> .
Adult <sup>e</sup>	238	Mean ACC value for collegiate swimmers <sup>d</sup> .	120	90 <sup>th</sup> percentile rate from Table 15-65 of EFH <sup>b</sup> .

ACC = American Chemistry Council, “An Analysis of the Training Patterns and Practices of Competitive Swimmers”, 2002.  
 EFH = Exposure Factors Handbook (U.S. EPA, 1997).

- a Mean value for younger competitive child. ACC (2002) assumed (2.5 events/week) x (52 weeks/year) x (6 month/year)/(12 months/year).
- b 90<sup>th</sup> percentile times spent in an outdoor pool or spa over a 24-hour period from EFH.
- c Mean value for older competitive child. ACC (2002) assumed (4 events/week) x (52weeks/year) x (11 months/year)/(12 months/year).
- d Mean values for master's and collegiate swimmers ranged from 187to 238 days/year. For collegiate swimmer, ACC assumed (5 events/week) x (52 weeks/year) x (11 months/year)/(12 months/year).
- e No gender preference.

Default values for exposure duration are shown, below, in Table 3-3.

**Table 3-3. Default exposure durations - number of years swimming (years).**

Age	Competitive		Non-competitive	
	# of years	Reference	# of years	Reference
7-10 years	4	Represents number of years in age range.	4	Represents number of years in age range.
11-14 years	4	Represents number of years in age range.	4	Represents number of years in age range.
Adult male	22	Based on ACC (2002). <sup>a</sup>	30	Table 15-176 of EFH. <sup>b</sup>
Adult female	22	Based on ACC (2002). <sup>a</sup>	30	Table 15-176 of EFH. <sup>b</sup>
Adult <sup>c</sup>	22	Based on ACC (2002). <sup>a</sup>	30	Table 15-176 of EFH. <sup>b</sup>

ACC = American Chemistry Council, “An Analysis of the Training Patterns and Practices of Competitive Swimmers”, 2002.  
 EFH = Exposure Factors Handbook (U.S. EPA 1997).

- a Represents 4 years of collegiate swimming plus 18 years of masters swimming.
- b Value represents the 95<sup>th</sup> percentile for population mobility (i.e., time that an individual would spend living at one residence).
- c No gender preference selected.

The SWIMODEL default inhalation rates are based on short-term exposure durations taken from the Exposure Factors Handbook (U.S. EPA, 1997). For competitive swimmers, rates based on a heavy

activity level are used. For non-competitive swimmers, rates based on a light activity level are used for all ages. Inhalation rates for pre-defined swimmers are shown in Table 3-4.

**Table 3-4. Default inhalation rates for pre-defined swimmer scenarios.**

Age	Competitive		Non-competitive	
	Inhalation rate	Reference	Inhalation rate	Reference
7-10 years	1.9	Table 5-23 of EFH; short-term exposures, heavy activity.	1.0	Table 5-23 of EFH; short-term exposures, light activity.
11-14 years	1.9	Table 5-23 of EFH; short-term exposures, heavy activity.	1.0	Table 5-23 of EFH; short-term exposures, light activity.
Adult male	3.2	Table 5-23 of EFH; short-term exposures, heavy activity.	1.0	Table 5-23 of EFH; short-term exposures, light activity.
Adult female	3.2	Table 5-23 of EFH; short-term exposures, heavy activity.	1.0	Table 5-23 of EFH; short-term exposures, light activity.
Adult	3.2	Table 5-23 of EFH; short-term exposures, heavy activity.	1.0	Table 5-23 of EFH; short-term exposures, light activity.

EFH = Exposure Factors Handbook (U.S. EPA, 1997).

Table 3-5 presents the recommended ingestion rates for the pre-defined and user defined scenarios. The SWIMODEL assumes an ingestion rate of 50 mL/hour for non-competitive children and 25 mL/hour for non-competitive adults. The 50 mL/hr value is the value used in EPA Office of Pesticide Programs' Standard Operating Procedures (2000), and is based on a recommendation from EPA's RAGs, Part A (U.S. EPA, 1989). The American Chemistry Council (ACC) report entitled "An Analysis of the Training Patterns and Practices of Competitive Swimmers" suggests that the pool water ingestion rate for recreational swimmers is approximately 21 mL/hour for adults and 49 mL/hour for children (based on an EPA pilot study). Based on ACC recommendations for competitive swimmers, ½ the ingestion rate of recreational swimmers was assumed.

**Table 3-5. Default ingestion rates for predefined swimmers.**

Age	Competitive		Non-competitive	
	Ingestion rate	Reference	Ingestion rate	Reference
7-10 years	50	½ the rate used for non-competitive swimmers, as recommended by ACC (2002).	50	EPA, 1989 and 1997; ACC, 2002 - based on EPA pilot study.
11-14 years	25	½ the rate used for non-competitive swimmers, as recommended by ACC (2002).	50	EPA, 1989 and 1997; ACC 2002 - based on EPA pilot study.
Adult male	12.5	½ the rate used for non-competitive swimmers, as recommended by ACC (2002).	25	ACC, 2002 - based on EPA pilot study.
Adult female	12.5	½ the rate used for non-competitive swimmers, as recommended by ACC (2002).	25	ACC, 2002 - based on EPA pilot study.
Adult	12.5	½ the rate used for non-competitive swimmers, as recommended by ACC (2002).	25	ACC, 2002 - based on EPA pilot study.

ACC = American Chemistry Council, "An Analysis of the Training Patterns and Practices of Competitive Swimmers", 2002.  
 Risk Assessment Guidance for Superfund, Volume 1, Human Health Evaluation Manual (Part A) (U.S. EPA, 1989).  
 Exposure Factors Handbook (U.S. EPA, 1997).

The SWIMODEL considers exposure in terms of two time frames: short-term and long-term. The Potential Dose Rate (PDR) is calculated to assess short-term exposure, using a high-end estimate of exposure time per event, in order to represent a maximum, one-time exposure. When longer exposures are considered, such as when calculating the Average Daily Dose (ADD) and Lifetime Average Daily Dose (LADD), the duration of each swimming event is assumed to be shorter, since, over time, event duration would represent an average of maximum and minimum exposures. Default swimming exposure times for short-term and long-term exposures are presented in Tables 3-6 and 3-7, respectively.

**Table 3-6. Default swimming exposure times (hours/event) for pre-defined swimmers for short-term exposures.**

Age	Competitive		Non-Competitive	
	Hours per event	Reference	Hours per event	Reference
7-10 years	1	Consistent with ACC survey and USA Swimming Guidelines.	5	90 <sup>th</sup> percentile value for time spent in an outdoor pool for age 5-11 yrs from Table 15-119 of EFH.
11-14 years	2	Consistent with ACC survey mean values and USA Swimming Guidelines.	3	90 <sup>th</sup> percentile value for time spent in an outdoor pool for age 12-17 yrs from Table 15-119 of EFH.
Adult Male	3	Upper-end of ACC survey mean values.	5	90 <sup>th</sup> percentile value for time spent in an outdoor pool from Table 15-119 of EFH.
Adult Female	3	Upper-end of ACC survey mean values.	5	90 <sup>th</sup> percentile value for time spent in an outdoor pool from Table 15-119 of EFH.
Adult	3	Upper-end of ACC survey mean values.	5	90 <sup>th</sup> percentile value for time spent in an outdoor pool from Table 15-119 of EFH.

ACC = American Chemistry Council, “An Analysis of the Training Patterns and Practices of Competitive Swimmers” (2002).  
 EFH = Exposure Factors Handbook (U.S. EPA, 1997).

**Table 3-7. Default swimming exposure times (hours/event) for pre-defined swimmers for long-term exposures.**

Age	Competitive		Non-competitive	
	Hours per event	Reference	Hours per event	Reference
7-10 years	1	Based on ACC survey chronic exposure times.	2.3	50 <sup>th</sup> percentile value for time spent in an outdoor pool for age 5-11 yrs from Table 15-119 of EFH.
11-14 years	1.65	Based on ACC survey chronic exposure times.	1.7	50 <sup>th</sup> percentile value for time spent in an outdoor pool for age 12-17 yrs from Table 15-119 of EFH.
Adult Male	1.83	Based on ACC survey chronic exposure times. <sup>a</sup>	1.3	50 <sup>th</sup> percentile value for time spent in an outdoor pool from Table 15-119 of EFH.
Adult Female	1.83	Based on ACC survey chronic exposure times. <sup>a</sup>	1.3	50 <sup>th</sup> percentile value for time spent in an outdoor pool from Table 15-119 of EFH.
Adult Male/Female	1.83	Based on ACC survey chronic exposure times. <sup>a</sup>	1.3	50 <sup>th</sup> percentile value for time spent in an outdoor pool from Table 15-119 of EFH.

ACC = American Chemistry Council, “An Analysis of the Training Patterns and Practices of Competitive Swimmers”, 2002.  
 EFH = Exposure Factors Handbook (U.S. EPA 1997).

a Weighted average of values for collegiate and masters swimmers:  
 $[4 \text{ years} \times (625 \text{ hrs/yr} / 238 \text{ events/yr}) + 22 \text{ years} \times (309 \text{ hrs/yr} / 187 \text{ events/yr})] / 22 \text{ years}$ .

Finally, the desired chemical should be selected from the list box labeled “**Chemical Used,**” found in the upper left corner of either the **Pre Defined Selections** or **Personal Information** screens. There are five chemicals to choose from in the original list. As with the “**Exposed Swimmer**” list box,

the assessor can input a new chemical by selecting the Generic entry in the “**Chemical Used**” list if all the associated values for the chemical are known. The five chemicals included in SWIMODEL are:

- Chloroform,
- Bromoform,
- Bromodichloromethane,
- Chlorodibromomethane, and
- Simazine.

After selecting a chemical and accepting the recommended values or making any desired changes, the assessor should click the “**Next**” button. This will display the **Oral Ingestion Exposure Route** screen.

### User-defined Age Ranges

If the assessor is interested in calculating exposures to a swimmer whose age is not represented by those of the pre-defined swimmer scenarios, the “**Other (Input age range)**” button from the **Pre Defined Selections** screen may be selected to define a custom age range. Figure 3-4 shows the **Pre Defined Selections** tab when a custom age range has been chosen for analysis. Two options are available when a custom age range is selected: exposure can be calculated for each age within the selected age range, or, alternately, the exposure for the average age of the selected age range can be calculated. The assessor should select the radio button representing the desired option shown beneath “How to use selected age range:” and select the “**Next**” button to continue to the **Personal Information** screen.

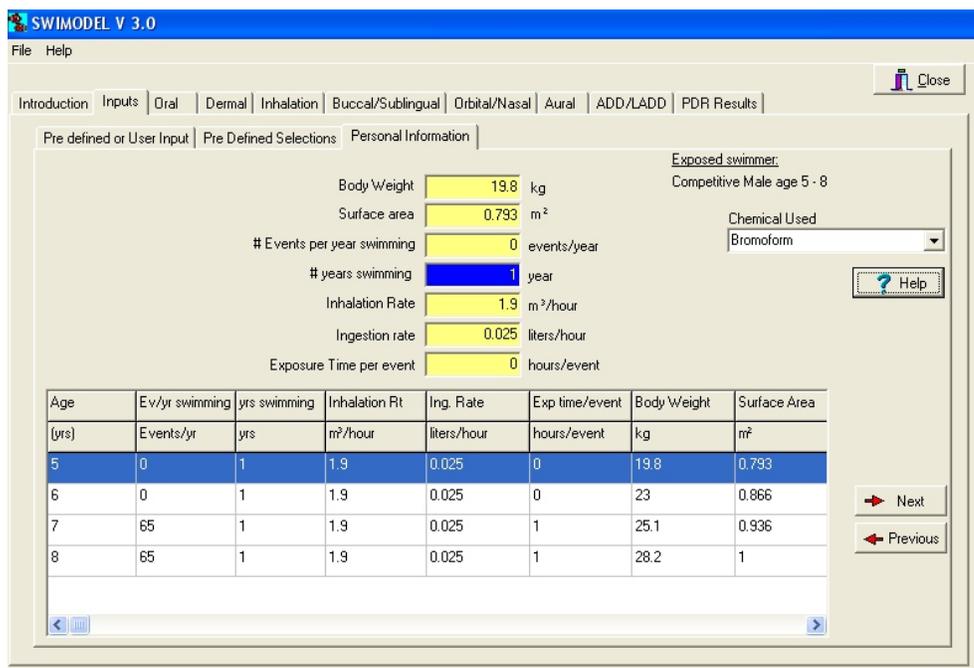
The screenshot shows the SWIMODEL V 3.0 software interface. The title bar reads "SWIMODEL V 3.0". Below the title bar is a menu bar with "File" and "Help". A tabbed interface is visible with tabs for "Introduction", "Inputs", "Oral", "Dermal", "Inhalation", "Buccal/Sublingual", "Orbital/Nasal", "Aural", "ADD/LADD", and "PDR Results". The "Oral" tab is active, and within it, the "Personal Information" sub-tab is selected. The main content area is titled "Personal Information" and contains the following fields:

Body weight	24.03	kg
Total body surface area	0.90	m <sup>2</sup>
# Events per year swimming (exposure frequency)	32.50	events/year
# Years swimming (exposure duration)	4.00	years
Inhalation rate	1.90	m <sup>3</sup> /hour
Ingestion rate	2.50E-02	liters/hour
Exposure time per event (short term for PDR)	0.50	hours/event
Exposure time per event (long term for ADD/LADD)	1.83	hours/event

Additional information on the right side of the screen includes: "Exposed swimmer: Competitive Male age 5 - 8", a dropdown menu for "Chemical Used" set to "Bromoform", a "Help" button, and "Next" and "Previous" navigation buttons at the bottom right.

**Figure 3-4. Pre Defined Selections Screen for Selected Age Range**

When “Use individual ages within range” button is selected, this screen will show the user-defined ages and the associated default values for each age (see Figure 3-5). Exposure parameters shown include body weight, body surface area, events per year swimming, years swimming, inhalation rate, ingestion rate, and exposure time per event. To modify any of the values, the assessor should highlight a desired age and



**Figure 3-5. Personal Information Screen for Selected Age Range**

modify the values in the yellow fields at the top of the screen. The recommended values for body weight and skin surface area for each age are shown in Table 3-8.

**Table 3-8. Recommended body surfaces areas and body weights for selected ages.**

Age (yrs)	Body surface area (m <sup>2</sup> )	Reference	Body weight (kg)	Reference
2<3	0.603 (male) 0.579 (female) 0.591 (no preference)	Tables 6-6 and 6-7 of EFH.	13.6 (male) 13.0 (female) 13.3 (no preference)	Tables 7-6 and 7-7 of EFH.
3<4	0.664 (male) 0.649 (female) 0.6565 (no preference)	Tables 6-6 and 6-7 of EFH.	15.7 (male) 14.9 (female) 15.3 (no preference)	Tables 7-6 and 7-7 of EFH.
4<5	0.731 (male) 0.706 (female) 0.7185 (no preference)	Tables 6-6 and 6-7 of EFH.	17.8 (male) 17.0 (female) 17.4 (no preference)	Tables 7-6 and 7-7 of EFH.
5<6	0.793 (male) 0.779 (female) 0.786 (no preference)	Tables 6-6 and 6-7 of EFH.	19.8 (male) 19.6 (female) 19.7 (no preference)	Tables 7-6 and 7-7 of EFH.

**Table 3-8. Recommended body surfaces areas and body weights for selected ages. (continued)**

<b>Age (yrs)</b>	<b>Body surface area (m<sup>2</sup>)</b>	<b>Reference</b>	<b>Body weight (kg)</b>	<b>Reference</b>
6<7	0.866 (male) 0.843 (female) 0.8545 (no preference)	Tables 6-6 and 6-7 of EFH.	23.0 (male) 22.1 (female) 22.55 (no preference)	Tables 7-6 and 7-7 of EFH.
7<8	0.936 (male) 0.917 (female) 0.9265 (no preference)	Tables 6-6 and 6-7 of EFH.	25.1 (male) 24.7 (female) 24.9 (no preference)	Tables 7-6 and 7-7 of EFH.
8<9	1.00 (male) 1.00(female) 1.00 (no preference)	Tables 6-6 and 6-7 of EFH.	28.2 (male) 27.9 (female) 28.05 (no preference)	Tables 7-6 and 7-7 of EFH.
9<10	1.07 (male) 1.06 (female) 1.065 (no preference)	Tables 6-6 and 6-7 of EFH.	31.1 (male) 31.9 (female) 31.5 (no preference)	Tables 7-6 and 7-7 of EFH.
10<11	1.18 (male) 1.17 (female) 1.175 (no preference)	Tables 6-6 and 6-7 of EFH.	36.4 (male) 36.1 (female) 36.25 (no preference)	Tables 7-6 and 7-7 of EFH.
11<12	1.23 (male) 1.30 (female) 1.265 (no preference)	Tables 6-6 and 6-7 of EFH.	40.3 (male) 41.8 (female) 41.05 (no preference)	Tables 7-6 and 7-7 of EFH.
12<13	1.34 (male) 1.40 (female) 1.37 (no preference)	Tables 6-6 and 6-7 of EFH.	44.2 (male) 46.4 (female) 45.3 (no preference)	Tables 7-6 and 7-7 of EFH.
13<14	1.47 (male) 1.48 (female) 1.475 (no preference)	Tables 6-6 and 6-7 of EFH.	49.9 (male) 50.9 (female) 50.4 (no preference)	Tables 7-6 and 7-7 of EFH.
14<15	1.61 (male) 1.55 (female) 1.58 (no preference)	Tables 6-6 and 6-7 of EFH.	57.1 (male) 54.8 (female) 55.95 (no preference)	Tables 7-6 and 7-7 of EFH.
15<16	1.70 (male) 1.57 (female) 1.635 (no preference)	Tables 6-6 and 6-7 of EFH.	61.0 (male) 55.1 (female) 58.05 (no preference)	Tables 7-6 and 7-7 of EFH.
16<17	1.76 (male) 1.60 (female) 1.68 (no preference)	Tables 6-6 and 6-7 of EFH.	67.1 (male) 58.1 (female) 62.6 (no preference)	Tables 7-6 and 7-7 of EFH.
17<18	1.80 (male) 1.63 (female) 1.715 (no preference)	Tables 6-6 and 6-7 of EFH.	66.7 (male) 59.6 (female) 63.15 (no preference)	Tables 7-6 and 7-7 of EFH.
18-24	1.94 (male) 1.69 (female) 1.815 (no preference)	Tables 6-2 and 6-3 of EFH.	73.8 (male) 60.6 (female) 67.2 (no preference)	Tables 7-4 and 7-5 of EFH.
25-34	1.94 (male) 1.69 (female) 1.815 (no preference)	Tables 6-2 and 6-3 of EFH.	78.7 (male) 64.2 (female) 71.45 (no preference)	Tables 7-4 and 7-5 of EFH.

**Table 3-8. Recommended body surfaces areas and body weights for selected ages. (continued)**

Age (yrs)	Body surface area (m <sup>2</sup> )	Reference	Body weight (kg)	Reference
35-44	1.94 (male) 1.69 (female) 1.815 (no preference)	Tables 6-2 and 6-3 of EFH.	80.9 (male) 67.1 (female) 74.0 (no preference)	Tables 7-4 and 7-5 of EFH.
45-54	1.94 (male) 1.69 (female) 1.815 (no preference)	Tables 6-2 and 6-3 of EFH.	80.9 (male) 68.0 (female) 74.45 (no preference)	Tables 7-4 and 7-5 of EFH.
55-64	1.94 (male) 1.69 (female) 1.815 (no preference)	Tables 6-2 and 6-3 of EFH.	78.8 (male) 67.9 (female) 73.35 (no preference)	Tables 7-4 and 7-5 of EFH.
65-74	1.94 (male) 1.69 (female) 1.815 (no preference)	Tables 6-2 and 6-3 of EFH.	74.8 (male) 66.6 (female) 70.7 (no preference)	Tables 7-4 and 7-5 of EFH.

EFH = Exposure Factors Handbook (EPA, 1997).

The recommended values for events per year swimming, years swimming, inhalation rate, ingestion rate, and exposure time per event are the same as those value shown in Tables 3-2 through 3-7. For events per year swimming and exposure time per event, no data are available for children under 7 years of age, and, thus, no values are recommended in SWIMODEL. The user must input assumed values for these two parameters in order to run the model.

If the assessor chooses the “Use as an average within range” button, the model will calculate exposures based on averaged values for body weight, surface body area, events per year swimming, years swimming, inhalation rate, ingestion rate, and exposure time per event using the model recommended values for the selected age range. In this instance, the **Personal Information** screen will look the same as that for the pre-defined swimmer (see Figure 3-3). Values can be modified by typing the desired value in the appropriate yellow fields. After accepting the recommended values or making any desired changes and selecting a chemical, the assessor should click the “**Next**” button to continue to the **Oral Ingestion Exposure Route** screen.

## 4.0 ORAL INGESTION EXPOSURE ROUTE

Figure 4-1, displayed below, represents the **Oral Ingestion Exposure Route** screen.

The screenshot shows the 'Oral Ingestion Exposure Route' screen in the SWIMODEL V 3.0 software. The interface includes a menu bar (File, Help) and a tabbed navigation system (Introduction, Inputs, Oral, Dermal, Inhalation, Buccal/Sublingual, Orbital/Nasal, Aural, ADD/LADD, PDR Results). The 'Oral' tab is active. The screen displays the following data and controls:

- Exposed swimmer:** Adult Competitive Male
- Chemical Used:** Bromoform (selected in a dropdown menu)
- Chemical concentration in water:** 50.00 µg/liter
- Ingestion rate:** 1.25E-02 liters/hour
- Exposure time:** 3.00 hours/event
- PDR<sub>oral</sub>:** 1.88E-03 mg/event
- Buttons:** View Final Results, Next, Previous
- Checkbox:** Use Oral route in calculations (checked)

**Figure 4-1. Oral Ingestion Exposure Route Screen**

The user must input the following values:

**Chemical concentration in water (µg/liter):** this is the concentration of the chemical selected in the “**Chemical Used**” list box. The value should reflect the maximum product use rate.

**Ingestion rate (liters/hour):** this is the amount of water that is actually swallowed by the swimmer. The default values are listed in Table 3-5 for various swimmers.

**Exposure time (hours/event):** this is the amount of time per event that the swimmer is actually in the pool. The default values for exposure time used to calculate PDR are listed in Table 3-6 for swimmer scenarios.

The total oral exposure per event is automatically calculated according to the following equation:

$$PDR_{\text{oral}} = ET \times IR \times C_w \times (1 \text{ mg}/1,000 \text{ } \mu\text{g})$$

where:

- PDR<sub>oral</sub> = Potential dose rate via oral exposure per event (mg/event),
- ET = Exposure time (hrs/event),
- IR = Ingestion rate (L/hr), and
- C<sub>w</sub> = Chemical concentration in water (µg/L).

Once all values for the **Oral Ingestion Exposure Route** screen have been entered, click the “**Next**” button to continue to the **Dermal Exposure Route** screen.

If the oral ingestion exposure route is not required, make sure to click the "**Use Oral route in calculations**" to deselect this route.

## 5.0 DERMAL EXPOSURE ROUTE

Figure 5-1 represents the **Dermal Exposure Route** screen.

**Figure 5-1. Dermal Exposure Route Screen**

The **Dermal Exposure Route** screen is used for organic chemicals only because this exposure calculation may generate overly conservative values for chemicals of concern that are inorganic or insoluble in water. For inorganic chemicals, it is recommended that this route be disabled by deselecting the "Use Dermal Route in calculations" check box.

The following values are required to calculate dermal exposure:

**Permeability Coefficient (Kp - cm/hr):** for pre-defined chemicals, a Kp value already exists. If the assessor is entering a new chemical, the Kp value for that chemical must be entered in cm/hour. The U.S. EPA recommends a default value of 1.0E-03 cm/hour for untested chemicals. Table 5-1 below lists the pre-defined chemicals and their associated Kp values (U.S. EPA, 1992).

**Table 5-1. Permeability coefficients (K<sub>p</sub>s) for available chemicals in SWIMODEL.**

Chemical Name	K <sub>p</sub> (cm/hour)
Chloroform	8.90E-03
Bromoform	2.60E-03
Bromodichloromethane	5.80E-03
Chlorodibromomethane	3.90E-03
Simazine	3.84E-03

**Chemical concentration in water (µg/liter):** chemical concentration in water is the concentration of the chemical that was selected in the “**Chemical Used**” list box. It should reflect the maximum product use rate.

**Total body surface area (SA) (m<sup>2</sup>):** Table 3-1 shows the type of swimmers and the associated body surface areas. The body surface area selected by the assessor is also shown in the **Personal Information** screen.

**Exposure time (hours/event):** exposure time is the amount of time per event that the swimmer is actually in the pool. Table 3-6 lists the types of swimmers and their associated exposure times (hours/event) used in calculating PDR.

The total dermal exposure per event is calculated according to the following equation:

$$PDR_{\text{dermal}} = ET \times SA \times K_p \times C_w \times (10,000 \text{ cm}^2/\text{m}^2) \times (0.001 \text{ L}/\text{cm}^3) \times (1 \text{ mg} / 1,000 \text{ } \mu\text{g})$$

where:

$PDR_{\text{dermal}}$	=	Potential dose rate via dermal exposure per day (mg/event),
ET	=	Exposure time (hrs/event),
SA	=	Surface area of exposed skin (m <sup>2</sup> ),
$C_w$	=	Concentration in water (µg/L), and
$K_p$	=	Chemical specific permeability coefficient (cm/hour).

Once all values for the **Dermal Exposure Route** screen have been entered, click the “**Next**” button to continue to the **Inhalation Exposure Route** screen.

If the dermal exposure route is not required, be sure to deselect the “**Use Dermal route in calculations**” checkbox.

## 6.0 INHALATION EXPOSURE ROUTE

Figure 6-1 below represents the **Inhalation Exposure Route** screen.

The screenshot shows the 'Inhalation Exposure Route' screen in SWIMODEL V 3.0. The interface includes a menu bar (File, Help) and a navigation bar with tabs for different exposure routes. The 'Inhalation' tab is selected. The screen displays various input fields and a calculated result. The 'Ambient vapor concentration' is 0.27 µg/m³. The 'Chemical concentration in water' is 50.00 µg/liter. The 'Vapor pressure of substance' is 5.51 torr. The 'Pool water temperature' is 25.00 °C. The 'Inhalation rate' is 3.20 m³/hour. The 'Exposure time (short term)' is 3.00 hours/event. The calculated 'PDR inhalation' is 2.56E-03 mg/event. The 'Chemical Used' is Bromoform. The 'Estimate Ambient vapor concentration' section has radio buttons for 'User Input', 'Henry's Law', and 'Raoult's Law' (selected). There are 'Next' and 'Previous' buttons. A checkbox 'Use Inhalation route in calculations' is checked. A 'View Final Results' button is at the bottom.

**Figure 6-1. Inhalation Exposure Route Screen**

The following values are input to calculate inhalation exposure:

**Ambient vapor concentration ( $C_{vp}$ ) ( $\mu\text{g}/\text{m}^3$ ):** the ambient vapor concentration is measured above the surface of the swimming pool (if available) or estimated using one of two methods: **Henry's Law** (preferred), or **Raoult's Law**. However, it is best to determine the ambient vapor concentration of the compound of interest above the surface of the indoor pool (or spa) at the maximum label use rate. The assessor should type this value directly into the **Ambient vapor concentration** box in the middle of the screen. The ambient vapor concentration should be in micrograms per cubic meter ( $\mu\text{g}/\text{m}^3$ ). Estimating the ambient vapor concentration from the chemical concentration in the water should be avoided if possible.

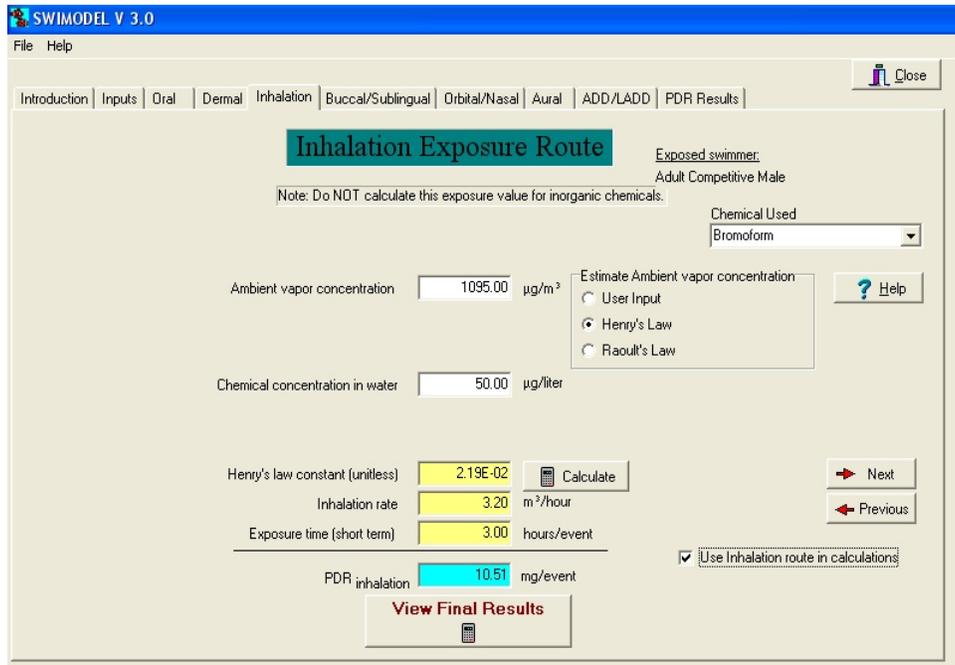
If the ambient vapor concentration cannot be measured and the chemical of concern is volatile and is not an acutely toxic irritant or reactive gas (like chlorine for example), then either Henry's Law or Raoult's Law can be used to estimate this value. It is recommended that Henry's Law be the preferred method, because Raoult's Law tends to be less reliable. If Henry's Law is used to estimate the ambient vapor concentration, click the **Henry's Law** radio button found beneath "Estimate ambient vapor concentration. The **Inhalation Exposure Route** screen will change to the screen shown in Figure 6-2. If one of the chemicals of concern provided in the pull down menu is being evaluated, the **Henry's law constant (unitless)** field will appear and the estimated ambient vapor concentration will be calculated as follows:

$$C_{vp} = H' \times C_w \times (1,000 \text{ L/m}^3)$$

where:

- $C_{vp}$  = Ambient air concentration ( $\mu\text{g/m}^3$ ),
- $H'$  = Unitless Henry's law constant, and
- $C_w$  = Concentration of chemical in water ( $\mu\text{g/L}$ ).

If the name of the chemical is not provided in the SWIMODEL and the unitless Henry's law constant value is not known, the user should click on the **Calculate** button next to the Henry's law constant field.



**Figure 6-2. Inhalation Exposure Route Screen Using Henry's Law Constant Calculations**

**Calculating the Henry's Law Constant in SWIMODEL**

6-3. The unitless Henry's law constant can be calculated using one of four choices shown in Figure



**Figure 6-3. Henry's Law Constant Calculation Screen**

**Choice A** requires the input of Henry's law constant in units of atm-m<sup>3</sup>/mole and the ambient air temperature in degrees C.

With these values, the unitless Henry's law constant is calculated as follows:

$$H' = HLC / (R \times (T + 273))$$

where:

- H' = Unitless Henry's law constant,
- HLC = Henry's law constant (atm-m<sup>3</sup>/mole),
- R = Gas constant (8.19e-05 atm-m<sup>3</sup>/mole-K), and
- T = Ambient air temperature (°C).

**Choice B** requires the input of solubility (mol/m<sup>3</sup>) and vapor pressure (torr). If neither H' or HLC (atm-m<sup>3</sup>/mol) values are available, the HLC may be estimated. However, this equation is ONLY valid when the data used to calculate HLC are for the same temperature and same physical state as the PURE compound. Knowing the solubility and vapor pressure, HLC first gets calculated as follows:

$$HLC = (V_p / 760) / Sol$$

where:

HLC = Henry's law constant (atm·m<sup>3</sup>/mole),  
 V<sub>p</sub> = Vapor Pressure (torr), and  
 Sol = Solubility (mole/m<sup>3</sup>).

Next, H' is calculated by using equation for **Choice A**.

**Choice C** relies on the solubility (mg/L), vapor pressure (torr), molecular weight of the chemical of concern, and the ambient air temperature (°C). With these values, H' is calculated as follows:

$$H' = (V_p \times MW) / (R \times Sol \times (T+273) \times (1 \text{ g}/1,000 \text{ mg}))$$

where:

V<sub>p</sub> = Vapor pressure (torr),  
 MW = Molecular weight (g/mole),  
 R = Gas constant (0.062 L-torr/mole-K),  
 Sol = Solubility (mg/L), and  
 T = Ambient air temperature (°C).

**Choice D** allows the use of a program called HenryWin to determine H'. The CAS number of the chemical or the SMILES notation needs to be entered and the **“Calculate”** button clicked. Then click the **“Save Results”** button to save the results to the default name of the file (e.g., henw0001.dat) and exit HenryWin. In some situations, the assessor may need to select between the bond and group estimation methods used in HenryWin. For more details on HenryWin, refer to the help screens within HenryWin.

Table 6-2 shows the chemicals available in SWIMODEL and their associated CAS numbers, molecular weights, vapor pressures, and unitless Henry's law constants.

**Table 6-1. Physical/chemical properties for chemicals available in SWIMODEL.**

Chemical	CAS #	MW (g/mole)	Vp (torr)	Henry's Law Constant (unitless)
Chloroform	67-66-3	119.4	197.6	0.15 @ 25°C
Bromoform	75-25-2	252.7	5.51	0.0219 @ 25°C
Bromodichloromethane	75-27-4	168.8	50.008	0.0667 @ 20°C
Chlorodibromomethane	124-48-1	208.3	4.864	0.0321 @ 20°C
Simazine	122-34-9	201.5	6.08E-9	1.75E-12 @ 20°C

If the ambient vapor concentration is being estimated using Raoult's Law, click on **Raoult's Law** radio button. Raoult's Law uses the vapor pressure (torr) of the chemical of concern and the pool temperature to calculate the ambient vapor concentration. The ambient vapor concentration will be estimated once the chemical concentration in water is entered. The following equation will be used by the SWIMODEL:

$$C_{vp} = C_w \text{ mg / L} * L / 1.0E + 06 \text{ mg water} * \left( \frac{MW_{\text{water}}}{MW_{\text{substance}}} \right) * \left( \frac{VP_{\text{substance}}}{760 \text{ mm Hg}} \right) * \left( \frac{273K}{\text{TempK}} \right) * \left( \frac{[MW_{\text{substance}} * 1,000 \text{ mg / g}]}{[22.4 \text{ L / mole} * \text{m}^3 / 1,000\text{L}]} \right)^w$$

here:

- VP<sub>substance</sub> = Vapor pressure of substance at a relevant temperature (see note below),
- MW<sub>water</sub> = Molecular weight of water (18 g/mole),
- TempK = Temperature of pool water (°K),
- C<sub>w</sub> = Concentration in water (µg/L), and
- C<sub>vp</sub> = Ambient air concentration (µg/m<sup>3</sup>).

Note: Since pool water and ambient air temperatures are usually warmer than 20°C or 25°C, this may be a potential source of error in the estimation calculations.

The **Inhalation rate (m<sup>3</sup>/hour)** and the **Exposure time (hours/event)** are dependent upon the swimmer's age and exercise level. The exposure time will be entered in automatically based on the person exposed option chosen. Table 3-4 shows the swimmer list and the corresponding default inhalation rates.

The total inhalation exposure per event is automatically calculated according to the following equation:

$$PDR_{\text{inhalation}} = C_{vp} \times ET \times IR \times (1 \text{ mg}/1,000 \text{ } \mu\text{g})$$

where:

- PDR<sub>inhalation</sub> = Potential dose rate via inhalation exposure per event (mg/event),
- C<sub>vp</sub> = Ambient concentration in air (µg/m<sup>3</sup> as vapor),
- ET = Exposure time (hours/event), and
- IR = Inhalation rate (m<sup>3</sup>/hour).

Once all values for the **Inhalation Exposure Route** screen have been entered, click the “**Next**” button to continue to the **Buccal/Sublingual Route** screen.

If the inhalation exposure route is not required, be sure to deselect the “**Use Inhalation route in calculations**” checkbox.

## 7.0 BUCCAL/SUBLINGUAL AND ORBITAL/NASAL ROUTES

The screen shown below (Figure 7-1) is the **Buccal/Sublingual Route** screen. This exposure calculation should not be performed if the chemical of concern is an inorganic or is not soluble in water.

SWIMODEL V 3.0

File Help

Introduction | Inputs | Oral | Dermal | Inhalation | Buccal/Sublingual | Orbital/Nasal | Aural | ADD/LADD | PDR Results

**Buccal/Sublingual Route**

Note: Do NOT calculate this exposure value for inorganic chemicals.

Exposed swimmer:  
Adult Competitive Male

Chemical Used  
Bromoform

Absorption rate 1.00E-02

Chemical concentration in water 50.00 µg/liter

Water intake 1.25 L/hour

Exposure time ((short term)) 3.00 Hours/event

PDR buccal/sublingual 1.88E-03 mg/event

View Final Results

Help

Next

Previous

Use Buccal route in calculations

Figure 7-1. Buccal/Sublingual Route Screen

This screen requires the following inputs:

**Absorption rate:** the default value for this field is 0.01 and is expressed as the fraction absorbed. The default is based on the rate of sublingual absorption of nitroglycerine and other drugs (conservative scenario). It does not account for excretion or metabolism of the chemical.

**Chemical concentration in water (µg/liter):** chemical concentration is the concentration of the chemical displayed in the “**Chemical Used**” list box. The value should reflect the maximum product use rate.

**Water intake (L/hour):** water intake refers to the amount of water taken into and out of the mouth during swimming. For children, it has been estimated that 15.8 L is taken in and out over 3 hours (5.27 L/hour). This value is used by default for competitive and non-competitive children. Approximately 50% of this value is used for adults (Dang, 1996).

**Exposure Time (hours/event):** Exposure time is the amount of time per event that the swimmer is actually in the pool.

Table 7-1 lists the types of swimmers and their associated water intake rates (liters/hour) and exposure times (hours/event).

**Table 7-1. Default water intake rates for buccal/sublingual exposure route**

Swimmer	Water Intake Rate (L/hr)	
	Competitive	Non-competitive
Adult male	1.25	2.5
Adult female	1.25	2.5
Adult	1.25	2.5
Older child (11-14 years)	2.5	5.0
Younger child (7-10 years)	2.5	5.0

The total buccal/sublingual exposure per event is calculated according to the following equations:

$$PDR_{\text{buccal/sublingual}} = ET \times WI \times C_w \times AR \times (1 \text{ mg}/1,000 \text{ }\mu\text{g})$$

where:

- PDR<sub>buccal/sublingual</sub> = Potential dose rate via buccal/sublingual route (mg/event),
- ET = Exposure time (hours/event),
- WI = Water intake (L/hour),
- C<sub>w</sub> = Concentration in water (μg/L), and
- AR = Absorption factor (unitless).

Once all values for the **Buccal/Sublingual** screen have been entered, click the “**Next**” button to continue to the **Orbital/Nasal Route** screen. If the Buccal/Sublingual route is not required, be sure to deselect the “**Use Buccal/Sublingual route in calculations**” check box.

If a non-competitive swimmer is being assessed, then the orbital/nasal exposure is assumed to be equal to the buccal/sublingual exposure. ACC (2002) showed that the vast majority of competitive swimmers wear goggles, and, thus, exposure via the orbital route is eliminated. Exposure via the nasal route remains. Thus, the orbital/nasal exposure for competitive swimmers is assumed to be one-half the buccal/sublingual exposure.

The orbital/nasal exposure per event is calculated according to the following equation:

$$PDR_{\text{orbital/nasal}} = ET \times WI \times C_w \times AR \times (1 \text{ mg}/1,000 \text{ }\mu\text{g})$$

where:

- PDR<sub>orbital/nasal</sub> = Potential dose rate via orbital/nasal route (mg/event),
- ET = Exposure time (hours/event),
- WI = Water intake (L/hour),
- C<sub>w</sub> = Concentration in water (μg/L), and
- AR = Absorption factor (unitless).

If the Orbital/Nasal route is not required, be sure to deselect the “**Use Orbital/Nasal route in calculations**” checkbox. Once all values for the **Orbital/Nasal Route** screen have been entered, click the “**Next**” button to continue to the **Aural Exposure Route** screen.

## 8.0 AURAL ROUTE

The screen displayed below (Figure 8-1) depicts the **Aural Route** screen.

**Figure 8-1. Aural Route Screen**

The following fields are required for input:

**Octanol/Water Partition Coefficient ( $K_{ow}$ ):**  $K_{ow}$  values are supplied for the pre-selected chemicals in the database. They are listed in Table 8-1.

**Table 8-1. Octanol/water partition coefficients ( $K_{ow}$ s) for available chemicals in SWIMODEL.**

Chemical	$K_{ow}$ (unitless)
Chloroform	93.33
Bromo form	234.42
Bromodichloromethane	125.89
Chlorodibromomethane	173.78
Simazine	97.72

For chemicals where the  $K_{ow}$  value is not known, the  $K_{ow}$  value can be calculated by clicking the **“Calculate”** button next to the  $K_{ow}$  field. This starts the KOWWIN program. The CAS number for the chemical or the SMILES notation needs to be known and entered. Once this information has been entered, click the **“Calculate”** button. Then click **“Save Results”** to save the results to the default name of the file (e.g., logpw001.dat) and exit KOWWIN.

The Log Octanol-Water Partition Coefficient Program (KOWWIN) estimates the logarithmic octanol-water partition coefficient (log P) of organic compounds. KOWWIN requires only a chemical structure to estimate a log P. Structures are entered into KOWWIN using SMILES (Simplified Molecular

Input Line Entry System) notation. The KOWWIN program and estimation methodology were developed at Syracuse Research Corporation. A discussion of the estimation methodology is available in Meylan and Howard (1995).

The octanol-water partition coefficient is a physical property used extensively to describe a chemical's lipophilic or hydrophobic properties. It is the ratio of a chemical's concentration in the octanol-phase to its concentration in the aqueous phase of a two-phase system at equilibrium. Since measured values range from  $<10^{-4}$  to  $>10^{+8}$  (at least 12 orders of magnitude), the logarithm (log P) is commonly used to characterize its value. Log P is a valuable parameter in numerous quantitative structure-activity relationships (QSAR) that have been developed for the pharmaceutical, environmental, biochemical, and toxicological sciences.

KOWWIN uses a "fragment constant" methodology to predict log P. In a "fragment constant" method, a structure is divided into fragments (atom or larger functional groups) and coefficient values of each group are summed together to yield the log P estimate. Coefficients for individual fragments and groups in KOWWIN were derived by multiple regression of more than 2400 reliably measured log P values. The estimated accuracy for the multiple regression has a statistical correlation coefficient ( $r^2$ ) of 0.98, a standard deviation of 0.22, and an absolute mean error of 0.16. The estimated accuracy of KOWWIN has been validated with a dataset of 8900 compounds (not included in the training dataset) with reliably measured values. This validation dataset has a statistical correlation coefficient ( $r^2$ ) of 0.954, a standard deviation of 0.42, and an absolute mean error of 0.32.

**Chemical concentration in water ( $\mu\text{g/liter}$ ):** chemical concentration is the concentration of the chemical displayed in the “**Chemical Used**” list box. The value should reflect the maximum product use rate.

**Surface area of the ears ( $\text{cm}^2$ ):** the default surface area for both ears is  $4 \text{ cm}^2$ .

**Permeability coefficient ( $\text{cm/hr}$ ):** the permeability coefficient values for the pre-selected chemicals are as follows:

**Table 8-2. Permeability coefficients ( $K_p$ s) for available chemicals in SWIMODEL.**

<b>Chemical</b>	<b><math>K_p</math> (<math>\text{cm/hr}</math>)</b>
Chloroform	8.9E-03
Bromoform	2.6E-03
Bromodichloromethane	5.8E-03
Chlorodibromomethane	3.9E-03
Simazine	3.84E-03

The permeability coefficient can also be calculated by clicking the “**Calculate**” button next to the permeability coefficient field. This will bring up the  **$K_p$  Calculation** screen.

**Exposure Time (hours/event):** exposure time is the amount of time per event that the swimmer is actually in the pool.

The potential dose rate via the aural route is automatically calculated according to the following equation:

$$PDR_{\text{aural}} = ET \times SA \times K_{ow} \times K_p \times C_w \times (1 \text{ L}/1,000 \text{ cm}^3) \times (1 \text{ mg}/1,000 \text{ }\mu\text{g})$$

where:

- PDR<sub>aural</sub> = Potential dose rate via aural route (mg/event),
- ET = Exposure time (hours/event),
- SA = Surface area of ears (cm<sup>2</sup>),
- K<sub>ow</sub> = Octanol/water partition coefficient (unitless),
- K<sub>p</sub> = Chemical-specific permeability coefficient (cm/hr), and
- C<sub>w</sub> = Concentration in water (μg/L).

### Calculating the Permeability Coefficient

The K<sub>p</sub> Calculation Form is shown below (Figure 8-2).

**Figure 8-2. Permeability Coefficient Calculation Form Screen**

To calculate the permeability coefficient, SWIMODEL requires the entry of the molecular weight of the chemical as well as the K<sub>ow</sub> (K<sub>ow</sub> can be calculated as discussed in the **Aural Route** screen). The K<sub>p</sub> value is calculated as follows:

$$\log K_p = -2.72 + 0.71 \times \log(K_{ow}) - 0.0061 \times MW$$

$$K_p = 10^{\log K_p}$$

where:

- K<sub>p</sub> = Permeability coefficient,
- logK<sub>p</sub> = Log(permeability coefficient),
- K<sub>ow</sub> = Octanol/water partition coefficient (unitless), and
- MW = Molecular weight of chemical (g/mole).

Once these values are entered, press “OK” to return to the **Aural Route** screen.

## 9.0 AVERAGE DAILY DOSE (ADD)/LIFETIME AVERAGE DAILY DOSE (LADD)

Figure 9-1 below shows the ADD/LADD Screen.

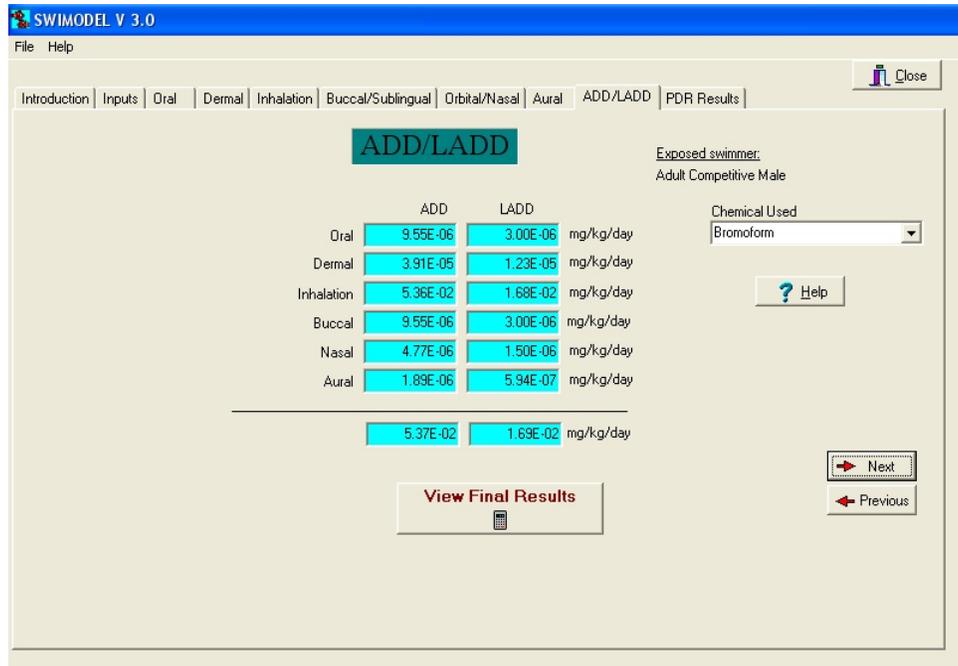


Figure 9-1. ADD/LADD Screen

The Average Daily Dose (ADD) and Lifetime Average Daily Dose (LADD) for each exposure route are calculated and displayed on this screen. Data entered on previous screens, primarily the Personal Input screen, is used in calculating the ADDs and LADDs.

The following equations are used to calculate the ADD and the LADD:

$$ADD_{\text{oral}} = \frac{ET \times IR \times C_w \times EF \times ED \times \frac{1 \text{ mg}}{1,000 \mu\text{g}}}{BW \times AT \times 365 \text{ d / yr}}$$

$$ADD_{\text{dermal}} = \frac{ET \times SA \times K_p \times C_w \times EF \times ED \times (10,000 \text{ cm}^2 / \text{m}^2) \times \frac{0.001 \text{ L}}{\text{cm}^3} \times \frac{1 \text{ mg}}{1,000 \mu\text{g}}}{BW \times AT \times 365 \text{ d / yr}}$$

$$ADD_{\text{inhalation}} = \frac{C_{\text{vp}} \times ET \times IR \times EF \times ED \times \frac{1 \text{ mg}}{1,000 \mu\text{g}}}{BW \times AT \times 365 \text{ d / yr}}$$

$$ADD_{\text{buccal/sublingual}} = \frac{ET \times WI \times C_w \times AR \times EF \times ED \times \frac{1 \text{ mg}}{1,000 \mu\text{g}}}{BW \times AT \times 365 \text{ d / yr}}$$

$$ADD_{\text{orbital/nasal}} = \frac{ET \times WI \times C_w \times AR \times EF \times ED \times \frac{1 \text{ mg}}{1,000 \mu\text{g}}}{BW \times AT \times 365 \text{ d / yr}}$$

where:

- ADD = Average Daily Dose (mg/kg-day),
- EF = Exposure frequency (events/year),
- ED = Exposure duration (years),
- BW = Body weight (kg), and
- AT = Averaging time (years).

When calculating ADD, the averaging time (AT) is equal to the exposure duration (ED). The total ADD is calculated by summing the ADD for each exposure route:

$$ADD_{\text{total}} = \sum ADD_{\text{route}}$$

If all the exposure routes are selected for an assessment,  $ADD_{\text{total}}$  is:

$$ADD_{\text{total}} = ADD_{\text{oral}} + ADD_{\text{dermal}} + ADD_{\text{inhalation}} + ADD_{\text{buccal/sublingual}} + ADD_{\text{orbital/nasal}} + ADD_{\text{aural}}$$

LADD (mg/kg-day) is calculated by using the same equations as for ADD, but averaging time (AT) is set equal to a lifetime of 70 years. The total LADD, as with the total ADD, is determined by summing the LADDs for each exposure route selected by the user.

## 10.0 PDR RESULTS

The **PDR Results** screen, as shown below in Figure 10-1, displays the Potential Dose Rate (mg/event) for all requested exposure routes along with the normalized PDR (mg/kg/event). The  $PDR_{normalized}$  is calculated by dividing the PDR by the swimmer's body weight (shown on the **Personal Information** sheet). A total PDR and total  $PDR_{normalized}$  are calculated by summing all the exposure routes assessed. The values are shown at the bottom of the screen.

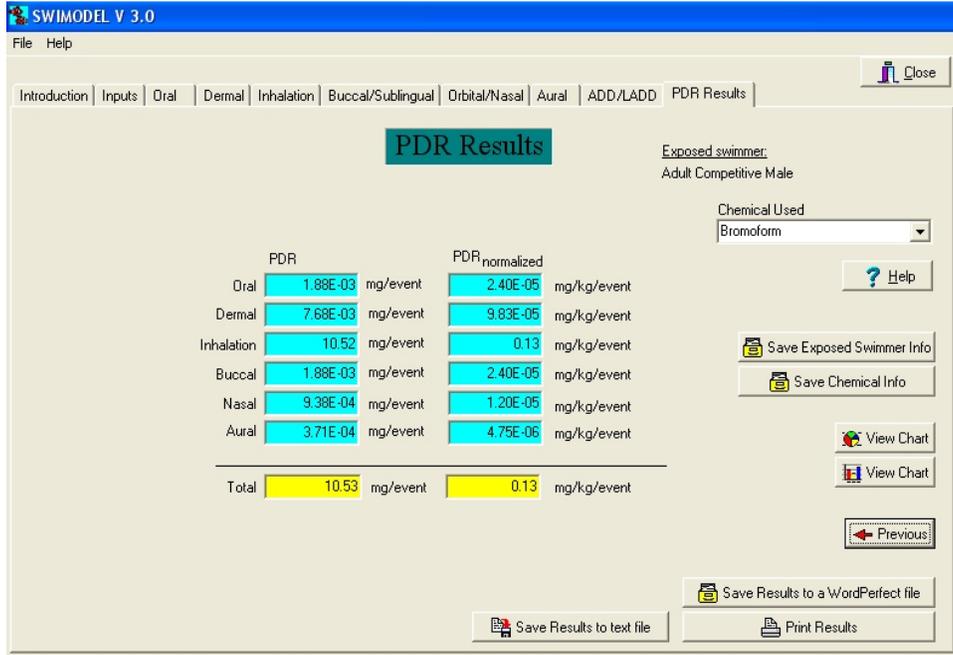


Figure 10-1. PDR Results Screen

A report can be printed by clicking **File** at the top of the screen and selecting the **“Print Results”** menu item. The report can also be saved as a WordPerfect file by clicking **“File”** then selecting the **“Save Results to a WordPerfect File”** menu item.

The data can be saved for the swimmer as well as for the selected chemical. When saving the data, care should be exercised because any overwrites of original data will be saved. The assessor can also view pie and bar chart representations of the exposures by clicking the **“View Chart”** buttons on the right. Data can also be saved as a comma delimited text file. This file can be imported into any spreadsheet such as Excel or Lotus 123. If the age distributions were used, the assessor can view a line graph of all exposures.

## 11.0 REFERENCES

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