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Database Tools for Modeling Emissions and Control of Air Pollutants from Consumer Products, Cooking, and Combustion

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ABSTRACT
In order to estimate building contaminant concentrations and associated occupant exposures, indoor air quality (IAQ) model users require data related to source strengths and other contaminant transport mechanisms (*e.g.* sinks, filters). Much of this information exists in the literature; however, it is not readily accessible, thereby requiring users to expend significant efforts in searching for this information. To support the modeling process, the National Institute of Standards and Technology (NIST) has created a series of model input databases for use in its multizone IAQ and ventilation model CONTAM. As part of this effort, a standard data entry format was developed, as well as a computer program to search the database for specific records and build a CONTAM input library. These databases and tools can serve as a basis for building an extensive collection of model input parameters, assessing the quality and completeness of existing data sets, and allow for identification of significant data gaps.

Keywords: database**,** indoor air quality, transport model, volatile organic compounds, particles, exposure

Table of Contents

INTRODUCTION

Indoor air quality (IAQ) models can be used to predict airflows, contaminant concentrations and building occupant exposures in a given indoor environment. In order to generate such results, however, IAQ models require the user to provide a wide range of input data including envelope leakage information, weather, ventilation system characteristics, contaminant source emission rates, sink removal rates, occupant schedules, and air cleaner removal rates. Many of the required model inputs are available in the literature; however, these data have generally not been compiled in a readily accessible source, thereby requiring users to search for model input parameters. To facilitate the IAQ modeling process and allow for assessment of the data quality and completeness, there is a need for well-designed databases of measured contaminant modeling data.

In response to this need, the National Institute of Standards and Technology (NIST) created several searchable databases for model input data. These databases may be used to organize volatile organic compound (VOC) emission rates from building materials, particle and inorganic gas emission rates from combustion sources, particle deposition rates, VOC sorption rates, and particle filtration. This process involved collecting representative data from the literature, designing a database format to standardize data entry, entering example data into the database, validating data entry, and developing a computer program to search the database for specific records to use in the multizone IAQ and ventilation model, CONTAM. The resulting databases and tools provide standardization that is needed for consistency and reliability in reporting, accessing, and manipulating IAQ model input data.

INDOOR AIR QUALITY MODELS AND INPUTS

Although the model input databases compiled as part of this effort can be used in any IAQ model, this report will focus on their use in NIST's airflow and pollutant transport model CONTAM (Walton and Dols, 2005). The CONTAM software and manual may be downloaded from the following website: http://www.bfrl.nist.gov/IAQanalysis/. In summary, CONTAM is a multizone model that treats a building as a system of interconnected, well-mixed zones between which airflow and pollutants are transported. This macroscopic approach is implemented by constructing a network of elements describing the flow paths (heating, ventilating, and air conditioning (HVAC) ducts, doors, windows, cracks, etc.) between the zones of a building. The network nodes represent the zones and duct segments, which are modeled with a single pressure, temperature, and pollutant concentration. CONTAM has a graphical interface that allows users to draw a building's zones and add airflow paths, ventilation systems, contaminant sources and sinks, and building occupants.

The program first calculates airflow rates between zones by solving for the pressure in each zone based on a mass balance of air. After calculating the airflow between zones and ambient, zonal pollutant concentrations are calculated by applying mass balance equations to the zones, which may also contain pollutant sources or sinks. The following mass balance may be used to describe contaminant transport in a multizone building:

$$\frac{dm_{\alpha,i}}{dt} = -R_{\alpha,i}C_{\alpha,i} - \sum_j F_{i,j}C_{\alpha,i} + \sum_j F_{j,i}\left(1-\eta_{\alpha,j,i}\right)C_{\alpha,j} + m_i\sum_\beta k_{\alpha,\beta}C_{\beta,i} + G_{\alpha,i} \tag{1}$$

where:

- $m_{\alpha,i}$ = mass of contaminant α in zone i (kg)
- $R_{\alpha,i}$ = removal coefficient for contaminant α in zone i (kg/s)
- $C_{\alpha,i}$ = concentration mass fraction of contaminant α in zone i (kg/kg)
- $F_{i,j}$ = rate of airflow from zone i to zone j (kg/s)
- $F_{j,i}$ = rate of airflow from zone j to zone i (kg/s)
- $\eta_{\alpha,j,i}$ = filter efficiency in the path from zone j to zone i (kg/kg)
- $C_{\alpha,j}$ = concentration mass fraction of contaminant α in zone j (kg/kg)
- m_i = mass of air in zone i (kg)
- $k_{\alpha,\beta}$ = kinetic reaction coefficient in zone i between species α and β (1/s)
- $C_{\beta,i}$ = concentration mass fraction of contaminant β in zone i (kg/kg)
- $G_{\alpha,i}$ = generation rate of contaminant α in zone i (kg/kg)

The user must supply data regarding airflow paths, contaminant source emission rates, contaminant removal rates, chemical reaction coefficients, filter efficiencies and occupant schedules. In a previous effort, NIST created a library of airflow leakage elements, wind pressure coefficients, and ventilation system schedules to aid the user when adding airflow path information (Persily and Ivy, 2001). The project described in this report focused on creating databases for the model input parameters needed to model exposure to air pollutants from consumer products, cooking, and combustion. These parameters include source emission rates ($G_{\alpha,i}$), contaminant sinks and deposition rates ($R_{\alpha,i}$), and particle filter efficiencies ($\eta_{\alpha,j,i}$).

Source Models

The generation rate of indoor contaminants has been described with several different source models. A summary of the source models currently available in CONTAM is provided in Table 1. It should be noted that there are additional source models available in the literature.

Table 1. Source models used to characterize source emission rates in CONTAM.

Source Model Name	**Equation**	**Example Uses**
Constant Coefficient Model	G G = generation rate	Dry VOC sources (*e.g.*, linoleum) Particles from cooking
Pressure Driven Model	$G^*\Delta P^n$ ΔP = pressure difference n = pressure exponent	Contaminated soil gas
Cutoff Concentration Model	$G\left(1-\frac{C}{C_{cut}}\right)$ C = current concentration C_{cut} = cutoff concentration at which emission ceases	Sources within a confined space (*e.g.*, mothballs in a closet)
Decaying Source Model	$G_0\exp(-t/t_c)$ G_0 = initial generation rate t = time since start of emission t_c = time constant	Wet VOC sources (*e.g.*, paint)
Boundary Layer Diffusion Model	$hdA\left(C_i-\frac{C_s}{k}\right)$ h = film mass transfer coefficient over sink d = film density of air A = surface area C_i = concentration in air C_s = concentration at surface of material k = partition coefficient	Reversible sinks
Burst Source Model	Fixed mass added to zone instantaneously	Occupant activities (*e.g.*, spraying an air freshener, changing kitty litter)

Power Law Model	If $t < t_p$, then
	$S(t) = at_p^{-b}$
	Else
	$S(t) = at^{-b}$
	t = time
	a, b, t_p = empirical coefficients
		"Dry" materials emissions

Peak Model	$S(t) = a\exp\left\{-0.5\left[\frac{\ln\left(\frac{t}{t_p}\right)}{b}\right]^2\right\}$ a, b, t_p = empirical coefficients	"Wet" material emissions

As shown in Table 1, each model is applicable to specific types of sources. For example, an exponential model better describes VOC emissions from a "wet" source than a constant source model. The modeler chooses which source model to apply; however, use of the different source models requires knowledge of the specific coefficients. The constant coefficient, first-order decay, power law and peak models in Table 1 are empirically-based. Thus, the user must find the model coefficients that are linked to specific experimental tests. The mass transfer approach (boundary layer diffusion model) is physically-based, thus its coefficients may be estimated using contaminant and material properties. However, the mass transfer values must still be determined.

To determine the empirical model coefficients or to validate the physical models, source emission rates have been experimentally measured for hundreds of consumer products and combustion appliances. Source emissions testing is typically completed in controlled laboratory chambers ranging in size from approximately 3.5 x 10^{-5} m^3 (field and laboratory emission cells) to larger than 10 m^3 (room size) (ASTM 1997). While there are currently no standard emission rate test methods for consumer products and combustion appliances, researchers typically report test facility characteristics, test conditions, and product/appliance characteristics.

Deposition Models

Deposition is a significant removal mechanism of particles indoors and needs to be accounted for when modeling particle transport. The rate of deposition depends on several factors including characteristics of the particle (*e.g.*, size and charge), room surfaces, and airflow (Nazaroff *et al*. 1993). Deposition of particles is typically reported in the literature in terms of a deposition velocity (υ_d) or a deposition rate (k_d). The deposition velocity sink model is:

$$R_\alpha(t) = \upsilon_d A_s \rho_{air}(t) C_\alpha(t) \tag{2}$$

where:

$R_\alpha(t)$	=	removal rate at time t (kg/s)
υ_d	=	deposition velocity (m/s)
A_s	=	deposition surface area (m^2)
$\rho_{air}(t)$	=	density of air in the source zone at time t (kg/m^3)
$C_\alpha(t)$	=	concentration of contaminant α at time t (kg/kg)

To use this model, the user must enter the deposition surface area and particle deposition velocity. Often it is difficult to estimate the deposition surface area, so it is lumped into a parameter known as the deposition rate, which is defined as:

$$k_d = \frac{\upsilon_d A_s}{V_z} \tag{3}$$

where:

V_z	=	zone volume (m^3)

Using the deposition rate parameter, the deposition sink model may be expressed as:

$$R_{\alpha}(t) = k_d V_z \rho_{air}(t) C_{\alpha}(t) \tag{4}$$

To use the deposition rate model, the user must provide a deposition rate.

Researchers have measured deposition velocities and deposition rates in several different test facilities, ranging from small chambers to real buildings. Common test parameters reported by researchers include the types of furnishings, air mixing mechanisms, air change rate, and particle characteristics. As with source emission rates, no standard test method yet exists for measuring particle deposition rates.

Sorption Model

Indoor contaminant calculations use sorption models to account for the transfer of gaseous contaminants between the air phase and the material phase. The rate of adsorption depends on characteristics of the adsorbent material, the adsorbing chemical, and the boundary layer that separates them. There are several sorption models available: CONTAM currently uses the boundary layer diffusion controlled (BLDC) reversible sink/source model. The BLDC model has been documented elsewhere (Axley, 1990). In summary, it accounts for the adsorption and desorption transport of chemicals between room air and room materials. The equation used to describe this transport is:

$$S = hdA\left(C_i - \frac{C_s}{k}\right) \tag{5}$$

where:

h	=	film mass transfer coefficient over the sink (m/s)
d	=	film density of air (kg/m^3)
A	=	surface area of the adsorbent (m^2)
C_i	=	concentration in air (kg/kg)
C_s	=	concentration in the adsorbent (kg/kg)
k	=	Henry adsorption constant or the partition coefficient (kg/kg)

To use the BLDC model in CONTAM, the user must provide the film mass transfer coefficient, film density of air, surface mass of adsorbent, and the partition coefficient. The first three parameters are based on physical constants and characteristics of the zone being modeled. The partition coefficient is chemical/material specific with limited values available for several indoor air chemical species and building materials in the literature (Zhang et al 2001).

Filter Model

CONTAM currently includes three filter models: constant removal efficiency, simple particle, and simple gaseous. The constant removal efficiency model describes the loss of particles or gases through a filter. As presented in Equation 6, the removal of contaminants through a filter is written as:

Filter removal = $F(1-\eta)C$ (6)

where:

F = airflow rate through the filter (kg/s)

η = single pass removal efficiency of filter (-)

C = contaminant removed by filter (kg/kg)

CONTAM also includes a particle filter element that allows the user to enter filter removal efficiencies as a function of particle size to create a filter performance curve for a single filter. The user is required to enter the filter data from which CONTAM generates a curve using a cubic spline fit. Another option is to choose an existing filter performance curve based on ASHRAE 52.2's Minimum Efficiency Reporting Value (MERV) System (ASHRAE 1999). Based on this evaluation system, Kowalski and Bahnfleth (2002) created several sets of filter performance curves using MERV test results. These filter performance curves have already been compiled into a CONTAM library. Users can therefore either enter their own filter curve data or choose an existing MERV curve to use in a CONTAM simulation.

CONTAM also has an air cleaner element for gaseous contaminants, which uses a removal efficiency for a given contaminant loading. As the mass of contaminant sorbed to the air cleaner media increases, the associated contaminant removal efficiency decreases. Again, CONTAM can generate a filter curve using a cubic spline fit based on user provided data. It is also possible to set a breakthrough efficiency for each contaminant.

MODEL INPUT DATA SOURCES

The model input data considered in this report include emission rates from consumer products, building materials, cooking and combustion appliances, particle deposition rates, chemical sorption rates, and particle filter removal. For each category, several key references were identified from which to build the database structures. It should be noted that the data sources identified for this project are not intended to be all-inclusive, but, rather, representative of the literature and to serve as examples for populating the databases in the future. A user may append any of the model input databases with his or her own data.

VOC Emission Rates from Consumer Products and Building Materials

There is a great deal of VOC source emission rate data available in the literature and other sources. Although there is not a comprehensive database available, there are several abridged versions that can provide the foundation for a sound database design. Based on completeness and accessibility, the NRC material emission database (Zhang *et al*. 1999) and the U.S. Environmental Protection Agency (EPA) database (U.S. EPA 1999) served as the sources of emission rate data for this project.

The NRC database is a material emission database assembled by the National Research Council of Canada (NRC). The NRC database was developed in Access and includes VOC emission rate data from tests conducted in their Indoor Environment Program laboratory chambers. This database currently contains over 2300 emission rates representing 152 contaminants and 69 different materials. Each record includes approximately 80 data fields including product manufacturer information, emissions testing conditions, chemical information, emission factors, emission profiles, and comments. NRC has also provided access to this emission rate data through its indoor air quality model IA-QUEST (http://irc.nrc-cnrc.gc.ca/ie/iaq/iaquest_e.html) (Sander *et al*. 2005). Since the NRC database represents a collection of data from a single testing facility and it is being managed by NRC, it was considered complete and exists on its own. However, its design was used to build a second database of emission rates from the published literature described below.

In order to provide a user interactive database of VOC source emission rates, a second VOC source database was created to add emission rates from the published literature and other sources. A collection of peer-reviewed source emission rates was compiled by the Indoor Environment Management Branch of the U.S. Environmental Protection Agency (EPA) (U.S. EPA 1999). The data were stored in an Excel spreadsheet that included approximately 8500 emission rate records from 72 references reviewed through May 1999. Records represent 78 types of materials in 17 source categories. Each record contains about 70 data fields including information regarding emission source classification, emission testing conditions, chemical information and analytical methods, emission factors, emission modeling parameters if available, and comments. For this NIST project, only the data published in first degree references (e.g., peer-reviewed journal articles as opposed to conference proceedings) were used. This data subset resulted in over 800 VOC emission rates from 16 references (Brown 1999a; Brown 1999b; Kelly *et al*. 1999; Lundgren *et al*. 1999; Horn *et al*., 1998; Chang *et al*. 1997; Van der Wal *et al*. 1997; Schaeffer *et al.* 1996; Nagda *et al.,* 1995; Chang and Guo 1994; Hodgson et al. 1993; Chang and Guo 1992; Hawkins et al. 1992; Colombo *et al*. 1990; Schlitt and Knoppel 1989; Wallace *et al.* 1987).

Cooking and Combustion Appliance Emission Rates

Unlike VOC emission rates, there is not an existing database of combustion appliance emission rates. Thus, a literature review was conducted to identify research papers with combustion related emission rates. As a result of this search, data from 21 references are included representing emissions from gas range tops (He *et al.* 2004; Wallace *et al.* 2004; Borazzo *et al.* 1987; Moschandreas *et al*. 1987; Billick *et al*. 1984; Caceres *et al*. 1983; Traynor *et al*. 1982; Yamanaka *et al*. 1979), gas ovens (He *et al*. 2004; Borazzo *et al.* 1987; Traynor *et al*. 1982), gas space heaters (Apte and Traynor 1986; Billick 1985; Traynor *et al.* 1985; Billick *et al*. 1984; Caceres *et al*. 1983; Girman *et al.* 1982; Yamanaka *et al*. 1979), kerosene space heaters (Tamura 1987; Traynor *et al.* 1987a; Apte and Traynor 1986; Porter 1984; Caceres *et al*. 1983; Girman et al. 1982; Yamanaka et al. 1979), wood stoves (McDonald et al. 2000; Nabinger *et al*. 1995; McCrillis and Burnet 1990; Traynor *et al*. 1987b; Knight *et al.* 1986), wood-burning fireplaces (McDonald *et al.* 2000), and candles (Fine *et al*. 1999).

Particle Deposition Rates

Although not compiled in a database, a literature review of particle deposition rates was recently published by Lai (2002). This review included 15 key indoor particle deposition references (Lai *et al*. 2002; Thatcher *et al.* 2002; Abadie *et al.* 2001; Cheng 1997; Fogh *et al.* 1997; Nomura *et al*. 1997; Morawska and Jamriska 1996; Byrne *et al.* 1995; Xu *et al*. 1994; Chen *et al*. 1992; Van Dingenen *et al*. 1989; Okuyama *et al*. 1986; Offermann *et al*. 1985; Crump *et al.* 1983; Harrison 1979). Lai's review includes graphs of deposition rate as a function of particle size as well as information regarding the experimental test conditions including test chamber dimensions, mixing mechanism, chamber type, and chamber surface textures. The published results from other deposition studies that have been completed at NIST (Howard-Reed *et al.* 2003; Emmerich and Nabinger 2001) and Lawrence Berkeley Laboratory (Thatcher and Layton 1995) are also included in the deposition data set.

Partition Coefficients

Another literature review was recently completed to compile data related to material sinks (Zhang 2001). In this review, several sink model inputs are provided including partition coefficients that are used in CONTAM's BLDC model. These partition coefficients are primarily from a single reference (Bodalal 1999) that was used to build a partition coefficient model input database. Of all the model input databases constructed for this project, this one has the least amount of available data, indicating an important research need.

Particle Filter Removal Efficiencies

As discussed earlier, Kowalski and Bahnfleth (2002) have created a series of filtration performance curves based on ASHRAE 52.2's Minimum Efficiency Reporting Value (MERV) System. These curves have recently been compiled in a CONTAM library and do not require a separate database.

MODEL INPUT DATABASE STRUCTURES AND TOOLS

The primary function of a database is to store a collection of information in a readily accessible format. A well-designed database should also allow for the assessment of data quality, trends in the observations, and data gaps. For this project, Access, a relational database management system (RDBMS), is used to create multiple searchable database structures for the compilation of IAQ model input data. The databases for this project are designed to expedite data entry by using tables of data fields that are linked by one-to-many relationships. To further aid data entry, forms were created to add data to the database tables. In most cases, the database fields for each type of model input are based on parameters reported in the published literature. To date, each model input database includes example entries from key references. The standard data format for the database also allows users to populate the databases with their own input data to build a model input library for CONTAM. Since a particle filtration database already exists in CONTAM, a separate database structure is not needed.

VOC Source Emission Rate Database

The format of the VOC source emission rate database is based on fields from both the NRC and EPA databases as well as parameters from several emission testing guides (ASTM 1997, 2001; European Guidelines 1991; and Matthews 1987). A summary of the test conditions recommended in these guides is provided in Table 2.

The resulting standard format includes the following nine tables: emission rate category (CATEGORY), type of material within category (TYPE), literature reference (REFERENCE), material properties (MATERIAL), contaminant properties (PROPERTY), environmental test conditions (TESTCOND), material test conditions (ETEST), source model equation (EQUATION), contaminant emission rate factors (CONTAMINANT). Each table contains information specific to that entity that is given in Figure 1. For example, the equation table provides a description of the equation, the equation itself, the number of required coefficients, and the corresponding source model type in CONTAM. The tables are linked to one another using a “one-to-many” relationship system (see Figure 1). For example, a single emission rate test can yield results for many different contaminants and a single reference can provide results for several different tests, etc.

Table 2. Summary of source emission rate testing conditions guidelines.

Parameter	ASTM Full-Scale Chambers[a]	ASTM Small-Scale Chambers[b]	European Guideline[c]	Matthews[d]
Small-scale chamber volume	not applicable	< 5 m^3	≤ 1 m^3	≤ 1 m^3
Large-scale chamber volume	room size	not applicable	> 10 m^3	> 15 m^3
Acceptable mixing criteria	tracer decay test, compare measured decay to theoretical decay curve	tracer decay test w/ mixing level > 80 %	tracer decay test, compare measured decay to theoretical decay curve	difference between concentration measurements in several locations should be within normal uncertainty
Clean air generation system	inlet conc. < 2 $\mu g/m^3$ for single VOC, < 10 $\mu g/m^3$ ΣVOCs	inlet conc. < 2 $\mu g/m^3$ for single VOC, < 10 $\mu g/m^3$ ΣVOCs	filtered/treated inlet air	not specified
Surface air velocity	mean: 0 to 0.25 m/s	typical indoor values	> 0.1 m/s	0.2 to 0.4 m/s
Turbulence kinetic energy	0 – 0.01 $(m/s)^2$	not specified	not specified	not specified
Temperature	23 °C ± 0.5 °C	not specified	23 °C ± 0.5 °C	23 °C ± 0.5 °C (std) 18 °C to 35 °C (typ)
Relative humidity	50 % ± 5 % RH	not specified	45 % ± 5 % RH	50 % ± 5 % RH (std) 20 % to 80 % (typ)
Total air change rate	0.5 h^{-1}	not specified	0.5 h^{-1} and/or 1.0 h^{-1}	not specified
Chamber pressure	0 Pa to 250 Pa above ambient	not specified	not specified	not specified
Product preparation	preconditioning for 48 h	seal product edges, use realistic substrates for liquid applications, preconditioning of product	seal product edges, use realistic substrates for liquid applications, preconditioning of product	size < 25 % of the transverse area of small-scale chamber, product edges coated, product preconditioning
Product history	record of product age, storage conditions, handling, transport	record of product age, treatment, storage conditions, handling, transport	record of product age, treatment, storage conditions, handling, transport	record of conditioning period
Miscellaneous	chamber background samples, duplicate samples (no fewer than 15 % of samples), routine calibrations	chamber background samples, routine calibration, internal standard, duplicate samples	chamber background samples, internal standard, duplicate samples, routine maintenance/ calibrations	blanks collected in chamber, total mass recover tests

a: ASTM 1997
b: ASTM 2001
c: European Communities 1991
d: Matthews 1987

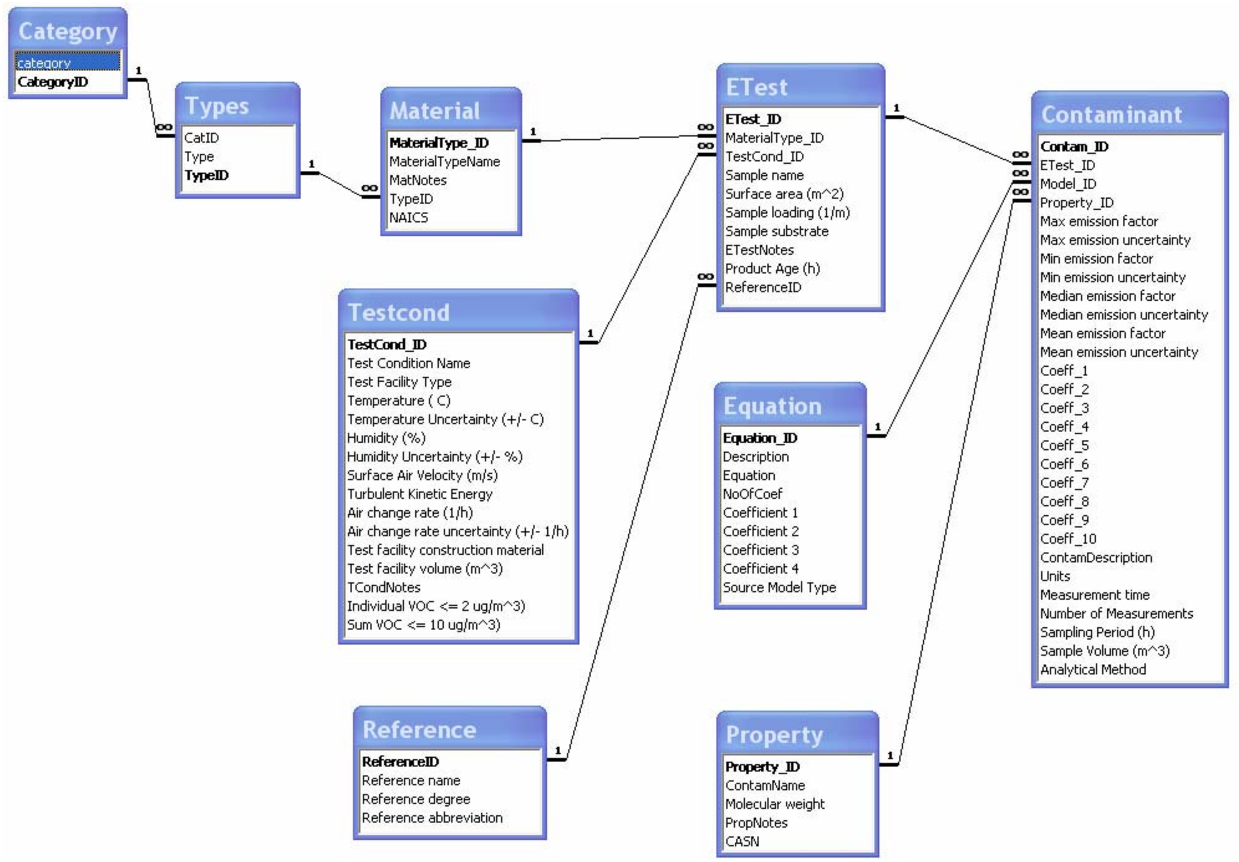

Figure 1. Relationships for tables in VOC source emissions database.

Based on the parameters in the tables in Figure 1, data entry forms were created (see Appendix A for description of form contents and example forms with data entered). As shown in Figure 1, certain parameters are assigned specific units to allow for number entries that could be used as search criteria. For example, the user could search for all records with experimental temperatures greater than 20 °C. This feature is discussed in more detail in a later section. A complete description of each data entry field is provided in Appendix A.

The NRC database was originally in Access with the 15 tables shown in Figure 2. NRC of Canada maintains this database, but has made the data contents available to CONTAM users. As a result, a link was created to transfer data to CONTAM but does not allow modification to the original NRC database structure.

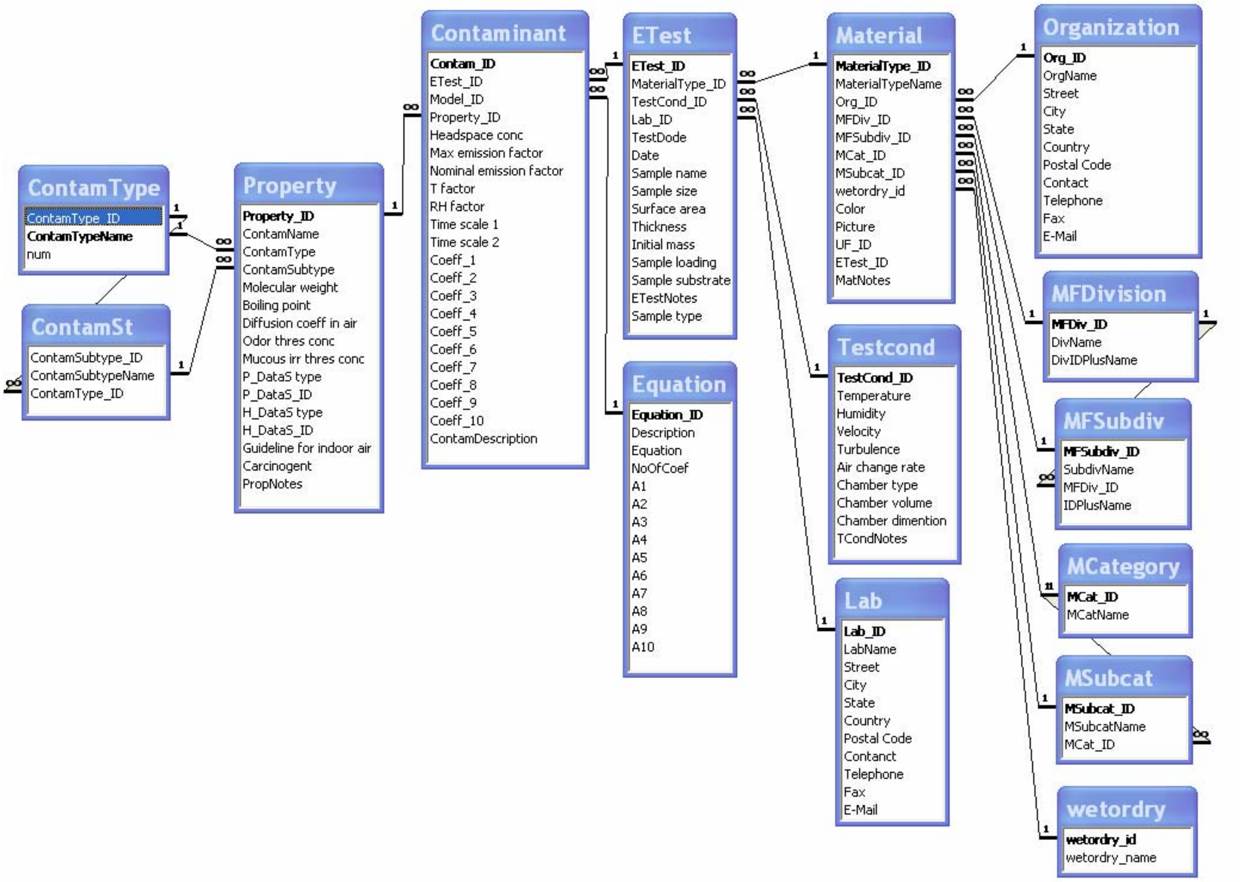

Figure 2. NRC database structure

Cooking and Combustion Appliance Database
The cooking and combustion appliance database consists of the following nine tables linked by one-to-many relationships (see Figure 3): combustion source category (CATEGORY), combustion source type (TYPE), reference (REFERENCE), test facility specifications (FACILITY SPECS), test appliance specifications (APPLIANCE SPECS), test conditions (TEST CONDITIONS), source emission rates (EMISSION FACTORS), contaminant information (CONTAMINANT PROPERTY), and source model (EQUATION). Due to the wide range of types of combustion appliances, numerous experimental parameters were added to the test conditions table. Thus, not all data fields will be applicable to all sources. A description of data entry forms and representative forms are available in Appendix A.

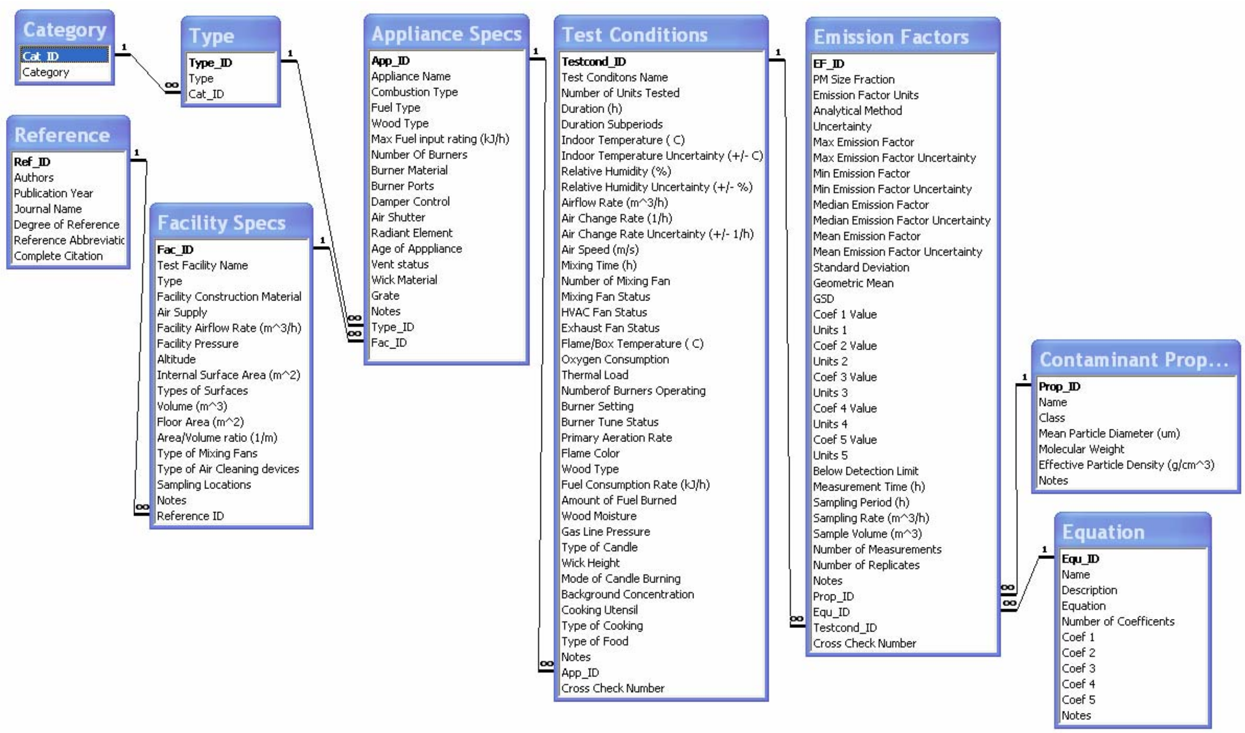

Figure 3. Cooking and Combustion Appliance Database Structure.

Particle Deposition Database

The deposition rate database is organized such that there are many deposition rates (DEPOSITION PARAMETERS) per test condition (TEST CONDITIONS) and particle characteristic (PARTICLE); many test conditions per test facility (TEST FACILITY), and many test facilities per reference (REFERENCE) (see Figure 4). Particles are distinguished by their mean or median diameter as measured by a specific type of analytical instrument. For example, the diameters of particles sized by an optical particle counter are given as equivalent light scattering (ELS) diameters, whereas the diameters of particles sized by an aerodynamic particle sizer were given as mass median aerodynamic diameters (MMAD). For a specific example, see the data entry forms in Appendix A.

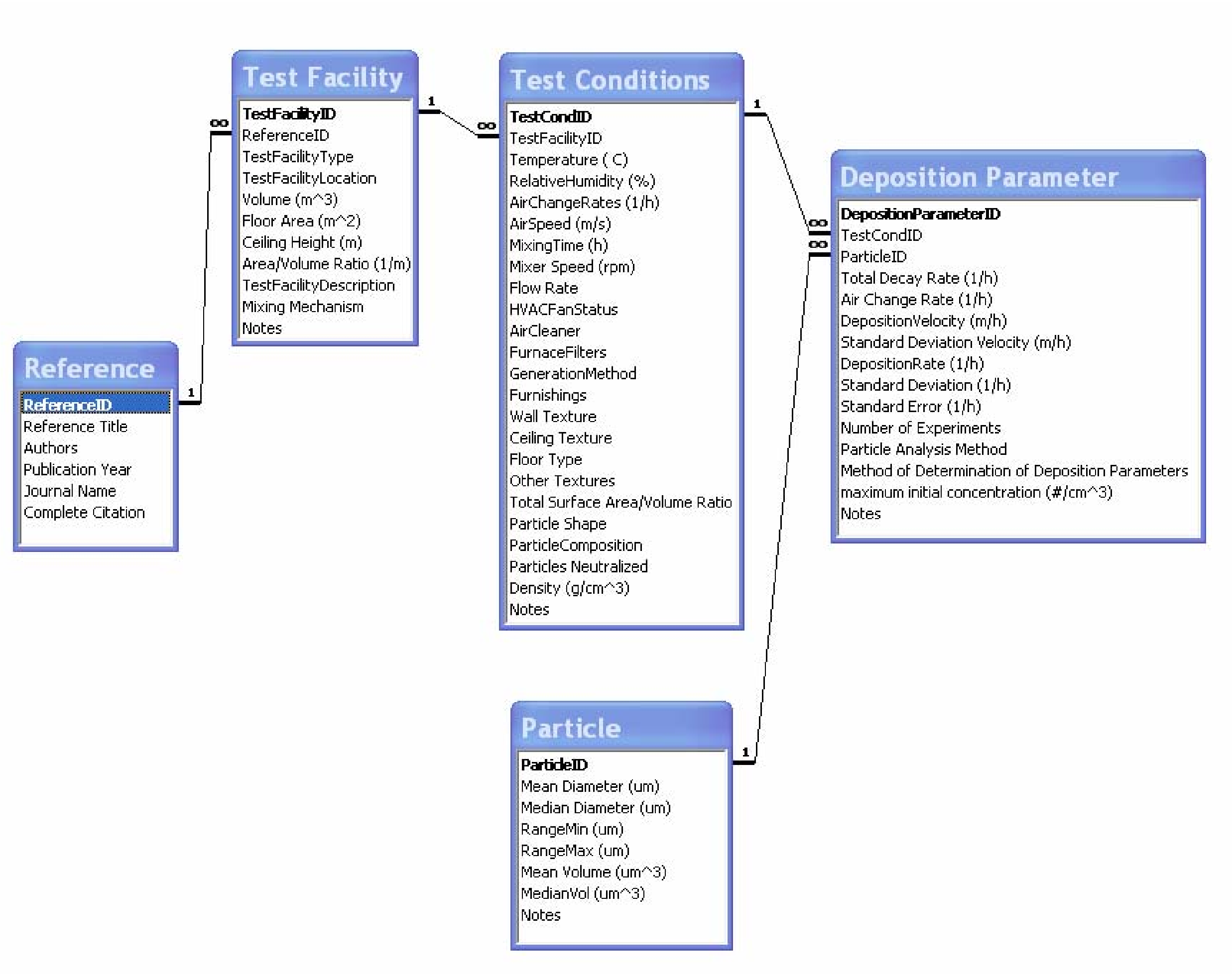

Figure 4. Particle Deposition Database Structure.

Partition Coefficient Database

The partition coefficient database consists of seven tables linked by one to many relationships. For every chemical (CHEMICAL), sorptive material (MATERIAL), and experimental test condition (TEST CONDITIONS), there can be multiple partition coefficients (PARTITION COEFFICIENTS). Each reference (REFERENCE) could include multiple test facilities (TEST FACILITY) and multiple test conditions. Each material is grouped by type (MATERIAL TYPE). Again there is only limited partition coefficient data available in the literature from which to build a database. As this data set grows, the database structure may need to be expanded. Currently available data entry forms are available in Appendix A.

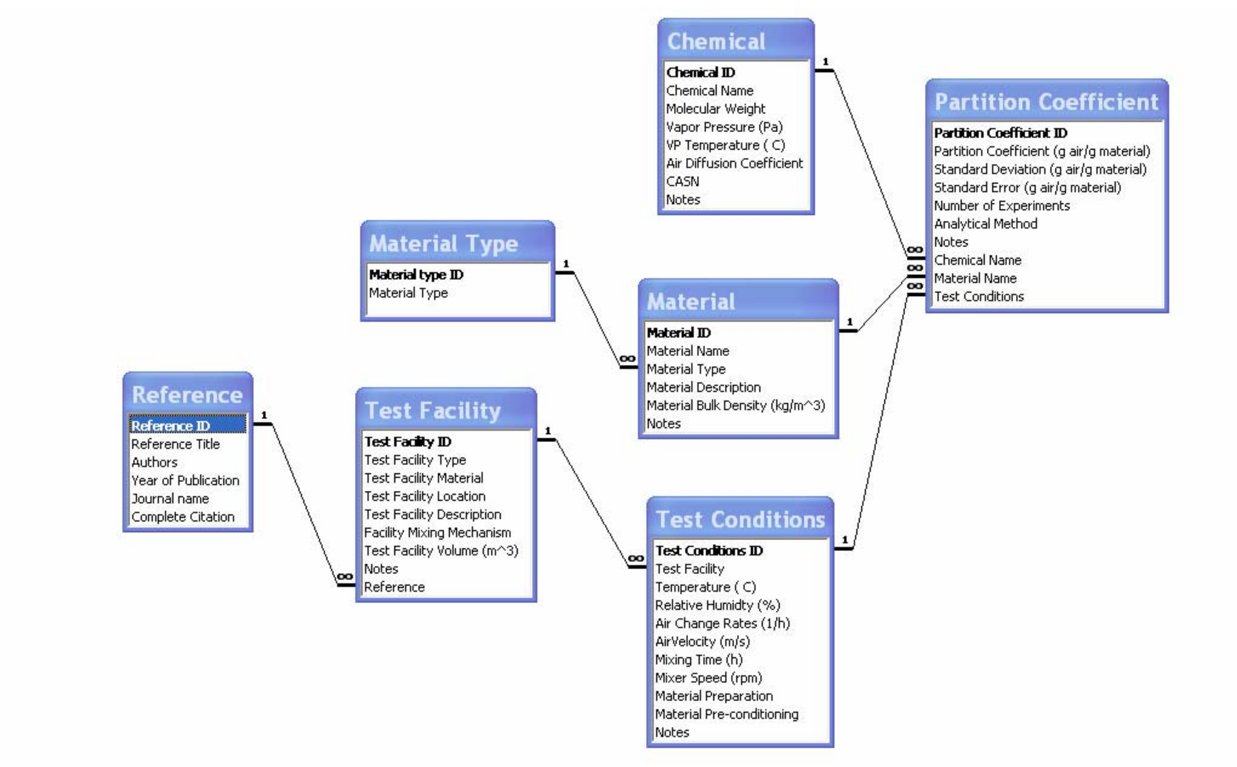

Figure 5. Partition Coefficient Database Structure.

CONTAM Data Link Manager

To aid the user in navigating the model input databases, the ContamLink 2.4 program was developed with the capabilities of browsing, searching, and selecting data for use in CONTAM. A complete description of ContamLink 2.4 and its user manual can be found in Appendix B. To download ContamLink 2.4, go to the CONTAM software page at: http://bfrl.nist.gov/IAQanalysis/software/index.htm.

DISCUSSION
Lessons Learned
Creation of accessible IAQ model input databases will undoubtedly make it easier for modelers to set up contaminant model scenarios. However, the convenience of such databases may also be a cause for concern. In particular, there is the potential for the data to be misinterpreted and misused, or the inclusion of poor quality data. While these are valid concerns, open access to all data is required for the verification and understanding of reported results. At this point, IAQ model input data should be considered "immature" and in need of being assessed. As such, the IAQ community could greatly benefit from model input databases that are readily accessible for assessments of data quality, trends, and gaps, as well as for convenient use in IAQ models. For example, a graph of the deposition rate data collected for the particle deposition database shows specific variations in deposition rates as a function of size (see Figure 6). In addition, by separating the data by analytical method, one can see that there is quite a bit more scatter in the deposition rates measured with a condensation nucleus counter (electrical mobility diameter) compared to an aerodynamic particle sizer (mass median aerodynamic diameter). Also, for particles of the same measured diameter, the deposition rates measured with optical particle counters (equivalent light scattering diameter) correlate well with those measured using a mass based instrument. One study reported activity mean aerodynamic diameters for submicron particles measured with a low-pressure impactor. Finally, the addition of a theoretical curve predicting deposition rates as a function of particle size shows most experimental data to follow the shape of that predictive curve but to be greater in magnitude, especially particles less than 0.1 µm in size.

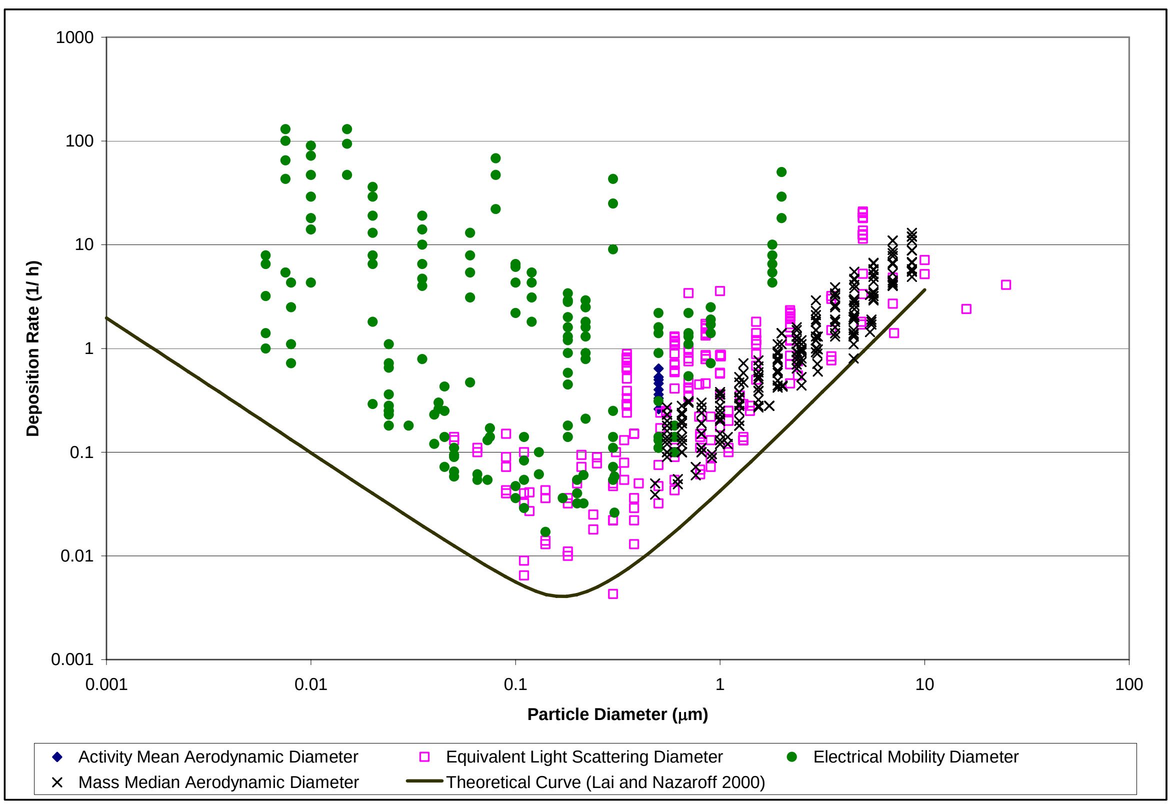

Figure 6. Particle deposition rates included in database (18 references) plotted as a function of particle size.

Another observation made during the course of this project is the lack of consistent format for reporting model input data in the literature. This lack of consistency adds time to data compilation efforts and increases the likelihood of missing data entries and misinterpreting data. One possible solution would be to create a set of standardized specifications for reporting data, perhaps through standards development organization (SDOs) such as the American National Standards Institute (ANSI), ASTM International, or International Standards Organization (ISO). Although the current databases contain a rather long list of required fields, only a subset of these values would need to be required. The required reporting variables could be based on the database search parameters (see Table 3) or other agreed upon criteria.

Future Directions

Based on the lessons learned for this project, several potential future directions were identified. For example, another approach for compiling the data would be to use MatML, an Extensible Markup Language (XML) developed to manage and exchange materials information on the Web (www.matml.org). Currently, most data on the Web are contained in documents using the hypertext markup language (HTML). HTML was developed simply to format the display of information/data on web pages, and it does not provide a description of the data themselves. As a result, it is not easy to automate the processing of data contained in HTML documents, thereby limiting their accessibility for use by software. To address this problem, XML was developed to portray data in a structure that is meaningful to both humans and computers. MatML is a customized markup language developed specifically for materials property data.

Recently, NIST completed a demonstration project to apply MatML to VOC source emission rate data (Begley and Howard-Reed 2005). Since MatML was designed to address any materials property data, it is well-suited for application to contaminant source emission rate databases. Thus, MatML would enable the IAQ community to use relevant tags for data management and exchange via the Web that could be accessed by any IAQ computer model. The challenge to this approach is convincing the IAQ community to adopt MatML for distributing data via the web. Using MatML requires learning the language and there is a need for more user-friendly editors.

Another need is to compile data related to occupant exposure. Occupant exposure assessments are an application that would benefit from the interaction between IAQ models and model input databases. Exposure assessment is based on contaminant air concentrations in a given set of locations and the duration of occupant exposure to those contaminants in those locations. CONTAM has the capability to predict occupant exposure using predicted contaminant concentrations and a user provided occupancy schedule. To date, there are no standard exposure scenarios available to conduct a representative exposure assessment. However, exposure related survey data has been collected such as the National Human Activity Pattern Survey (NHAPS) (Tsang and Klepeis 1996). The NHAPS dataset contains 24 hour activity data for 9386 randomly selected respondents. Based on these data, it would be possible to build representative exposure scenarios that would include daily activities as well as length of stay in a specific room location.

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DISCLAIMER
In an effort to enhance the scientific study of indoor air quality, published model input data are accessible on this site. However, care must be taken when using these data as they are intended for research use. Users of these data assume sole responsibility for determining the appropriateness of their use in any particular application and for any conclusions drawn from results of their use. NIST used its best efforts to deliver a high quality copy of the Database and to verify that the data contained therein have been selected on the basis of sound scientific judgment. However, NIST makes no warranties to that effect, and NIST shall not be liable for any damage that may result from errors or omissions in the Database.

Certain trade names and company products are mentioned in the text to specify adequately the products and equipment used in the test and those needed to use this software. In no case does such identification imply endorsement by the National Institute of Standards and Technology of these products and equipment, nor does it imply that the products are necessarily the best available for the purpose.

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APPENDIX A – DATA ENTRY FORMS

EPA VOC Source Emission Rate Database Entry Forms

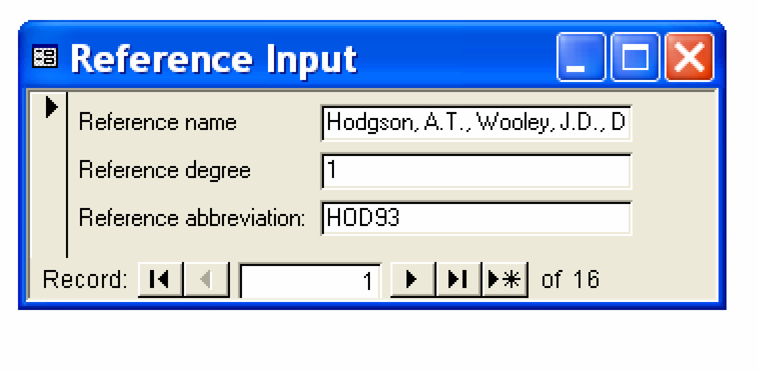


Table Name: Reference

Data Field	Field Description	Data Type	Units
Reference name	Complete citation for reference	Text	
Reference degree	Reflects peer review status of reference. For example, a 1st degree reference indicates journal level review, 2nd degree reference indicates conference level review, and 3rd degree reference indicates internal review.	Number	
Reference abbreviation	Consists of the first three letters of the first author's last name and abbreviated year of publication.	Text	

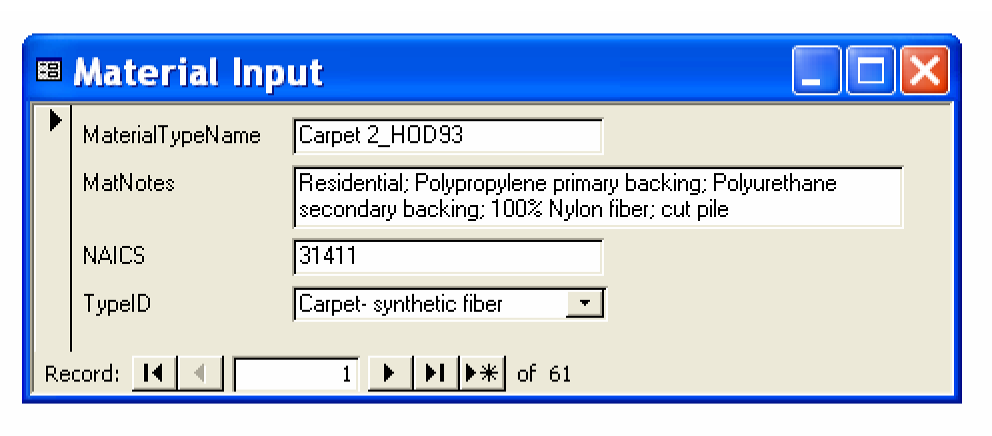


Table Name: Material

Data Field	Field Description	Data Type	Units
MaterialTypeName	Internal reference descriptor with Reference abbreviation	Text	
MatNotes	Relevant information describing material	Text	
NAICS	North American Industry Classification System number	Text	
TypeID	Link to material type	Number	

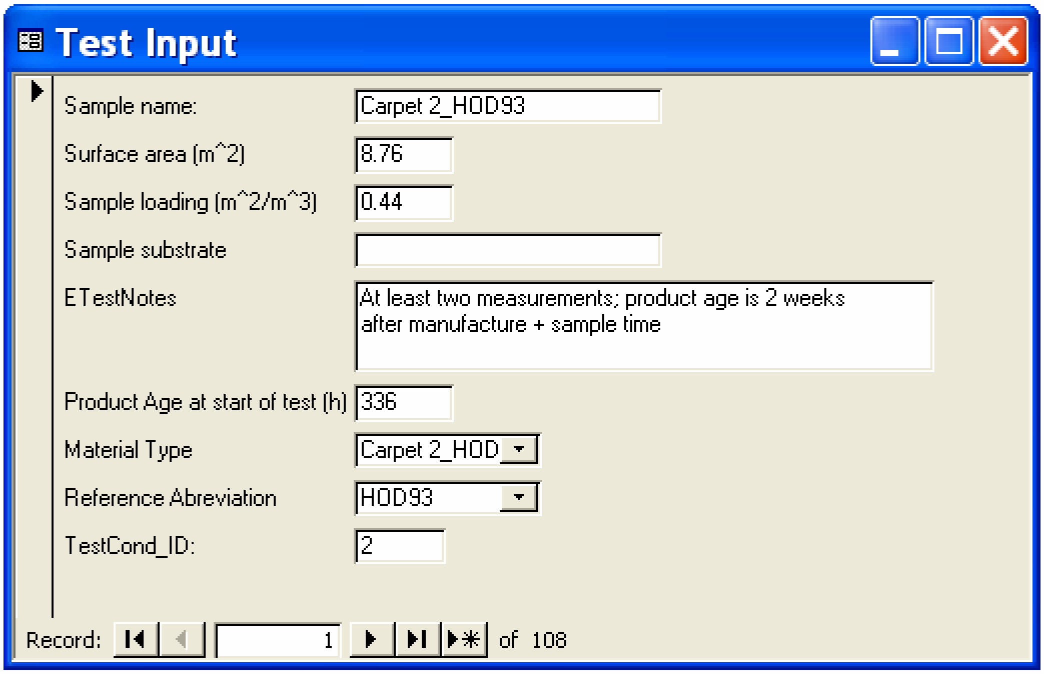


Table Name: ETest

Data Field	**Field Description**	**Data Type**	**Units**
Sample name	Internal reference descriptor with Ref. abbreviation	Text	
Surface area	Product surface area exposed in test facility	Number	m^2
Sample loading	Product surface area to test facility volume ratio	Number	m^2/m^3
Sample substrate	Composition of material on which test product is applied	Text	
ETestNotes	Clarifying and additional information regarding sample	Text	
Product Age at start of test	Age of sample at star of test	Number	h
Material Type	Link to material type name	Number	
Reference Abbreviation	Link to reference abbreviation	Number	
TestCond_ID	Link to test conditions number	Number	

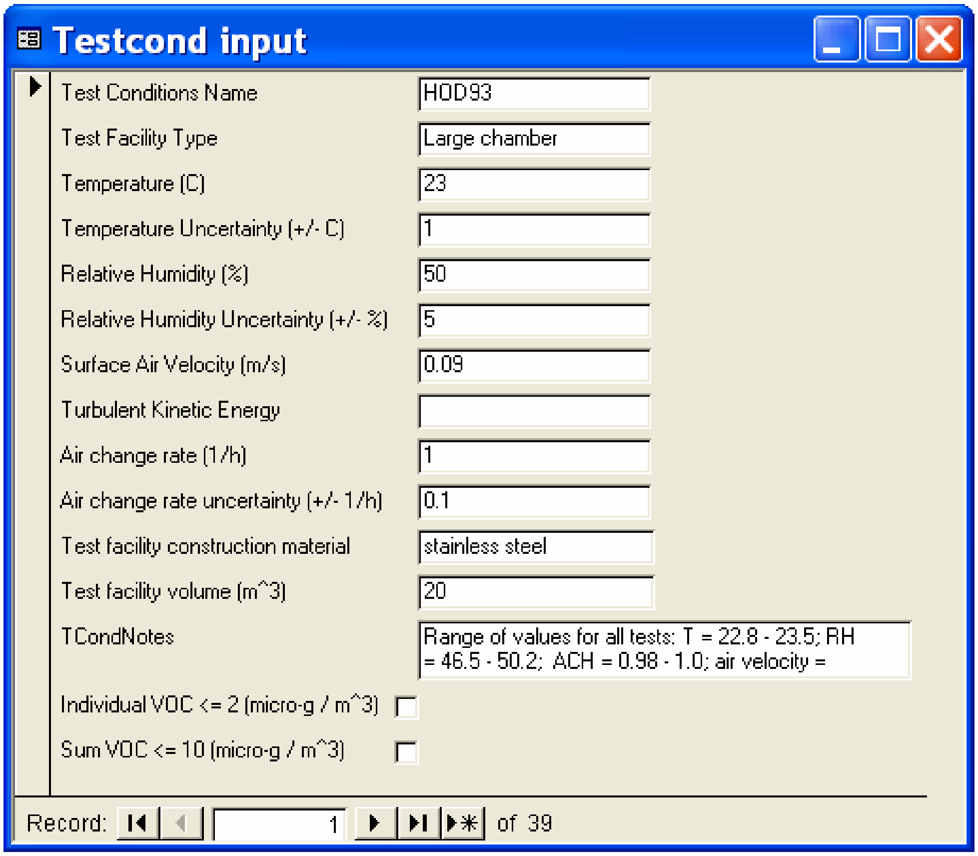


Table Name: Testcond

Data Field	Field Description	Data Type	Units
Test Conditions Name	Same as reference abbreviation	Text	
Test Facility Type	Description of test facility	Text	
Temperature	Temperature of test facility air	Number	° C
Temperature Uncertainty	Uncertainty of temperature measurement	Number	± ° C
Relative Humidity	Relative Humidity of test facility air	Number	%
Relative Humidity Uncertainty	Uncertainty of relative humidity measurement	Number	± %
Surface Air Velocity	Air velocity in test facility near sample surface	Number	m/s
Turbulent Kinetic Energy	Turbulent kinetic energy of test facility air	Number	
Air change rate	Air change rate of test facility	Number	1/ h
Air change rate uncertainty	Uncertainty of air change rate measurement	Number	±1/ h
Test facility construction material	Material covering test facility walls, ceiling and floor	Text	
Test facility volume	Volume of air in test facility	Number	m^3
TCondNotes	Clarifying and additional information regarding test conditions	Text	
Individual VOCs ≤ 2 μg/m^3	Is concentration of each VOC measured in background air of test facility less than or equal to 2 μg/m^3?	Yes/No	
Sum VOCs ≤ 10 μg/m^3	Is concentration of all VOCs measured in background air of test facility less than or equal to 10 μg/m^3?	Yes/No	

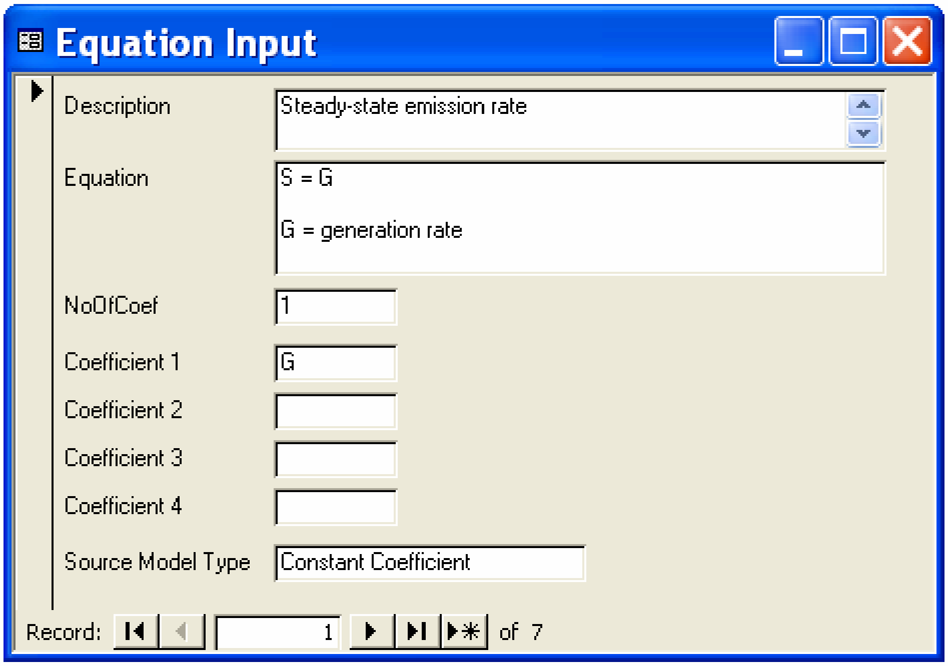


Table Name: Equation

Data Field	**Field Description**	**Data Type**	**Units**
Description	Description of emissions model	Text	
Equation	Model equations with definition of coefficients	Text	
NoOfCoef	Number of model coefficients	Number	
Coefficient 1	Parameter defined as model coefficient 1	Text	
Coefficient 2	Parameter defined as model coefficient 2	Text	
Coefficient 3	Parameter defined as model coefficient 3	Text	
Coefficient 4	Parameter defined as model coefficient 4	Text	
Source Model Type	CONTAM Name of source model	Text	

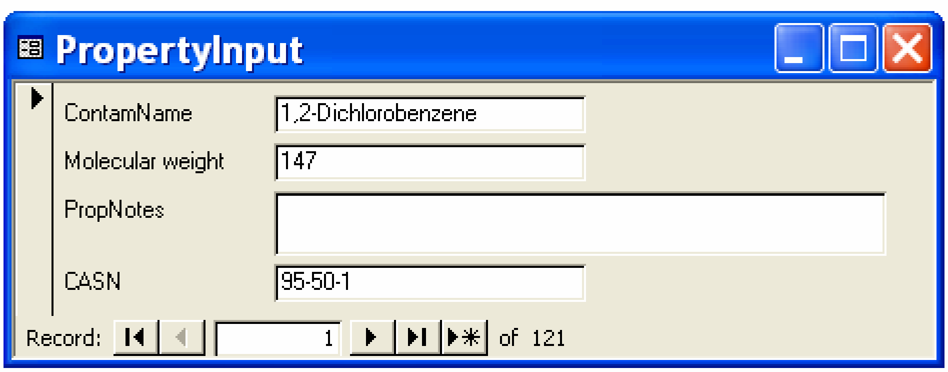


Table Name: Property

Data Field	**Field Description**	**Data Type**	**Units**
ContamName	Name of contaminant	Text	
Molecular weight	Molecular weight of contaminant	Number	
PropNotes	Clarifying or additional information regarding the contaminant	Text	
CASN	Chemical Abstract Service Number	Text	

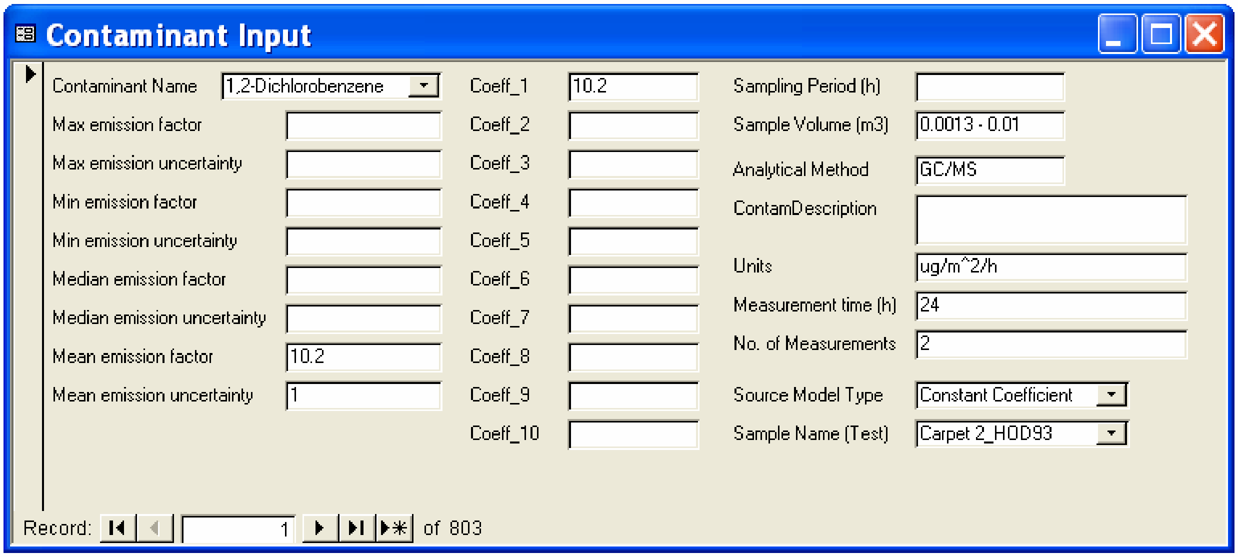
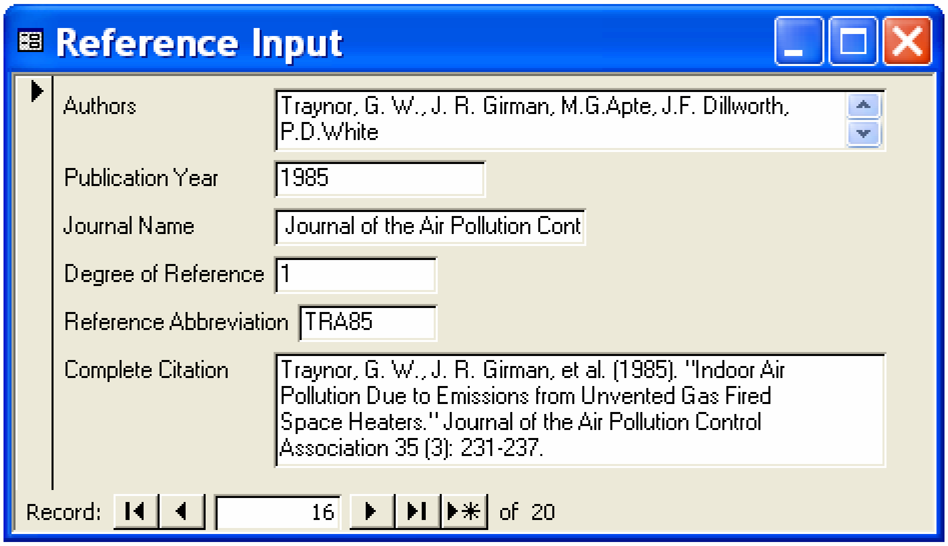


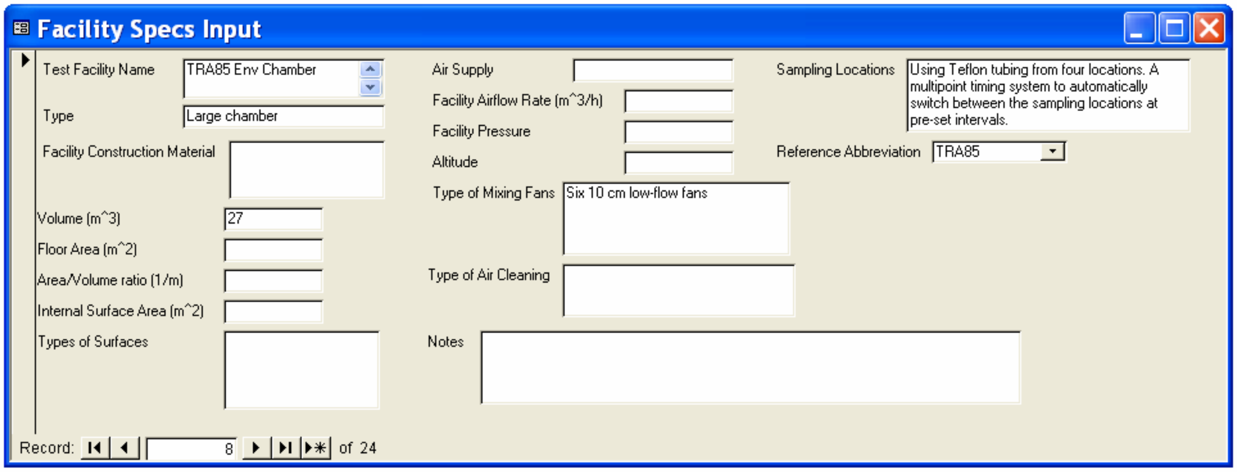
Table Name: Contaminant

Data Field	Field Description	Data Type	Units
Contaminant Name	Link to contaminant name	Text	
Max emission factor	Maximum emission rate for sample period	Number	
Max emission uncertainty	Uncertainty of maximum emission rate measurement	Number	
Min emission factor	Minimum emission rate for sample period	Number	
Min emission uncertainty	Uncertainty of minimum emission rate measurement	Number	
Median emission factor	Median emission rate for given sample time	Number	
Median emission uncertainty	Uncertainty of median emission rate measurement	Number	
Mean emission factor	Mean emission rate for given sample time	Number	
Mean emission uncertainty	Uncertainty of mean emission rate measurement	Number	
Coeff_1	Value of model coefficient 1	Number	
Coeff_2	Value of model coefficient 2	Number	
Coeff_3	Value of model coefficient 3	Number	
Coeff_4	Value of model coefficient 4	Number	
Coeff_5 – Coeff_10	Value of model coefficients 5 – 10, if necessary	Number	
Sampling Period	The length of time sample was collected	Text	h
Sample Volume	Volume of sample collected	Text	m^3
Analytical Method	Detector used to measure concentration	Text	
Contam Description	Clarifying or additional information regarding emission rate data	Text	
Units	Units of coefficients listed in order	Text	
Measurement time	Time sample was collected	Text	h
No. of Measurements	Number of samples included in reported emission factor	Text	
Source Model Type	Link to source model	Number	
Sample Name (Test)	Link to test conditions	Number	

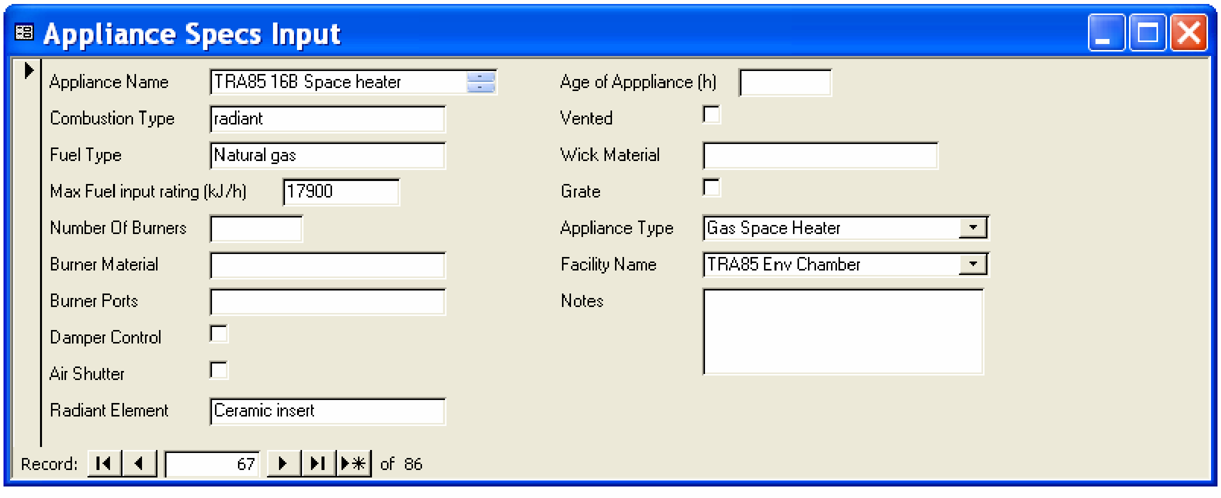
Combustion Source Emission Rate Data Entry Forms



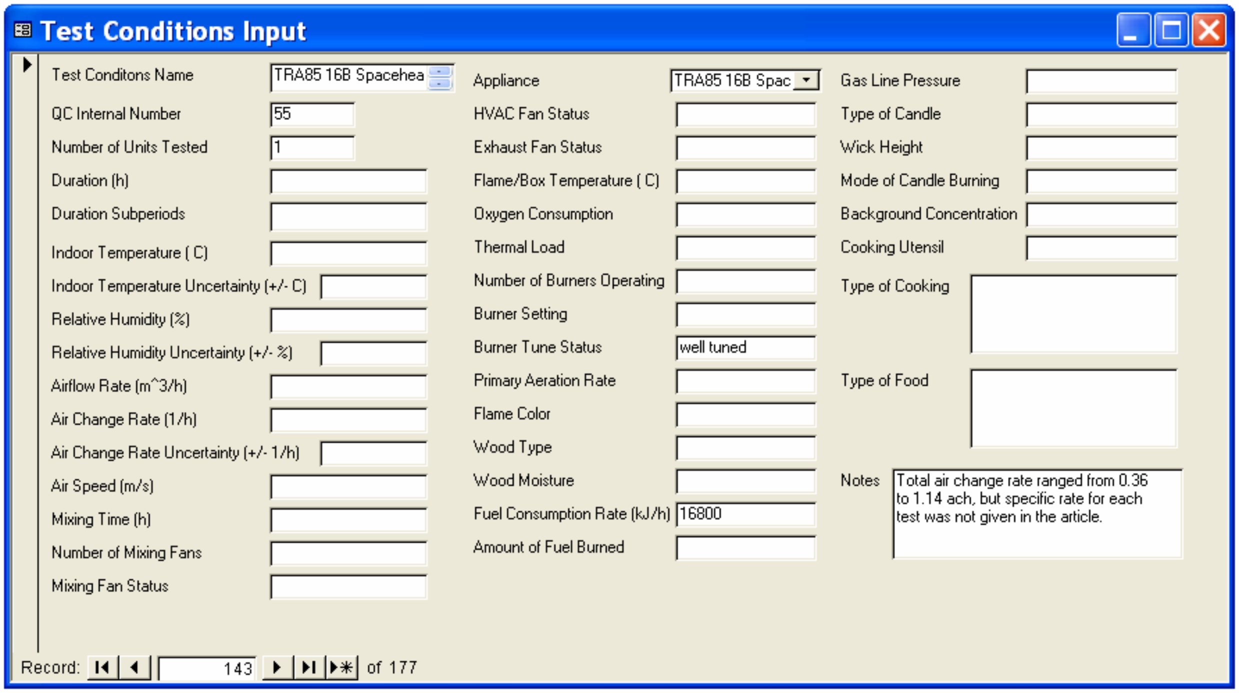
Data Field	Field Description	Data Type	Units
Authors	Authors of reference	Text	
Publication Year	Year reference was published	Text	
Journal Name	Title of journal or other document where reference was published	Text	
Degree of Reference	Reflects peer review status of reference. For example, a 1st degree reference indicates journal level review, 2nd degree reference indicates conference level review, and 3rd degree reference indicates internal review.	Number	
Reference Abbreviation	Consists of the first three letters of the first author's last name and abbreviated year of publication.	Text	
Complete citation	Complete citation for reference	Text	



Data Field	Field Description	Data Type	Units
Test Facility Name	Reference Abbreviation with internal descriptor of test facility	Text	
Type	Type of test facility	Text	
Facility Construction Material	Material covering test facility walls, ceiling and floor	Text	
Volume	Volume of air in test facility	Number	m^3
Floor Area	Surface area of test facility floor	Number	m^2
Area/Volume ratio	Surface area of test facility to volume of test facility ratio	Number	m^2/m^3
Internal Surface Area	Surface area of test facility walls, ceiling and floor	Number	m^2
Type of Surfaces	Description of surfaces in test facility, in addition to walls, ceiling and floor	Text	
Air Supply	Source of air added to test facility	Text	
Facility Airflow Rate	Airflow rate measured in test facility	Number	m^3/h
Facility Pressure	Air pressure measured in test facility	Text	
Altitude	Altitude of test facility	Text	
Type of Mixing Fans	Description of mixing fans in test facility	Text	
Type of Air Cleaning	Description of filtration/air cleaning devices used in test facility	Text	
Notes	Clarifying or additional information regarding test facility	Text	
Sampling Locations	Description of sample locations in test facility	Text	
Reference Abbreviation	Link to reference abbreviation	Number	

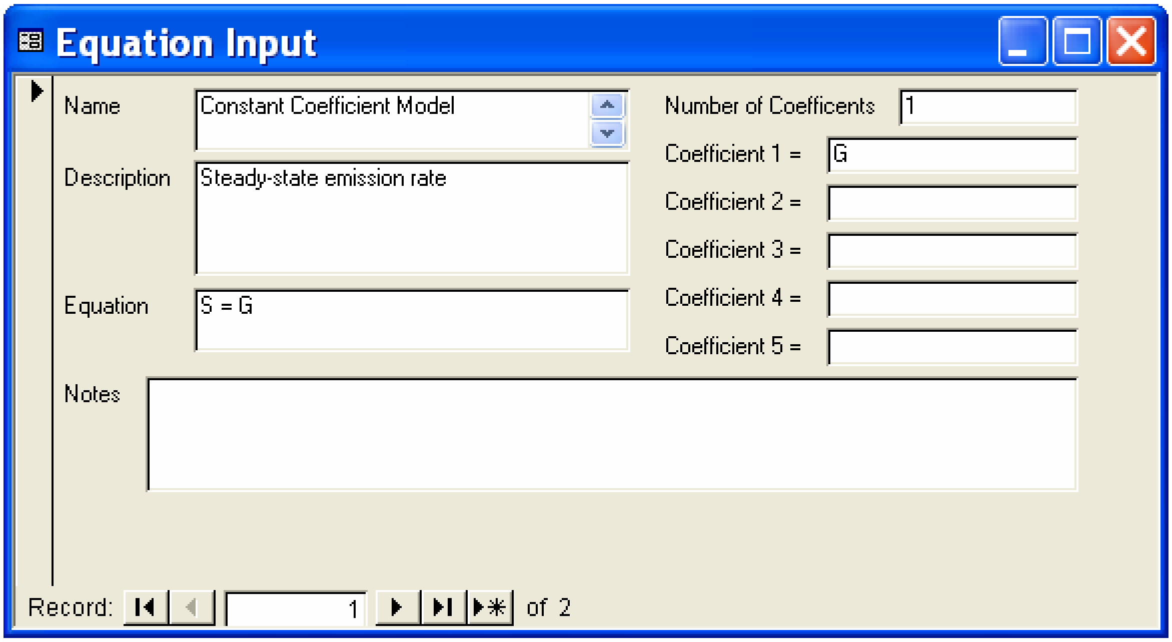


Data Field	Field Description	Data Type	Units
Appliance Name	Reference abbreviation and internal appliance descriptor	Text	
Combustion Type	Combustion mechanism	Text	
Fuel Type	Fuel used in appliance	Text	
Max Fuel input rating	Maximum fuel input rating for appliance	Number	kJ/h
Number of Burners	Number of burners operated during test	Number	
Burner Material	Material of burners used in test	Text	
Burner Ports	Type of burner port in appliance	Text	
Damper Control	Does the appliance have damper control?	Yes/No	
Air Shutter	Does the appliance have an air shutter?	Yes/No	
Radiant Element	Type of radiant element	Text	
Age of Appliance	Appliance age at time of test	Number	h
Vented	Is the appliance vented?	Yes/No	
Wick Material	Type of candle wick	Text	
Grate	Does the appliance have a grate?	Yes/No	
Appliance Type	Link to appliance type	Number	
Facility Name	Link to facility name	Number	
Notes	Clarifying or additional information regarding appliance specifications	Text	

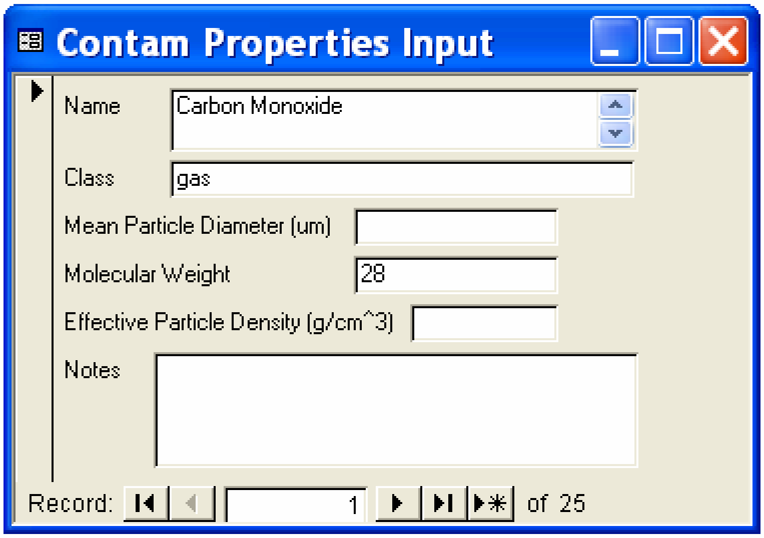


Data Field	Field Description	Data Type	Units
Test Conditions Name	Reference ID and internal descriptor	Text	
QC Internal Number	Internal record keeping number for quality assurance checks	Number	
Number of Units Tested	Number of appliances tested for given emission factor	Number	
Duration	Length of experiment	Text	h
Duration Subperiods	Any distinction of experiment time periods	Text	
Indoor Temperature	Temperature of room air in test facility	Number	° C
Indoor Temperature Uncertainty	Uncertainty of temperature measurement	Number	± ° C
Relative Humidity	Relative humidity of test facility	Number	%
Relative Humidity Uncertainty	Uncertainty of relative humidity measurement	Number	± %
Airflow Rate	Flow rate of air through test facility	Number	m^3/h
Air Change Rate	Volumetric air change rate of test facility	Number	1/h
Air Change Rate Uncertainty	Uncertainty of air change rate measurement	Number	± 1/h
Air Speed	Velocity of air near surface of test appliance	Number	m/s
Mixing Time	Period of mixing prior to first sample	Number	h
Number of Mixing Fans	Number of mixing fans in test facility	Number	
Mixing Fan Status	Description of mixing fan use during the test	Text	
Appliance	Link to appliance name	Number	
HVAC Fan Status	Description of facility HVAC use during the test	Text	
Exhaust Fan Status	Description of facility exhaust fan use during the test	Text	
Flame/Box Temperature	Temperature of heated chamber (e.g., fire box, oven, etc.)	Number	° C

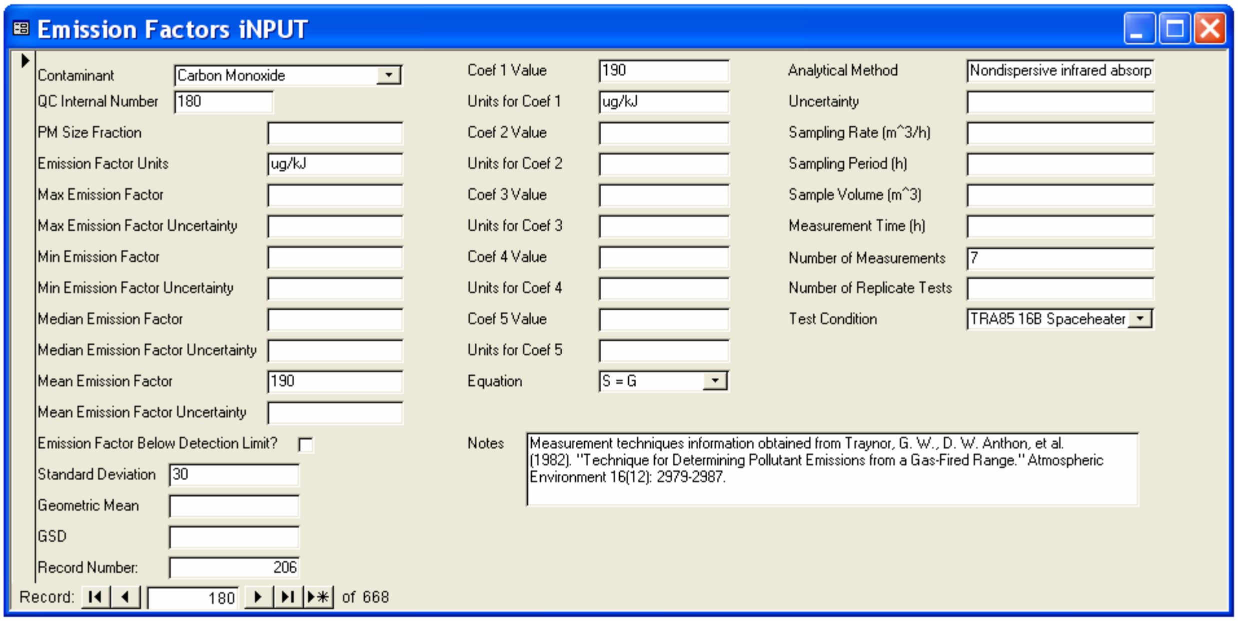
Oxygen Consumption	Appliance oxygen consumption rate	Text	
Thermal Load	Thermal load of appliance	Number	
Number of Burners Operating	Number of burners on during the test	Number	
Burner Setting	Level of burner setting according to appliance (e.g., low, medium, high)	Text	
Burner Tune Status	How well-tuned are the appliance burners	Text	
Primary Aeration Rate	Allowance of primary air to appliance	Text	
Flame Color	Color of appliance flame	Text	
Wood Type	Type of wood burned	Text	
Wood Moisture	Moisture content of wood burned	Text	
Fuel Consumption Rate	Rate of fuel consumption for appliance	Number	kJ/h
Amount of Fuel Burned	Mass of fuel burned for test	Text	
Gas Line Pressure	Pressure of gas in input line	Text	
Type of Candle	Type of candle burned for test	Text	
Wick Height	Height of candle wick	Text	
Mode of Candle Burning	Description of candle burn (e.g, sooting, etc.)	Text	
Background Concentration	Room air concentration in test facility prior to test	Text	
Cooking Utensil	Type of utensil used in cooking test	Text	
Type of Cooking	Description of cooking style for test	Text	
Type of Food	Description of food cooked during test	Text	
Notes	Clarifying or additional information regarding test conditions	Text	



Data Field	**Field Description**	**Data Type**	**Units**
Name	CONTAM name of source model	Text	
Description	Description of emissions model		
Equation	Model equations with definition of coefficients	Text	
Notes	Clarifying or additional information regarding source model equations	Text	
Number of Coefficients	Number of model coefficients	Number	
Coefficient 1	Parameter defined as model coefficient 1	Text	
Coefficient 2	Parameter defined as model coefficient 2	Text	
Coefficient 3	Parameter defined as model coefficient 3	Text	
Coefficient 4	Parameter defined as model coefficient 4	Text	
Coefficient 5	Parameter defined as model coefficient 5	Text	



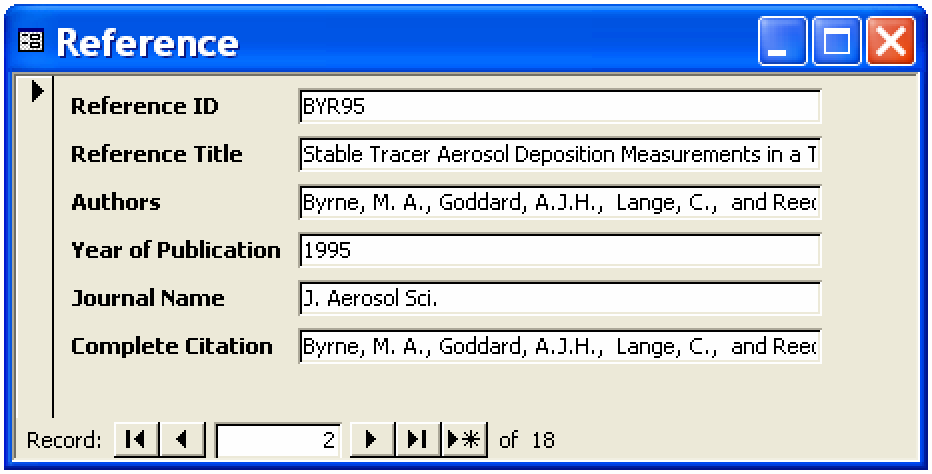
Data Field	Field Description	Data Type	Units
Name	Name of contaminant	Text	
Class	Physical state of contaminant	Text	
Mean Particle Diameter	Mean diameter of particle measured	Number	µm
Molecular Weight	Molecular weight of contaminant	Text	
Effective Particle Density	Effective density of particle	Number	g/cm^3
Notes	Clarifying or additional information regarding contaminant properties	Text	



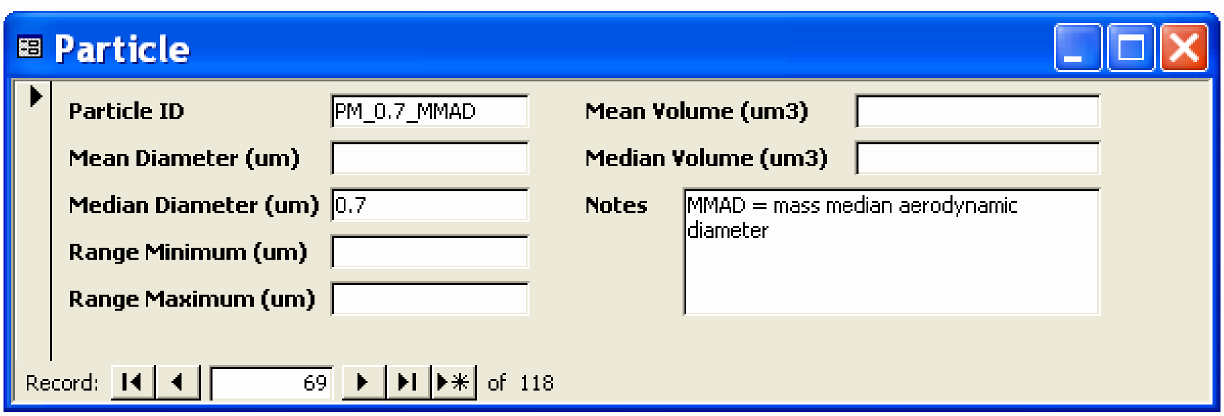
Data Field	Field Description	Data Type	Units
Contaminant	Link to contaminant ID	Number	
QC Internal Number	Internal record keeping number for quality assurance checks	Number	
PM Size Fraction	Range of particle diameters for given emission factor	Text	
Emission Factor Units	Units of reported emission factors	Text	
Max Emission Factor	Maximum emission rate for sample period	Number	
Max Emission Factor Uncertainty	Uncertainty of maximum emission rate measurement	Number	
Min Emission Factor	Minimum emission rate for sample period	Number	
Min Emission Factor Uncertainty	Uncertainty of minimum emission rate measurement	Number	
Median Emission Factor	Median emission rate for sample period	Number	
Median Emission Factor Uncertainty	Uncertainty of minimum emission rate measurement	Number	
Mean Emission Factor	Mean emission rate for sample period	Number	
Mean Emission Factor Uncertainty	Uncertainty of mean emission rate measurement	Number	
Emission Factor Below Detection Limit?	Are the measured concentrations less than the minimum detection limit?	Yes/No	
Standard Deviation	Standard deviation of mean emission rate for sample period	Number	
Geometric Mean	Geometric mean emission rate for sample period	Number	
GSD	Geometric standard deviation of emission rate for sample period	Number	
Record Number	Database automatic record number	Autonumber	
Coef 1 Value	Value of first coefficient in model equation	Number	
Units for Coef 1	Units of first coefficient in model	Text	
Coef 2 Value	Value of second coefficient in model equation	Number	
Units for Coef 2	Units of second coefficient in model	Text	

Coef 3 Value	Value of third coefficient in model equation	Number	
Units for Coef 3	Units of third coefficient in model	Text	
Coef 4 Value	Value of fourth coefficient in model equation	Number	
Units for Coef 4	Units of fourth coefficient in model	Text	
Coef 5 Value	Value of fifth coefficient in model equation	Number	
Units for Coef 5	Units of fifth coefficient in model	Text	
Equation	Link to equation ID	Number	
Notes	Clarifying or additional information regarding the emission rate measurements	Text	
Analytical Method	Instrument used to measure contaminant concentrations	Text	
Uncertainty	Uncertainty of analytical method used to measure contaminant concentrations	Text	
Sampling Rate	Volumetric airflow sample rate of instrument	Number	m^3/h
Sampling Period	Duration of sample collection	Text	
Sample Volume	Air volume of sample collected	Number	m^3
Measurement Time	Time sample was collected	Text	
Number of Measurements	Number of samples collected for emission rate estimate	Number	
Number of Replicate Tests	Number of replicate experiments included in emission rate estimate	Number	
Test Condition	Link to Test Condition ID	Number	

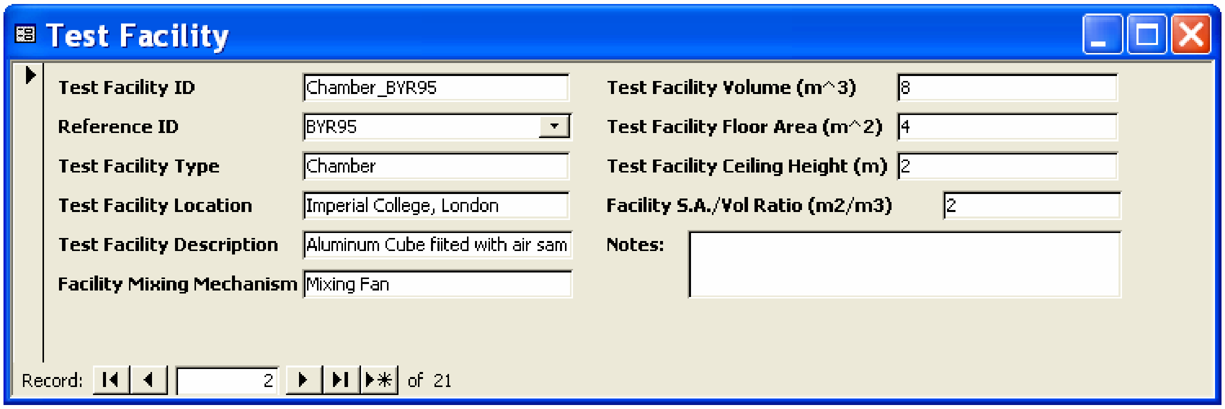
Particle Deposition Rate Entry Forms



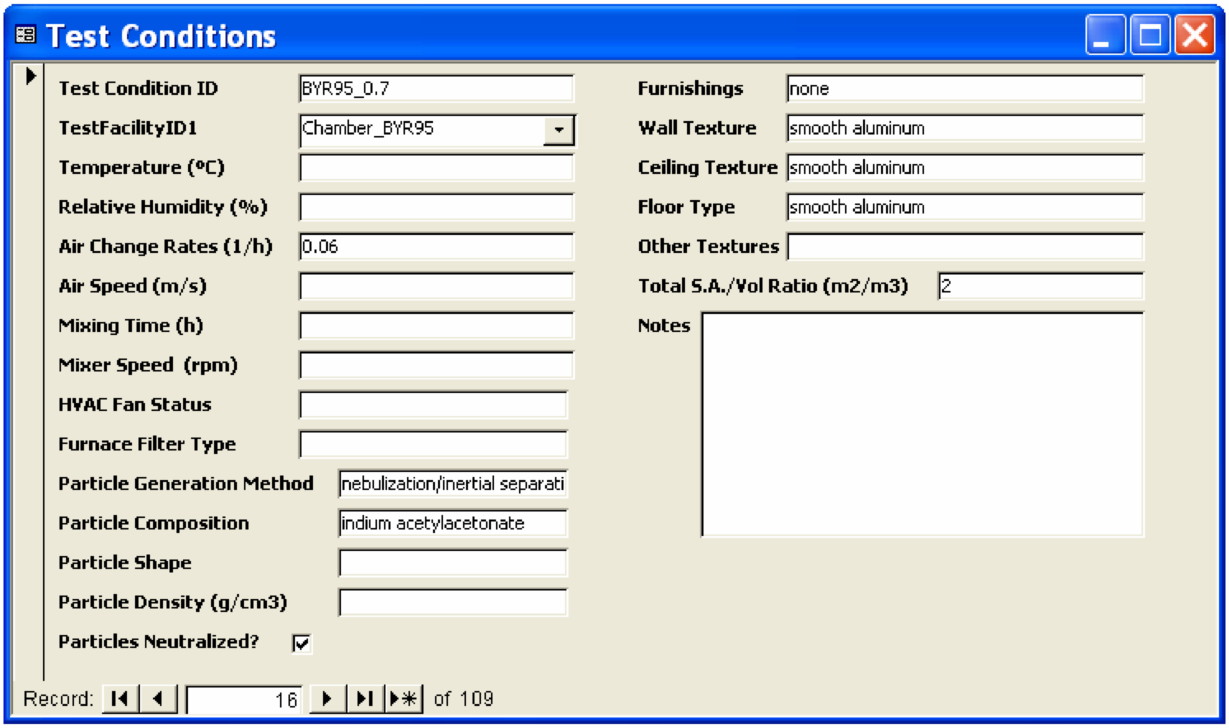
Data Field	Field Description	Data Type	Units
Reference ID	Consists of the first three letters of the first author's last name and abbreviated year of publication	Text	
Reference Title	Title of reference	Text	
Authors	Authors of reference	Text	
Year of Publication	Year reference was published	Text	
Journal Name	Title of journal or other document where reference was published	Text	
Complete citation	Complete citation for reference	Text	



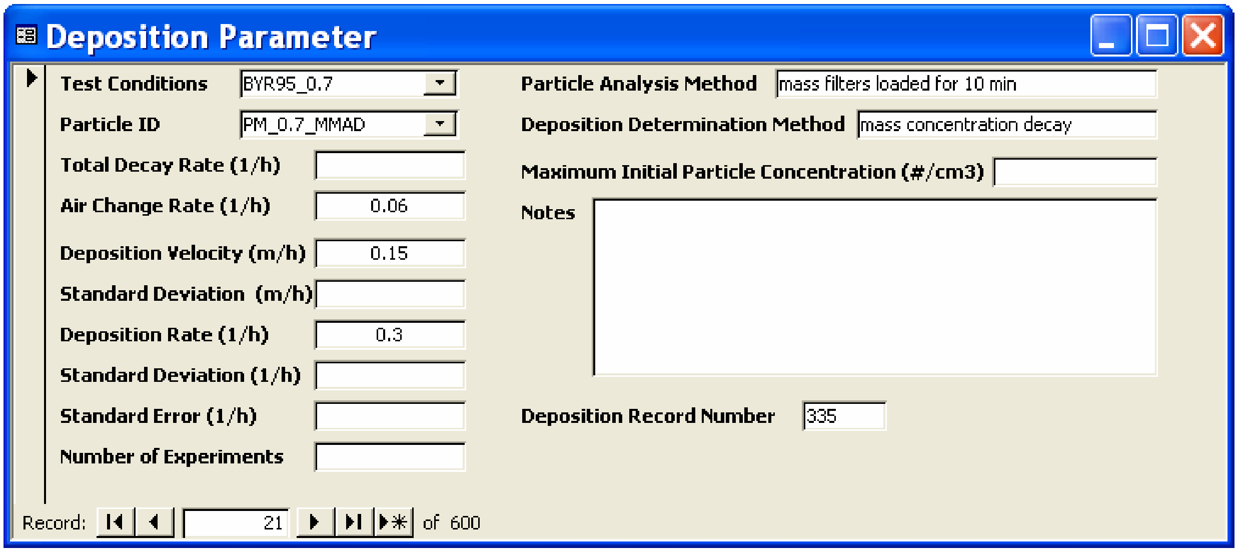
Data Field	Field Description	Data Type	Units
Particle ID	Consists of PM_particle diameter_type of diameter based on analytical method	Text	
Mean Diameter	Mean particle diameter	Number	μm
Median Diameter	Median particle diameter	Number	μm
Range Minimum	Minimum particle diameter for range of sizes	Number	μm
Range Maximum	Maximum particle diameter for range of sizes	Number	μm
Mean Volume	Mean volume of particle	Number	μm^3
Median Volume	Median volume of particle	Number	μm^3
Notes	Clarifying or additional information regarding the particle properties	Text	



Data Field	**Field Description**	**Data Type**	**Units**
Test Facility ID	Test facility type and Reference ID	Text	
Reference ID	Link to Reference ID	Number	
Test Facility Type	Type of test facility	Text	
Test Facility Location	Geographical location of test facility	Text	
Test Facility Description	General description of test facility	Text	
Facility Mixing Mechanism	Air mixing mechanisms in test facility	Text	
Test Facility Volume	Air volume of test facility	Number	m^3
Test Facility Floor Area	Surface area of the test facility floor	Number	m^2
Test Facility Ceiling Height	Average height from floor to ceiling of test facility	Number	m
Facility S.A./Vol Ratio	Total surface area of the test facility to volume of test facility ratio	Number	m^2/m^3
Notes	Clarifying or additional information related to the test facility	Text	

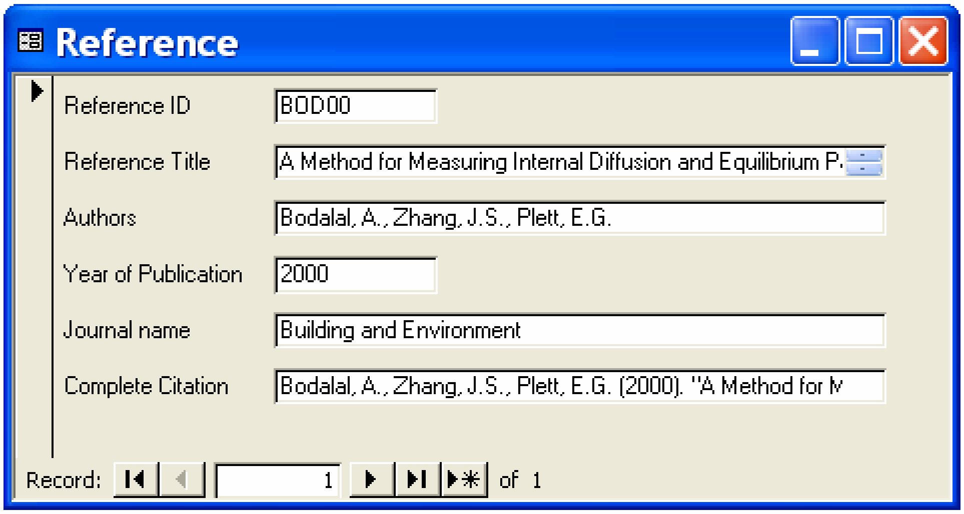


Data Field	Field Description	Data Type	Units
Test Condition ID	Reference ID and internal test condition descriptor	Text	
TestFacilityID1	Link to Test Facility ID	Number	
Temperature	Air temperature in test facility	Number	° C
Relative Humidity	Relative humidity of room air in test facility	Number	%
Air Change Rates	Range of air change rates for test condition	Text	1/h
Air Speed	Room air velocity	Number	m/s
Mixing Time	Period of particle mixing in test facility prior to deposition measurements	Number	h
Mixer Speed	Mixing fan speed	Number	rad/s
HVAC Fan Status	Was HVAC fan operating during test?	Text	
Furnace Filter Type	If HVAC fan was operating, what type of filter was present	Text	
Particle Generation Method	Mechanism or device used to generate particles	Text	
Particle Composition	Composition of particles	Text	
Particle Density	Effective density of particles	Number	g/cm^3
Particles Neutralized?	Were the generated particles neutralized before release?	Yes/No	
Furnishings	General description of furnishings in test facility	Text	
Wall Texture	Material covering test facility walls	Text	
Ceiling Texture	Material covering test facility ceiling	Text	
Floor Type	Material covering test facility floor	Text	
Other textures	Additional test facility textures worth noting	Text	
Total S.A./Vol Ratio	Total surface area of test facility to volume of test facility ratio	Number	m^2/m^3
Notes	Clarifying or additional information related to test conditions	Text	

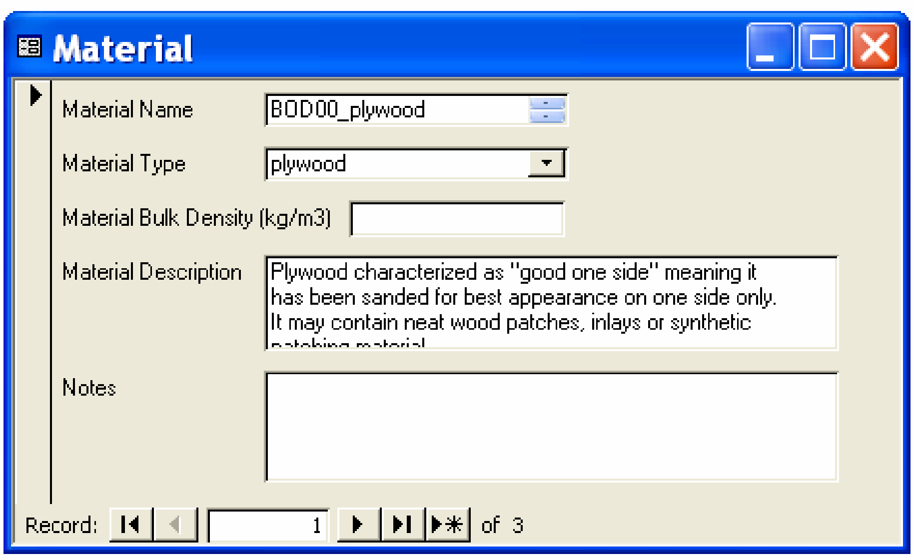


Data Field	Field Description	Data Type	Units
Test Conditions	Link to Test Condition ID	Number	
Particle ID	Link to Particle ID	Number	
Total Decay Rate	Total decay rate of particle including all loss mechanisms	Number	1/h
Air Change Rate	Air change rate of test facility for specific test	Number	1/h
Deposition Velocity	Measured deposition velocity of particle	Number	m/h
Standard Deviation	Standard deviation of measured deposition velocity	Number	m/h
Deposition Rate	Measured deposition rate of particle	Number	1/h
Standard Deviation	Standard deviation of measured deposition rate	Number	1/h
Standard Error	Standard error of measured deposition rate	Number	1/h
Number of Experiments	Number of experiments included in deposition value	Number	
Particle Analysis Method	Method to collect and analyze particle mass or concentrations for a specific particle diameter	Text	
Deposition Determination Method	Mathematical method used to determine particle deposition rate	Text	
Maximum Initial Particle Concentration	Maximum particle concentration at start of deposition experiment to indicate effect of coagulation	Number	$\#/cm^3$
Notes	Clarifying or additional information regarding deposition values	Text	
Deposition Record Number	Internal tracking number for quality assurance checks	Autonumber	

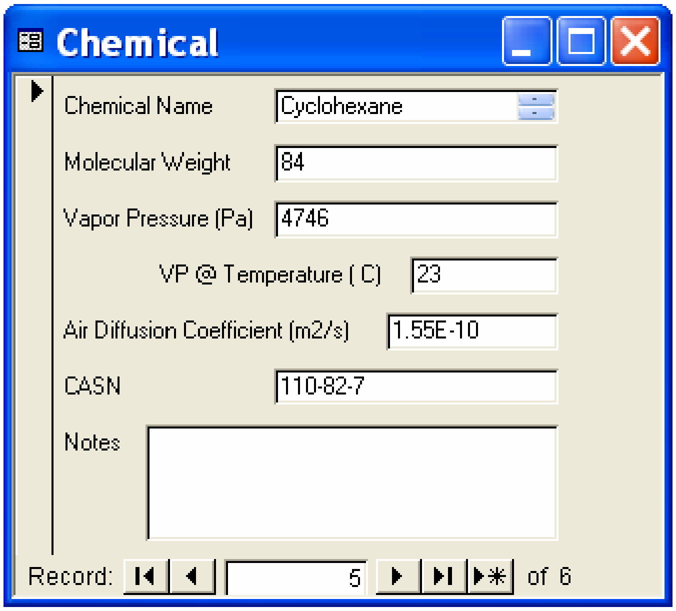
Partition Coefficient Data Entry Forms



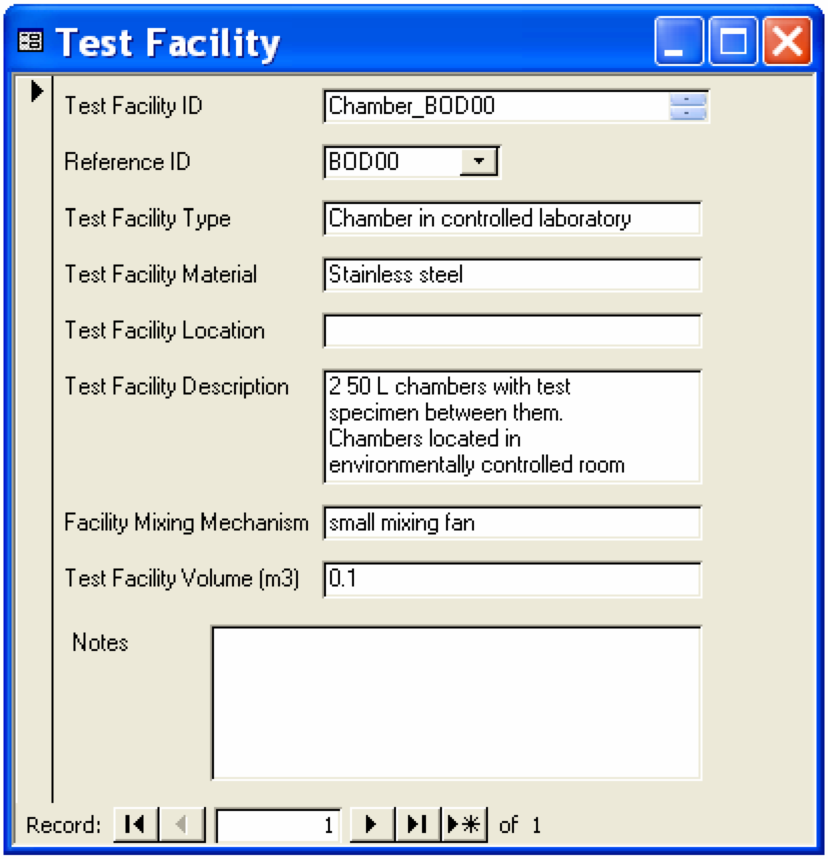
Data Field	Field Description	Data Type	Units
Reference ID	Consists of the first three letters of the first author's last name and abbreviated year of publication	Text	
Reference Title	Title of reference	Text	
Authors	Authors of reference	Text	
Year of Publication	Year reference was published	Text	
Journal Name	Title of journal or other document where reference was published	Text	
Complete citation	Complete citation for reference	Text	



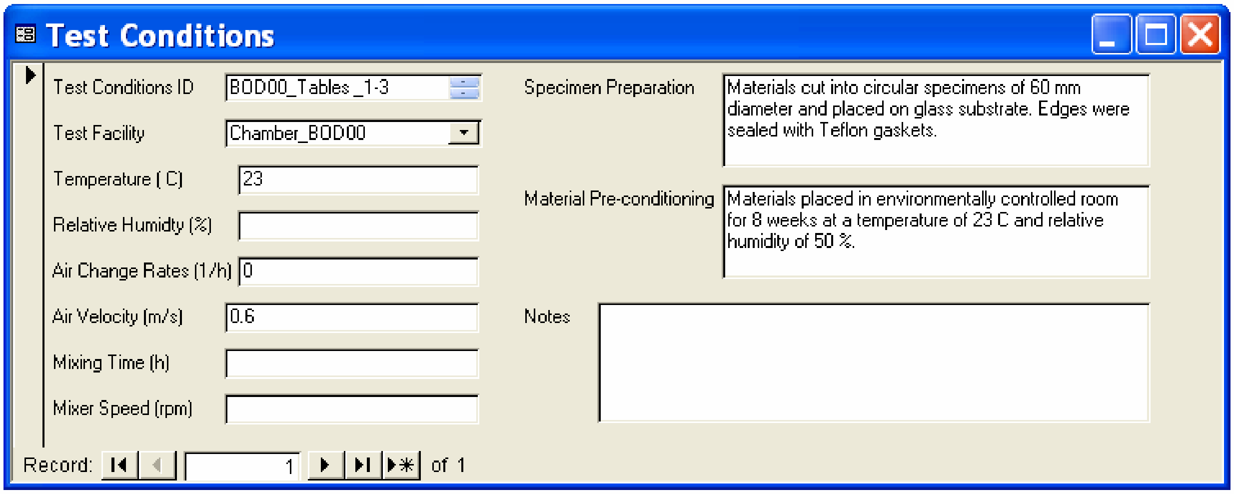
Data Field	Field Description	Data Type	Units
Material Name	Consists of Reference ID and internal material descriptor	Text	
Material Type	Link to sorbent material type	Number	
Material Bulk Density	Bulk density of sorbent material	Number	kg/m^3
Material Description	Description of material used in experiment	Text	
Notes	Clarifying or additional information related to sorbent material	Text	



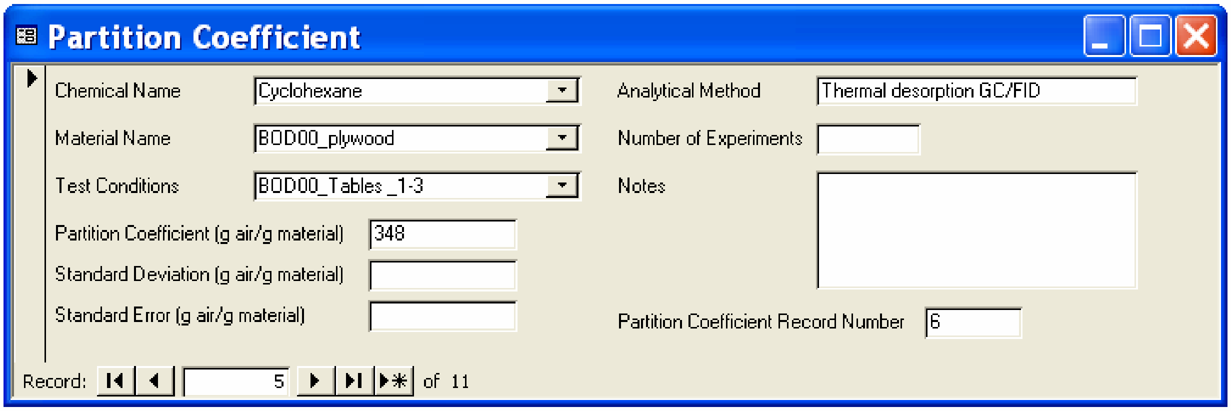
Data Field	**Field Description**	**Data Type**	**Units**
Chemical Name	Name of chemical used in sorption experiment	Text	
Molecular Weight	Molecular weight of chemical	Text	
Vapor Pressure	Vapor Pressure of chemical at specific temperature	Number	Pa
VP@ Temperature	Specific temperature for vapor pressure value	Number	° C
Air Diffusion Coefficient	Diffusion coefficient of chemical in air	Number	m^2/s
CASN	Chemical Abstract Service Number	Text	
Notes	Clarifying or additional information regarding chemical used in experiment	Text	



Data Field	Field Description	Data Type	Units
Test Facility ID	Internal test facility descriptor and Reference ID	Text	
Reference ID	Link to Reference ID	Number	
Test Facility Type	Type of test facility	Text	
Test Facility Material	Material covering test facility walls, ceiling and floor	Text	
Test Facility Location	Geographical location of test facility	Text	
Test Facility Description	General description of test facility	Text	
Facility Mixing Mechanism	Mechanism used to mix test facility room air	Text	
Test Facility Volume	Volume of test facility air	Number	m^3
Notes	Clarifying or additional information related to test facility	Text	



Data Field	Field Description	Data Type	Units
Test Conditions ID	Reference ID and internal descriptor of test conditions	Text	
Test Facility	Link to Test Facility ID	Number	
Temperature	Temperature of test facility air	Number	° C
Relative Humidity	Relative humidity of test facility air	Number	%
Air Change Rates	Air change rate of test facility	Number	1/h
Air Velocity	Velocity of test facility air near surface of material	Number	m/s
Mixing Time	Mixing time of test facility air	Number	h
Mixer Speed	Rotational speed of test facility mixing mechanism	Number	rad/s
Specimen Preparation	General description of preparation of materials for experiment	Text	
Material Pre-conditioning	Any pre-experimental procedures for the material specimen	Text	
Notes	Clarifying or additional information regarding test conditions	Text	



Data Field	Field Description	Data Type	Units
Chemical Name	Link to Chemical ID	Number	
Material Name	Link to Material ID	Number	
Test Conditions	Link to Test Conditions ID	Number	
Partition Coefficient	Measure partition coefficient for given chemical and material	Number	g air/ g material
Standard Deviation	Standard deviation of partition coefficient measurement	Number	g air/ g material
Standard Error	Standard error of partition coefficient measurement	Number	g air/ g material
Analytical Method	Method used to measure chemical concentration	Text	
Number of Experiments	Number of experiments included in partition coefficient value	Number	
Notes	Clarifying or additional information regarding partition coefficient value	Text	
Partition Coefficient Record Number	Internal tracking number for quality assurance checks	Text	

APPENDIX B: ContamLink 2.4 User Manual

Introduction

ContamLink is a tool that is used to facilitate the transfer of information from contaminant emission databases to CONTAM as CONTAM source/sink elements. These databases contain experimental contaminant modeling data, including source emission rates for volatile organic compounds, inorganic gases and particles, particle deposition rates, sorption rates, and air cleaning removal.

Getting ContamLink

ContamLink can be downloaded from CONTAM's homepage (http://bfrl.nist.gov/IAQanalysis/software/index.htm). Installation instructions can be found on ContamLink's download page.

Using ContamLink

The ContamLink main window has three parts: the menubar, the sidebar and the data viewer (see Figure 1).

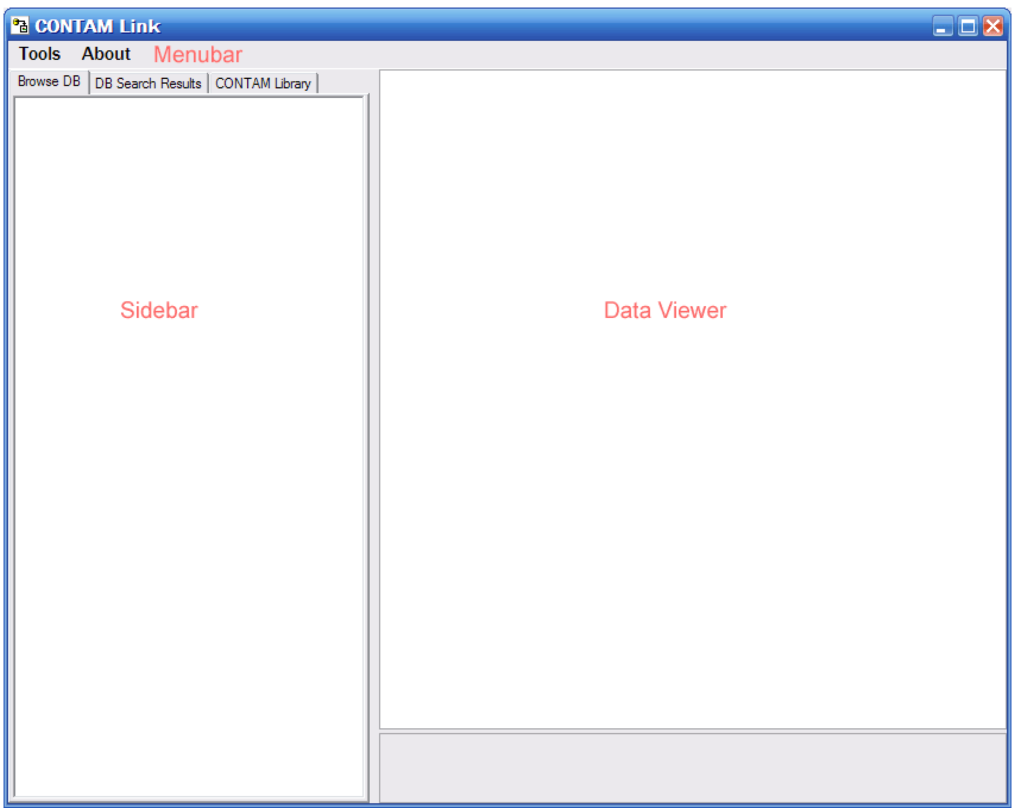


Figure 1. ContamLink main window.

Menubar

The Tools dropdown menu on the window bar includes the commands to open or search a database, create a source/sink or super source/sink, or exit the program.

Sidebar

The sidebar has three functions. The first is to browse a database's contents. This is done with a tree to show the hierarchy of the database. The second function of the sidebar is to show results of searching the database. The third function is the library manager. This library manager is similar to the one found in ContamW (Walton and Dols, 2005). Species and source/sinks that are created in ContamLink can be managed here.

Data Viewer

The data viewer displays information from the database. The data shown depends on what is selected when browsing or searching the database. The data viewer is not used with the library manager.

Loading a database

A database can be loaded using Tools ⇒ Open Database from the menu or using the Ctrl+O keyboard shortcut. The dialog shown in Figure 2 is then presented.

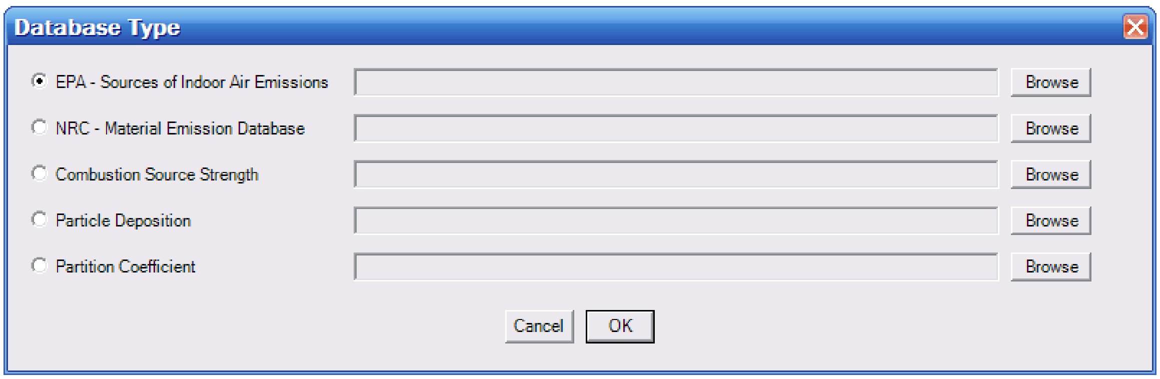


Figure 2. Choosing a database window.

Pick the type of database file to use on the left. Then use the corresponding browse button to pick the database file to use. Databases are available on the CONTAM homepage (http://bfrl.nist.gov/IAQanalysis/software/CONTAMLINKdatabases.htm) and the database filenames match the respective "database type". For example, the Particle Deposition filename is "Particle Deposition." After the database is successfully loaded, a dialog box will appear. Click OK to begin using the database.

Browsing a database

After a database is loaded the contents of the database can be browsed. The browse tab, on the sidebar, is used to show the hierarchy of the database. Most items in the hierarchy show information in the data viewer, which correspond to a record in a table or multiple tables that are joined together from the database. Each database has a slightly different hierarchy which is presented below:

EPA Database

The first level of the EPA VOC source database shows the categories of materials contained in the database. The next level provides the types of materials in this category (e.g., water-based paint is a type of Paint and Coating). Below each material type are specific studies that generated emission results. Clicking on a study name shows a more detailed description of the material used in the study. The different test conditions used for a specific study are listed in the next level, with details in the data viewer window. Finally, all of the chemical compounds measured are listed. Clicking on each compound shows emission rate results and model information in the data viewer. Figure 3 shows the EPA VOC source database hierarchy with the test conditions highlighted for the data viewer window.

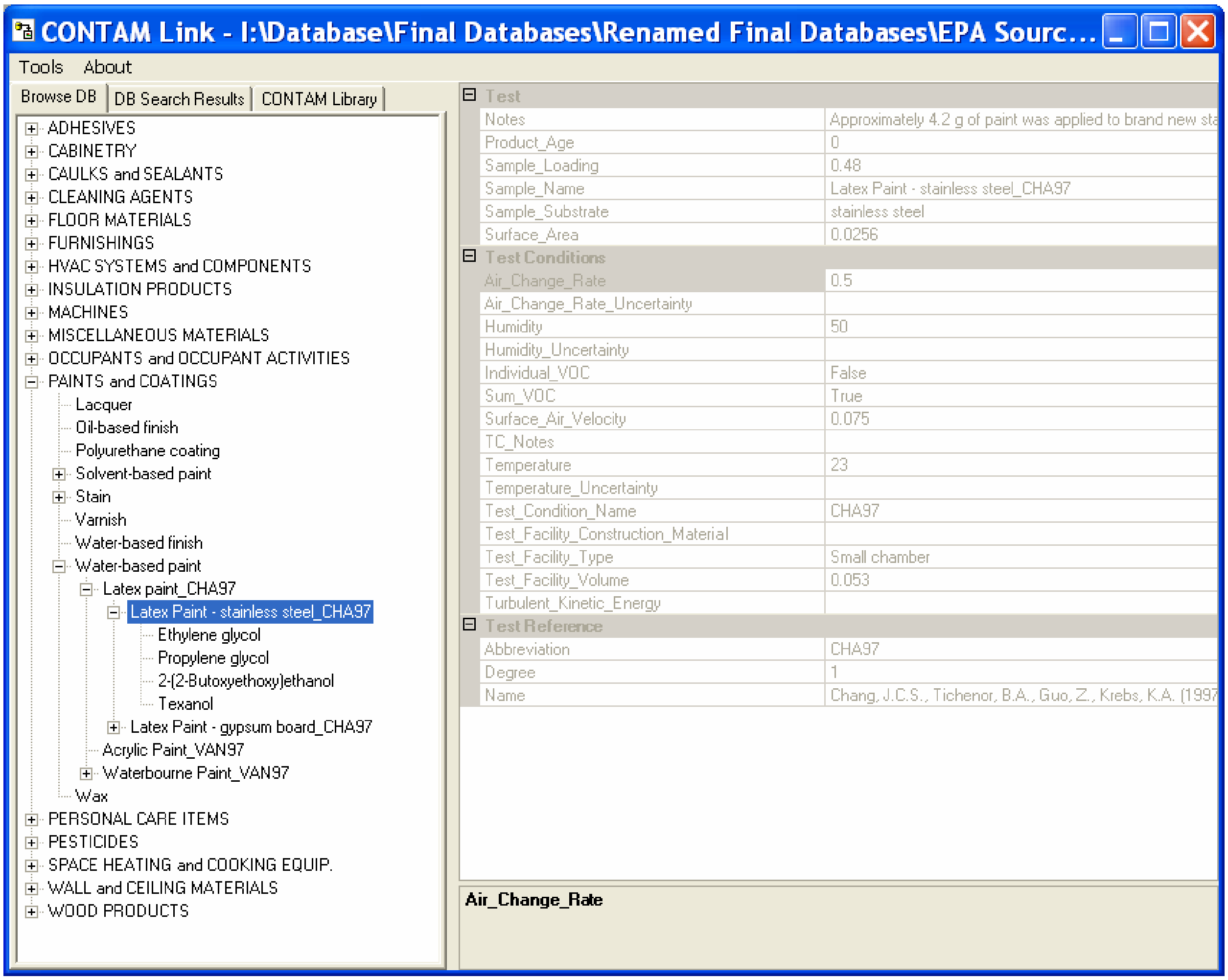


Figure 3. Browsing capabilities of VOC source emissions database with ContamLink and material test conditions results display.

NRC Database

The NRC VOC Source emission database has a similar hierarchy to the EPA VOC source database (see Figure 4).

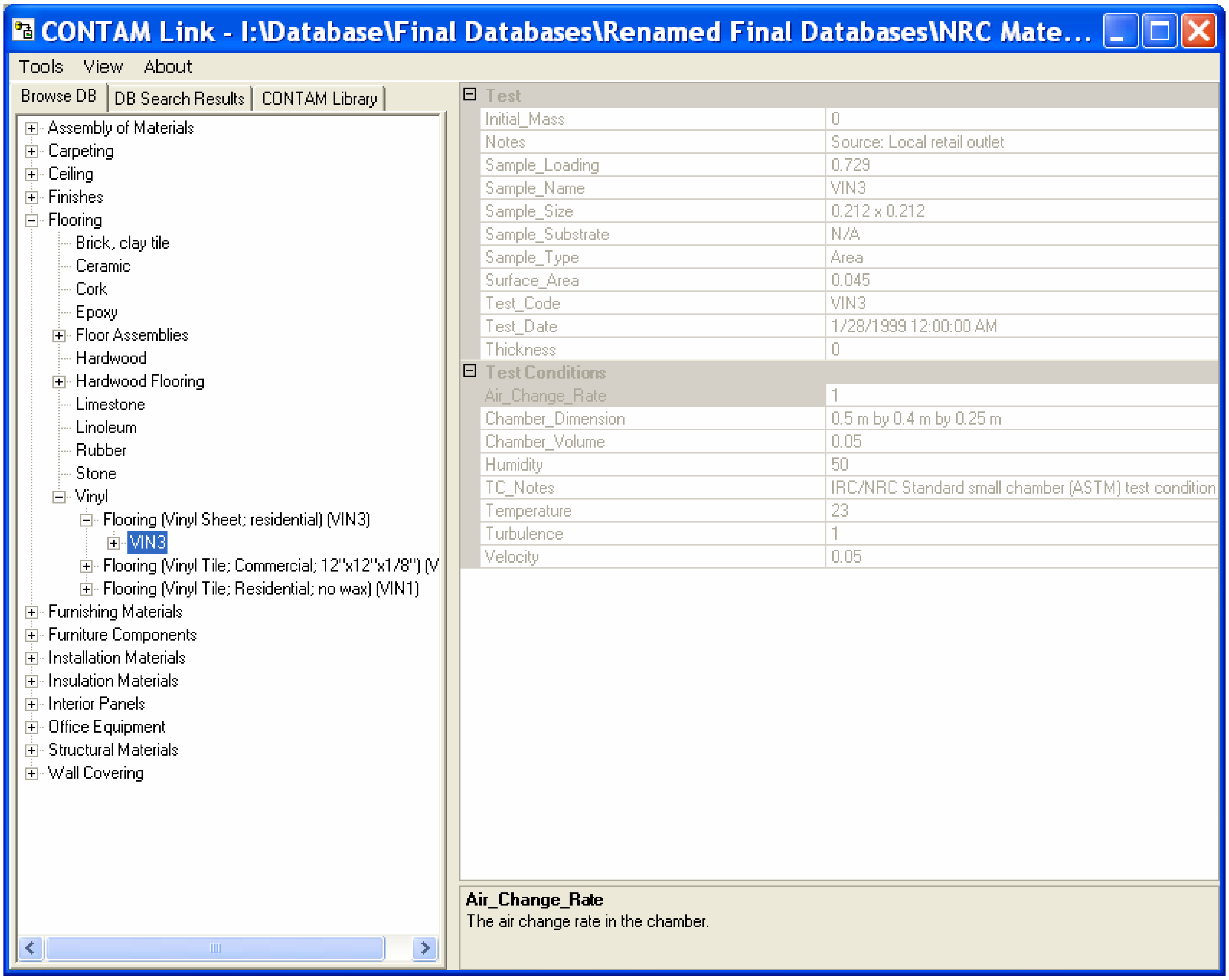


Figure 4. Browsing capabilities of NRC VOC source emissions database with ContamLink and environmental test conditions results display.

Combustion Source Strength Database

The first level of the combustion source strength database hierarchy is category of combustion appliance (see Figure 5). The next level includes the different types of appliances in each category (e.g., kerosene space heater is type of space heater). Under each appliance type is a list of specific studies, which, when highlighted, show the appliance and test facility specifications in the data viewer. The next level lists different test conditions for each study with the specific values given in the data viewer. The final level lists all contaminants measured in each study with contaminant properties, emission factors, and model information in the data viewer.

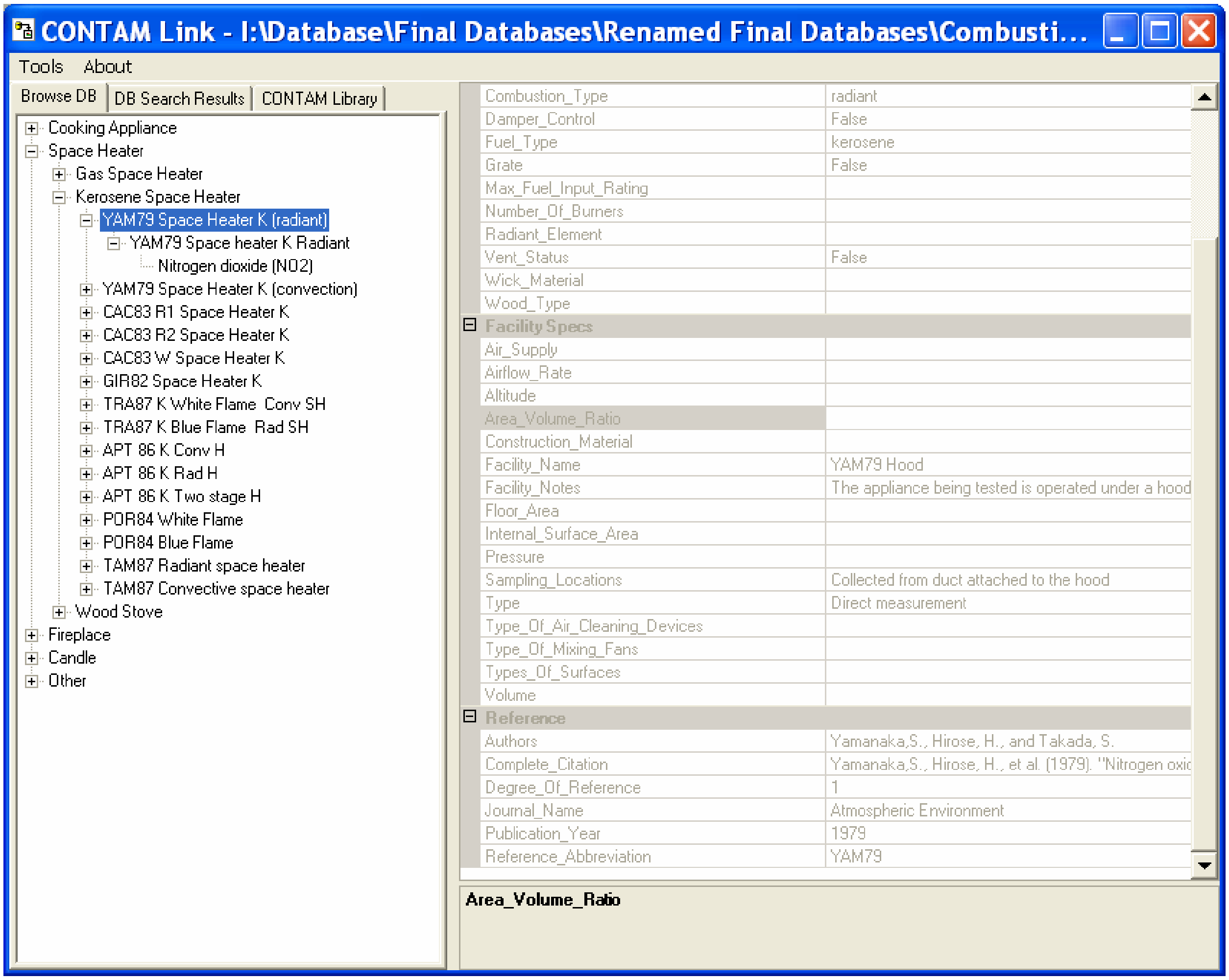


Figure 5. Browsing capabilities of Combustion Source Strength database with ContamLink and appliance and test facility specification in results display.

Particle Deposition Database

The particle deposition database is first organized according to the type of test facility used for each deposition study (see Figure 6). The next level lists each deposition study for that type of facility with reference and test facility details in the data viewer. The different test conditions for each study is provided in the next level with specific values given in the data viewer. Finally, specific particle sizes are listed with the associated deposition rates given in the data viewer.

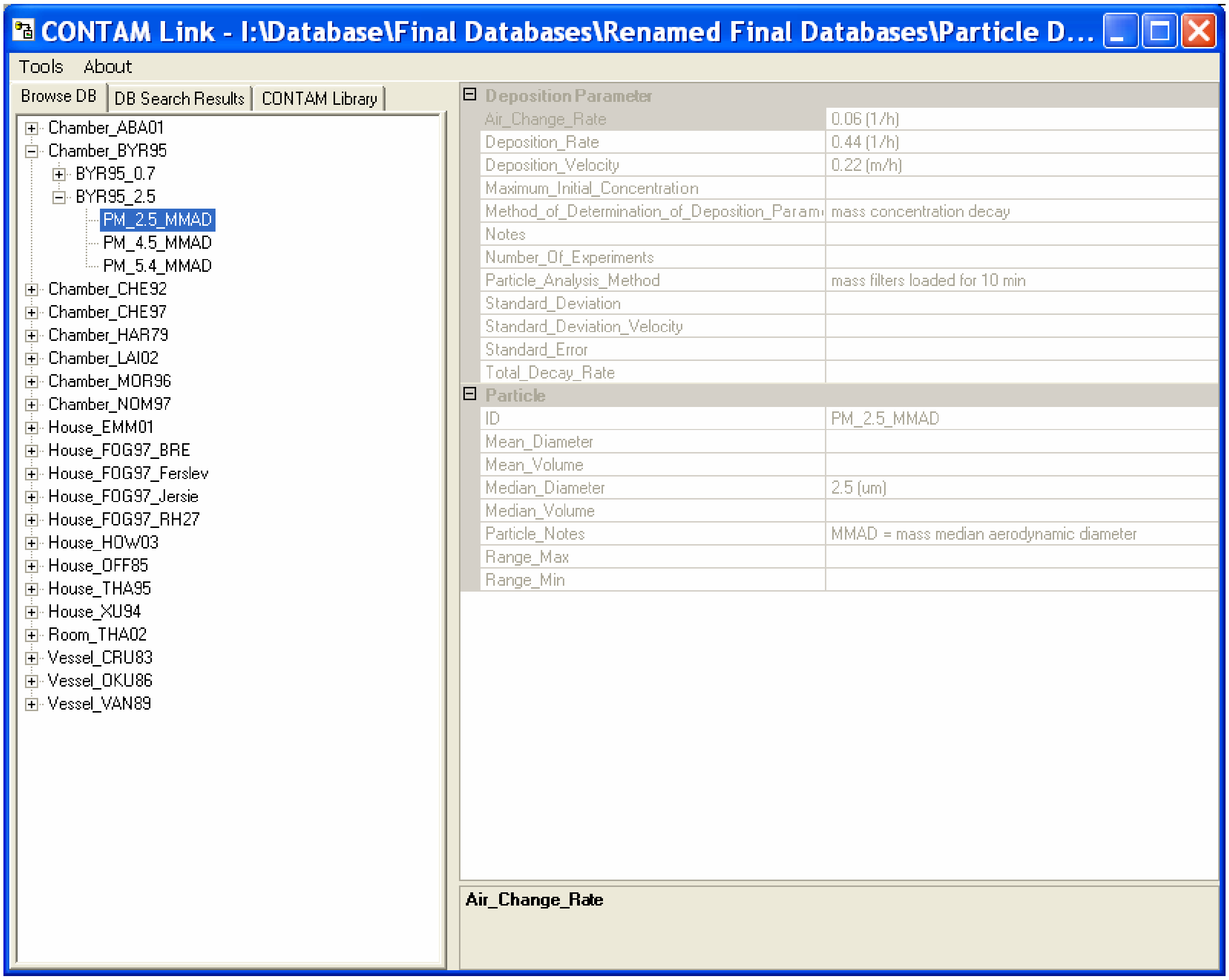


Figure 6. Browsing capabilities of Particle Deposition database with ContamLink and particle deposition results in results display.

Partition Coefficient Database

The first level of the Partition Coefficient database hierarchy is a list of sorptive indoor materials (see Figure 7). Under each material type is a list of sorption studies which displays more information about the material in the data viewer. The next level lists the chemicals used in the sorption study with information about the tests in the data viewer.

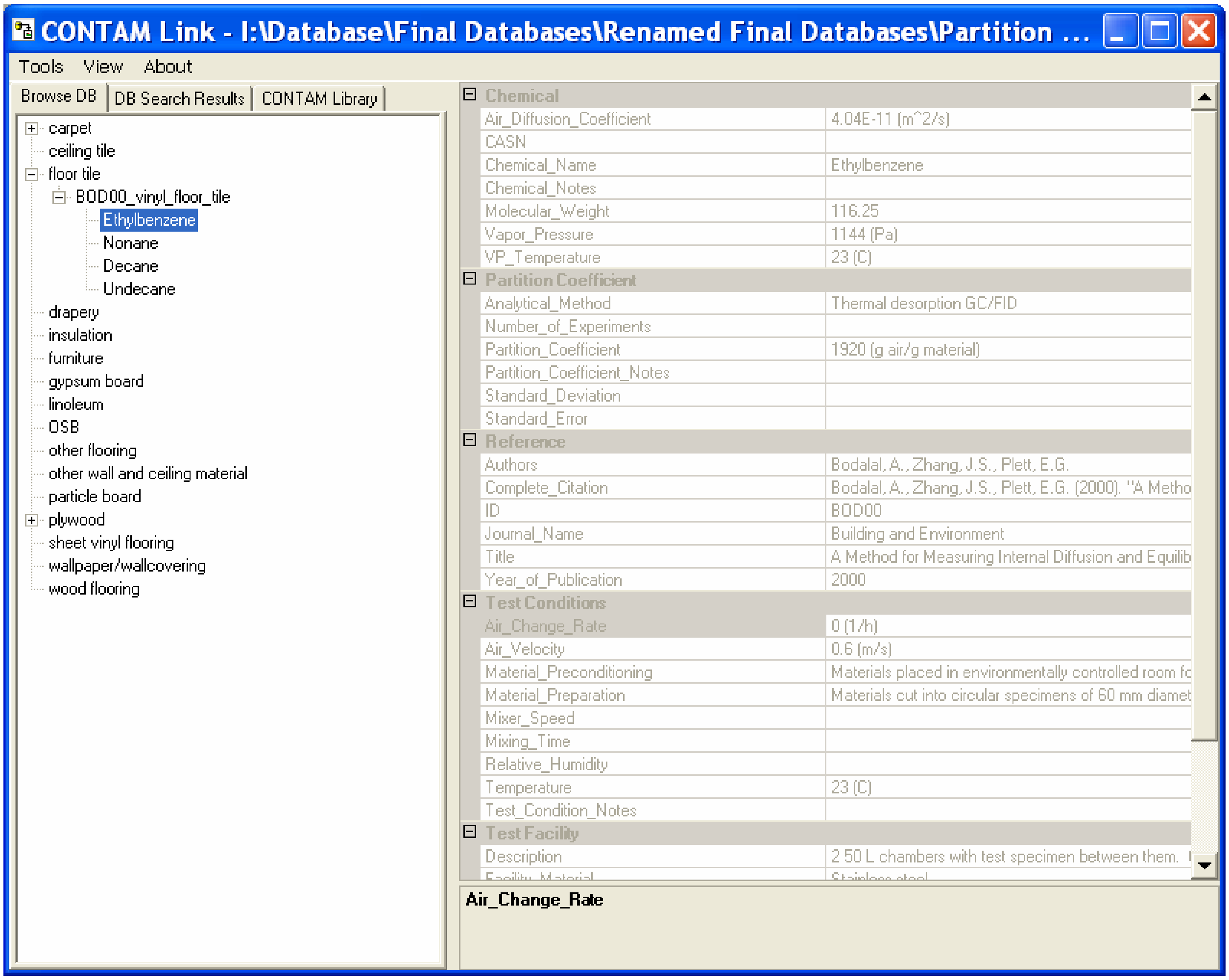


Figure 7. Browsing capabilities of Partition Coefficient database with ContamLink and partition coefficient results in results display.

Searching a database

Searching the database makes it easier to find records in the database. Search the database by using Tools ⇒ Search Database from the menu or using the Ctrl+S keyboard shortcut. The dialog shown in Figure 8 is then presented.

The first step is to define the search parameters. The search parameters available vary depending on the database that is used. Table 1 lists all of the available search parameters for each database. On the dialog select a parameter, an operator and enter a value for the parameter. Then add that parameter set to the query by pressing the Add button. When using more than one parameter you also need to select if the parameters are to be used together using the AND operator. Or if the parameters are to be used separately using the OR operator.

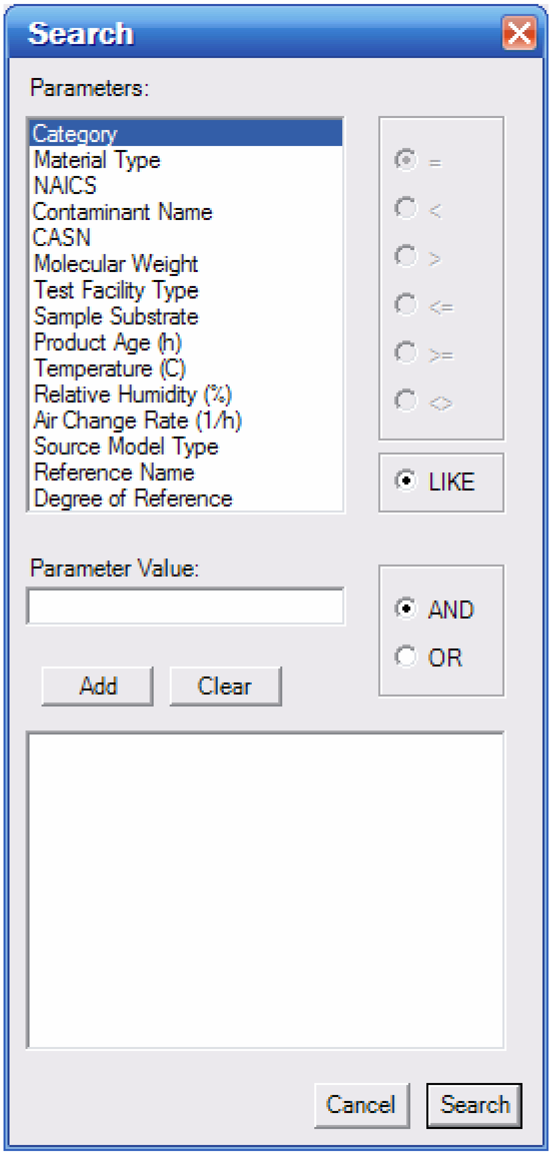


Figure 8. Searching capabilities for VOC emissions database.

Initiate the search by pressing the Search button. A message bow will give the number of records that matched the search parameters. The records can be found in the Search tab of the sidebar. The search tab shows the same hierarchy as the browse tab but only includes the records that matched the search query. The search results can also be browsed like the browse tab.

Table 1. Search Parameters for each Model Input Database

VOC Emission Rates	Combustion Emission Rates	Particle Deposition Rates	Partition Coefficients
Category Material Type NAICS Contaminant Name CASN Molecular Weight Test Facility Type Sample Substrate Product Age (h) Temperature (°C) R.H. (%) Air Change Rate (1/h) Source Model Type Reference Authors Year of Publication Degree of Reference	Category Combustion Type Fuel Type Contaminant Name Contaminant Class Molecular Weight Test Facility Type Facility Altitude Fuel Consumption Rate (kJ/h) Equation Name Reference Authors Year of Publication Degree of Reference	Test Facility Type Area/Volume Ratio (1/m) Air Change Rate (1/h) Mixing Mechanism Particle ID Mean Diameter (μm) Median Diameter (μm) Particle Analytical Method Generation Method Particle Composition Neutralized Particles? Reference Authors Year of Publication Degree of Reference	Material Type Contaminant Name Molecular Weight Vapor Pressure (Pa) CASN Test Facility Type Temperature (°C) R.H. (%) Air Change Rate (1/h) Reference Authors Year of Publication Degree of Reference

Library Manager

The third function of the side bar is the library manager. CONTAM libraries are external files whose purpose is to store pre-defined/user-defined simulation elements (schedules, wind pressure profiles, airflow elements, and duct elements) for use in multiple CONTAM simulations. The library manager is a way to easily create and manage these library files. ContamLink allows the user to only manage species and sources, since these are the only elements that are needed by ContamLink. Other elements like filters that can use the species in these libraries need to be defined in ContamW. Those elements will remain in the library when it is saved.

Library File

The user may either open an existing species-related library file or create a new one through ContamLink. To open an existing file press the "Browse" button and select the appropriate library file. The name of the library file opened and any description provided in the file will be displayed in the respective name and description fields. To manually create a new library file press the "New" button (see “Creating CONTAM Sources/sinks from a Database” to automatically add species and sources to library file). This will provide a clear field in the Library Elements part of the dialogue box. After adding new elements to the Element name list the list may be saved as a new CONTAM Library file.

Species and Source/Sinks

This is a list of species and source/sink elements present in the current library file. A more detailed description of the element will be displayed below the Element name list, if a description for the element is available.

There are a few options to add and remove elements from the list. A new element may be created by pressing the new button then following the appropriate steps to create a new element. Elements already in the library file may be modified by first selecting them from the list and pressing the edit button. If a species is not used by a source/sink in the library file it may be removed by selecting it from the element list and then pressing the delete button. Source/Sinks can always be deleted from a library.

Creating CONTAM sources/sinks from a database

CONTAM source/sinks are created using a wizard to define species and source/sink elements. By either searching or browsing a database, records from the database are chosen to be the basis for a CONTAM source/sink element. The lowest items in the browse tree or search tree (either contaminant names or particle sizes) correspond to a CONTAM source/sink element. Right click on one of these items and select Create Source/Sink from the context menu (see Figure 9). A wizard is started to create a source/sink. The wizard can also be started using Tools ⇒ Create Source/Sink from the menu or using the Ctrl+C keyboard shortcut.

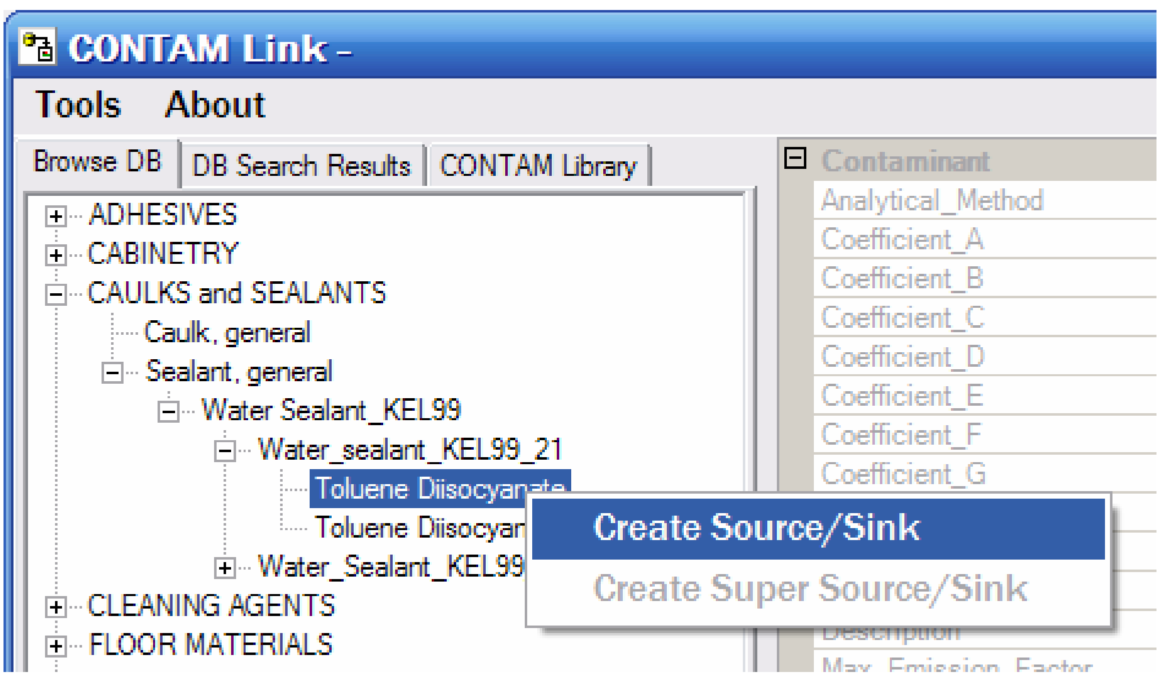


Figure 9. Automatically adding a source/sink to library manager using ContamLink wizard.

Pick a species

If a species exists in the current library then you will be given the opportunity to reuse a species for the source being created. Otherwise the wizard will start with the next step. You can select to create a new species or use an existing species. Information about the species selected from the database is shown on the left side of the window (see Figure 10).

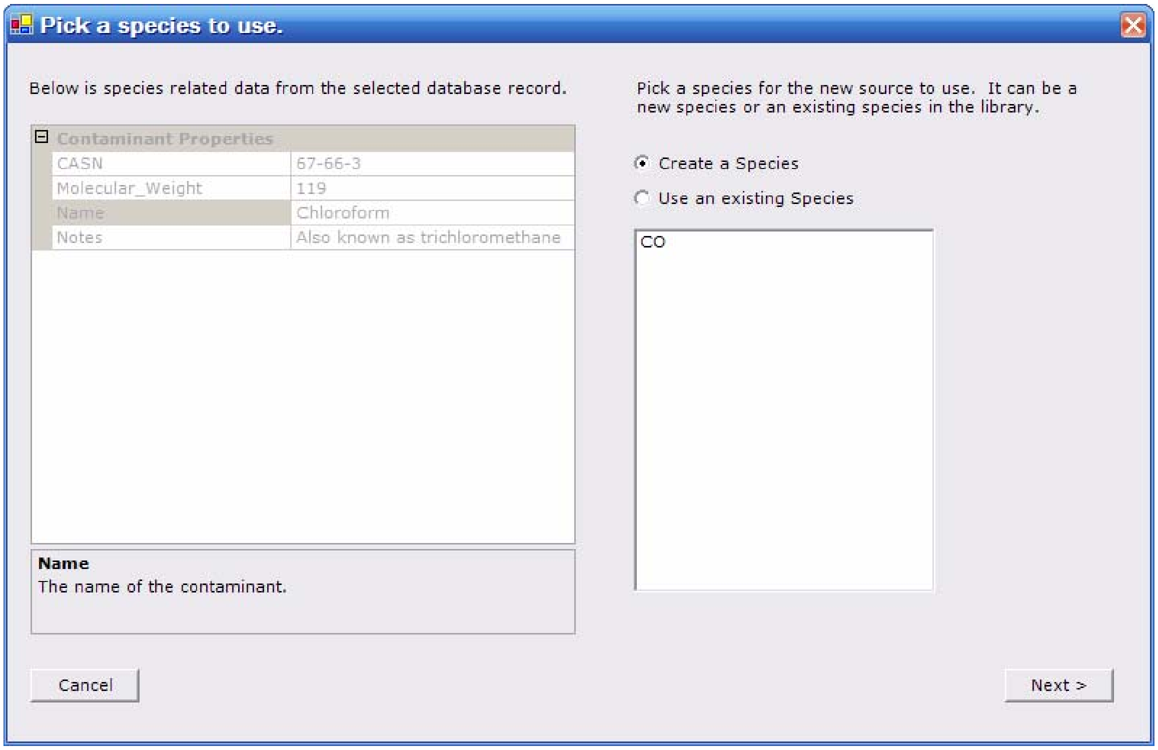


Figure 10. Selecting a species for library file.

Define a Species

If there is no existing species or an existing species was not used then you have to define a species for the source/sink to use (see Figure 11). The species being defined can be edited on the right side of the window. Information about the selected species from the database is shown on the left side of the window. The name of the species from the database is reused. Because there is a limit on the length of a species name the name may be trimmed. Also, there cannot be any spaces in the species name. The full name is put into the description. If available the molecular weight is also taken from the database.

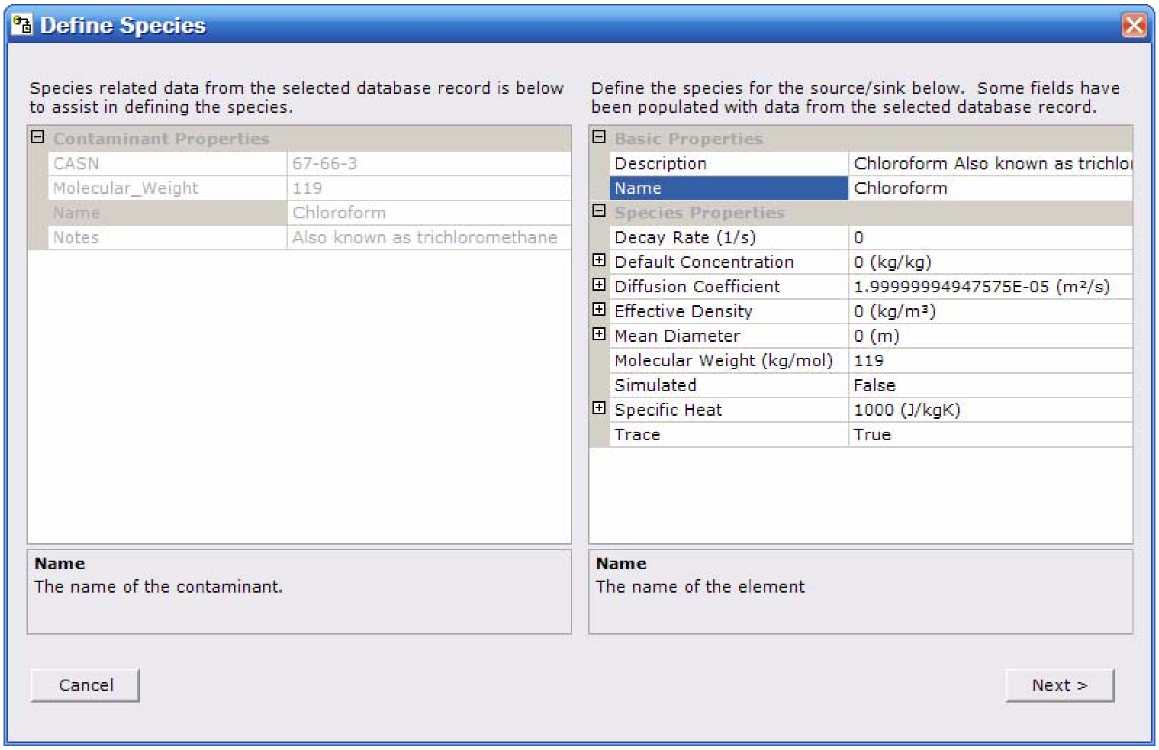


Figure 11. Defining a species using ContamLink wizard.

Picking a Source/Sink Model

Next a source/sink model must be chosen. Some model selections may be limited depending on the database being used due to what is expected to be in those databases. Information about the model from the database is shown on the left hand side of the wizard (see Figure 12).

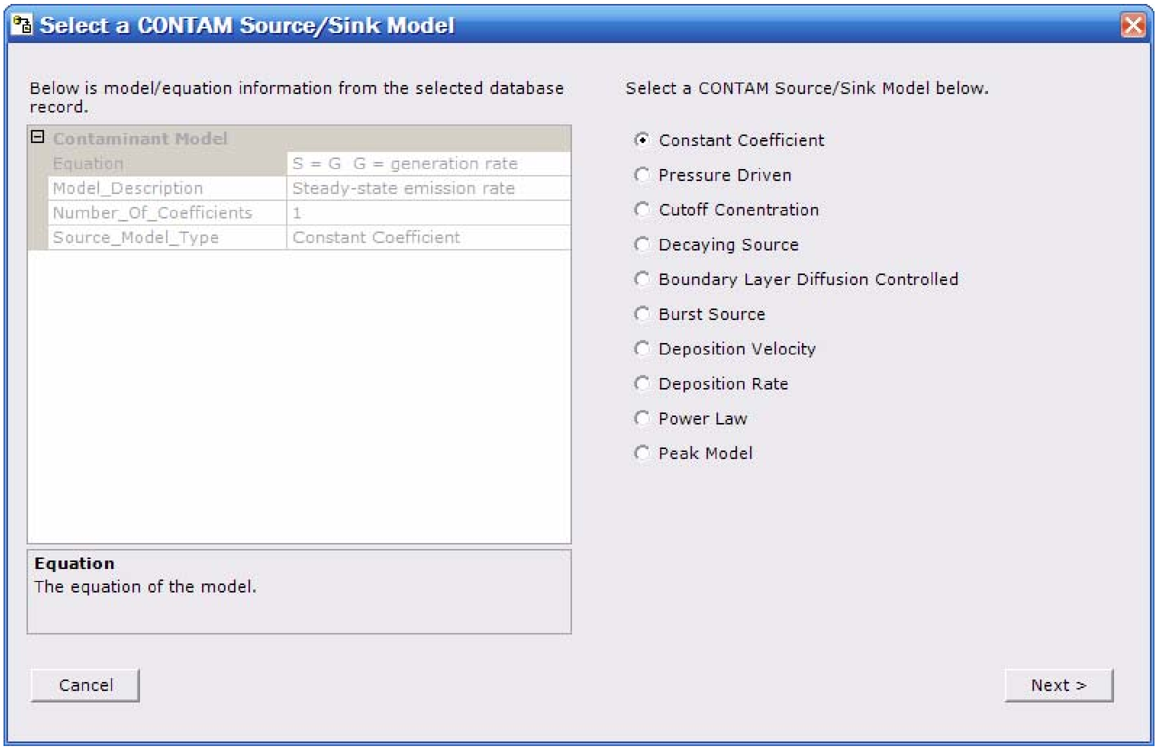


Figure 12. Selecting a CONTAM source/sink model using ContamLink wizard.

Defining the Source/Sink

When defining the source/sink some fields will be initialized with values from the database record. Some of the information from the database records is shown on the left side of the window (see Figure 13). After defining the source, the wizard is complete and the new species and source/sink will be shown in the library manager.

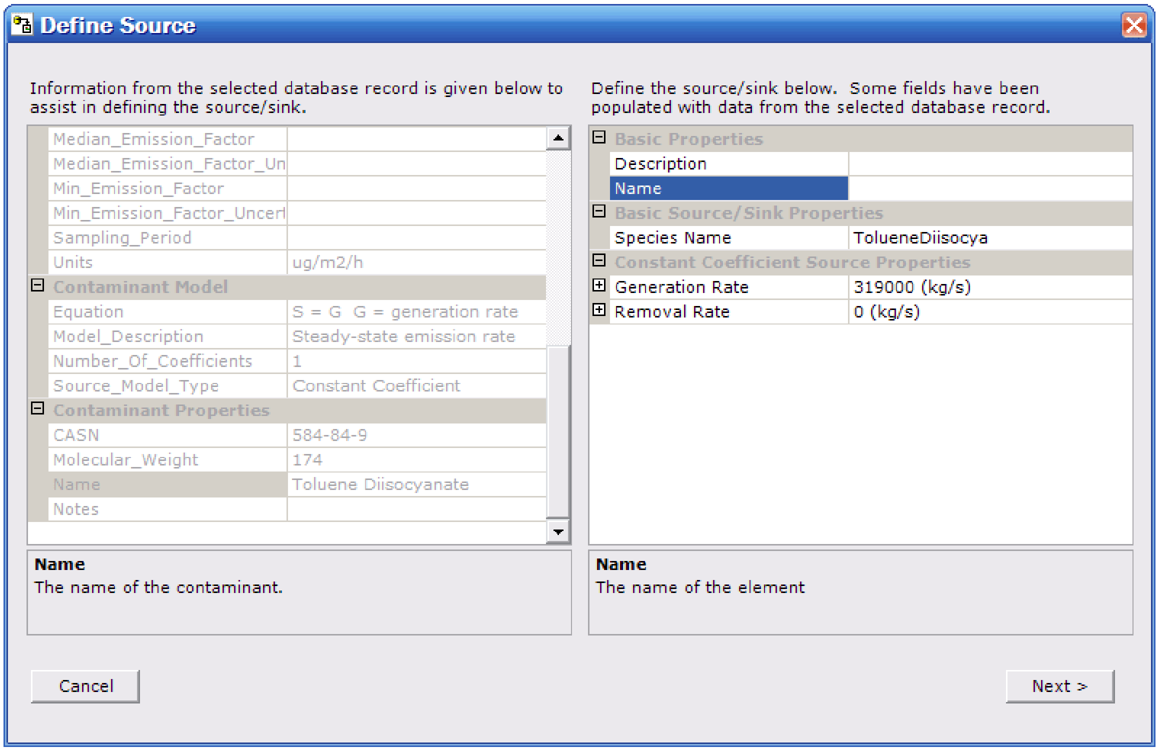


Figure 13. Defining a source/sink using ContamLink wizard.

Creating a Super Source/Sink from a database

The super element allows multiple elements of the other types to be combined into a single element. This can reduce repetitious work required to create multiple sources throughout a building by allowing multiple sources to be represented by a single icon on the SketchPad. Creating a super source/sink is similar to creating a simple source/sink, however the process is started at a different level in the Browse or Search tree (see Figure 14). To create a super source/sink you select the level that corresponds to study test conditions, which is one level above the selection point for a simple source/sink.

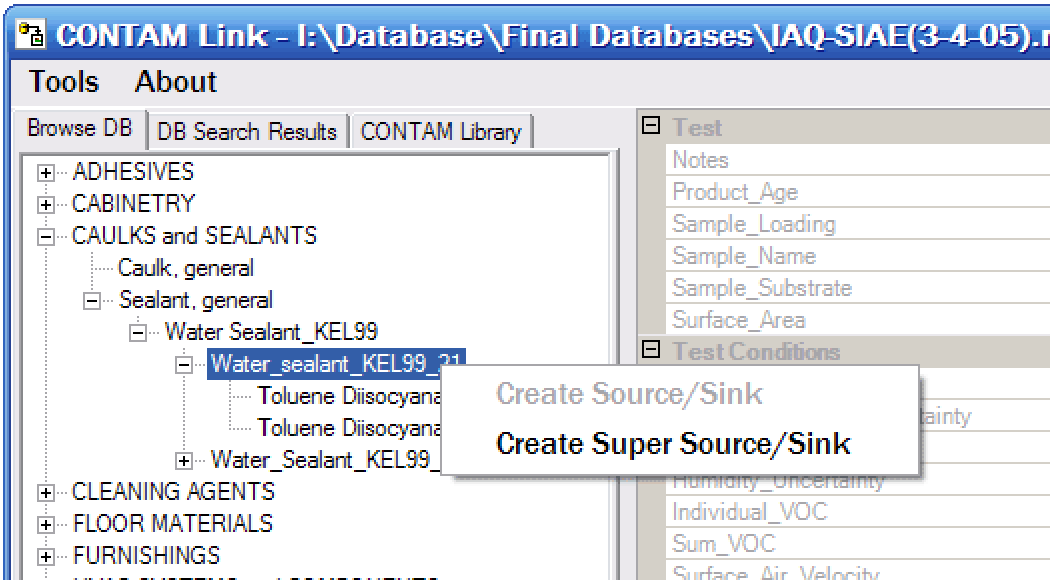


Figure 14. Creating a super source/sink using ContamLink Wizard.

Another difference when creating a super source/sink is that there is an additional step that is done first in the wizard. This step entails selecting which contaminants to include in the super source/sink (see Figure 15).

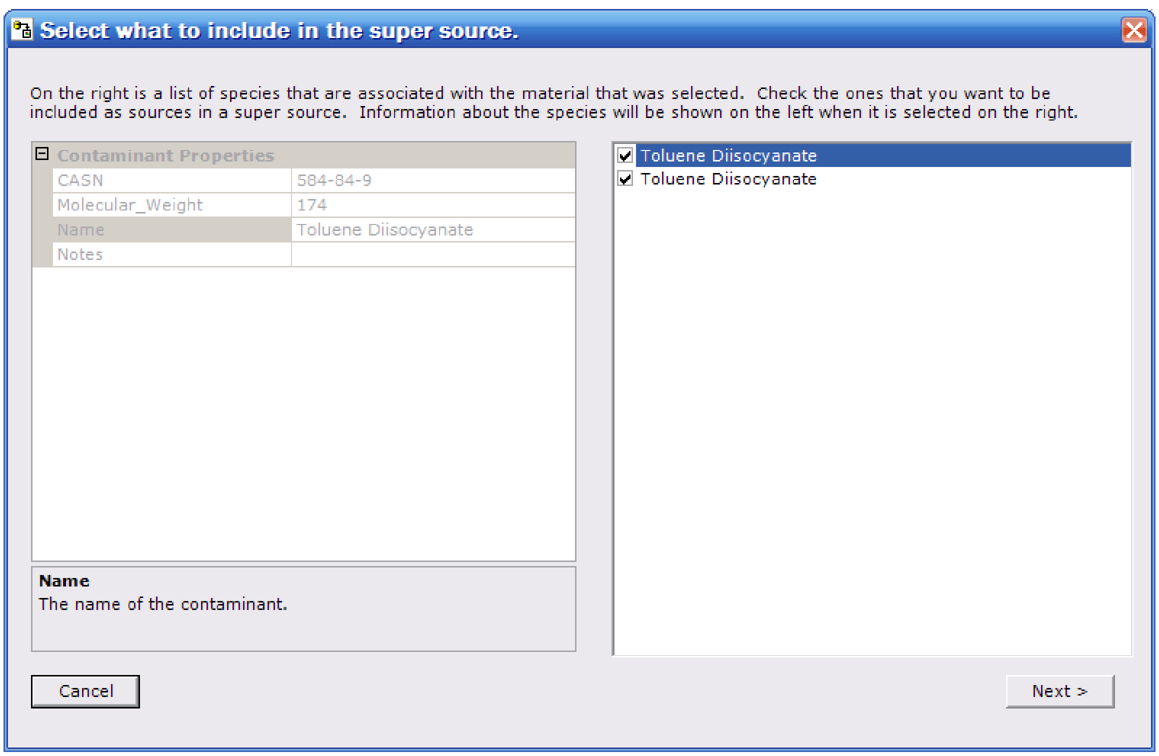


Figure 15. Selecting contaminants to include in the super source using ContamLink wizard.

Each of these contaminants will have to have a species and a simple source/sink defined. The definition of these species and source/sinks has the same procedure as defining any other simple source/sink. These simple source/sinks will then be included in the super source/sink. After the simple source/sinks are defined you define the super source.

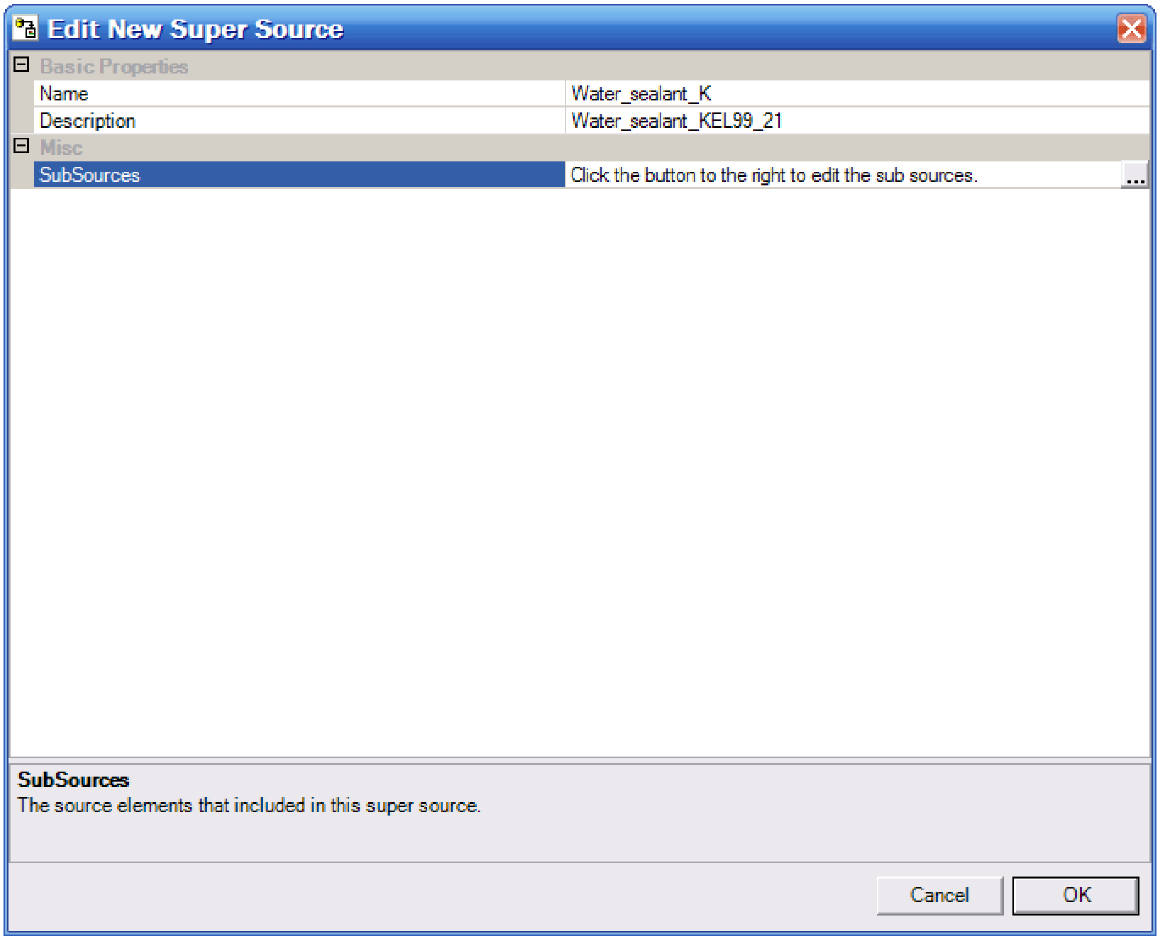


Figure 16. Defining subsources that make up super source using ContamLink wizard.

You can edit the sub source/sinks by pressing the small button by the right edge of the window, which is present in the SubSources row when it is selected. It will bring up the dialog box in Figure 17.

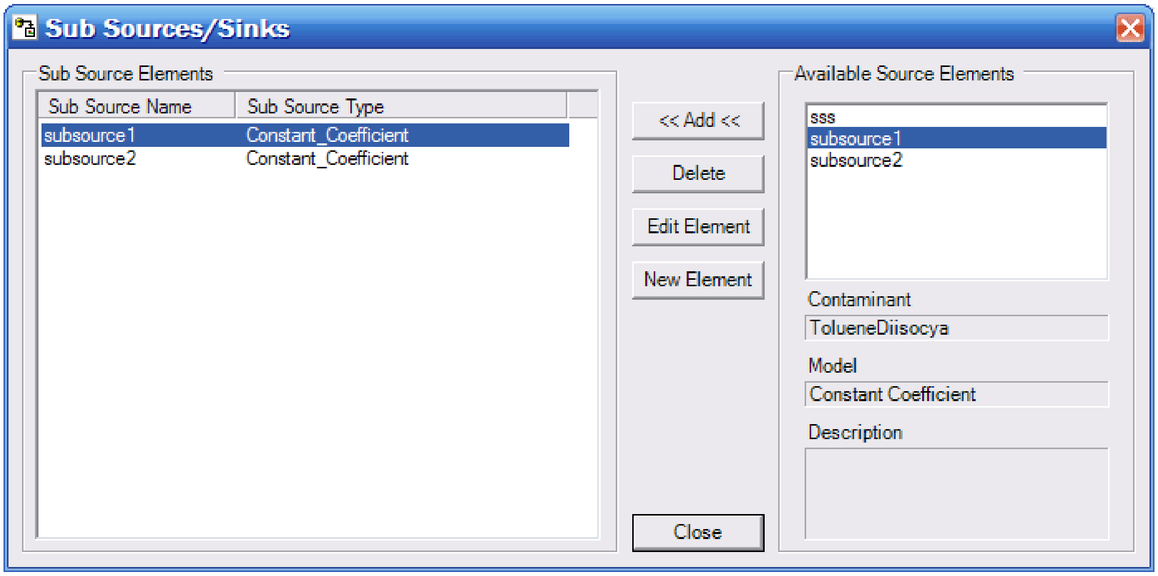


Figure 17. Defining subsources that make up super source using ContamLink wizard.

The simple source/sinks included in the super source/sink are shown on the left side of the window. On the right side of the window is a list of the available simple source/sinks that can be included in the super source/sink. One can edit the simple sources or create new simple source/sinks from this dialog. The user can also add or delete simple source/sinks to/from the super source/sink.

When finished defining the super source/sink and closing the dialog box with the OK button, the super source/sink will appear in the library manager.