

Development of IAQ Model Input Databases: Volatile Organic Compound Source Emission Rates

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ABSTRACT

Indoor air quality (IAQ) models can be used to predict airflows, contaminant concentrations and personal exposures for a given indoor environment. In order to generate such results, these 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 data are available in the literature; however, this information has generally not been compiled in a convenient form for use in an IAQ model. As a result, finding appropriate model data can be a repetitive and laborious process for the user.

To make this effort more efficient, the National Institute of Standards and Technology (NIST) has begun an effort to compile model input data needs into searchable databases. The process involves collecting data from the literature, designing a database format to standardize data entry, entering the information into the database, and developing a computer program to search the database for specific records to use in an IAQ model. This process has been completed for airflow leakage elements, wind pressure coefficients, and ventilation system schedules and is currently underway for VOC source emission rates. With these databases, CONTAMW users and other modelers will be able to simulate a wide range of exposure scenarios in different types of buildings as well as simulate the impacts of potential control strategies. In addition, as a result of this work, it will be possible to identify important gaps in the data.

INTRODUCTION

The U.S. Department of Housing and Urban Development (HUD) has identified a need to improve urban housing conditions to protect children's health. One critical area of HUD's Healthy Homes Initiative (HHI) is to address a wide range of indoor air quality (IAQ) concerns (*e.g.*, inadequate ventilation, moisture problems, combustion by-products, *etc.*). HUD is funding several demonstration projects across the country to implement interventions that correct many of these IAQ problems in lower income urban homes. Due to the costs of fieldwork, however, the demonstration projects will only be able to implement a limited number of interventions in a small number of homes. A more feasible way to prioritize the hazards and identify the best intervention strategies is with an IAQ model.

In order to estimate building contaminant concentration levels and associated occupant exposures, IAQ model users require data related to source strengths and other contaminant transport mechanisms (*e.g.* sinks, filters). Such analyses, and practical findings to improve residential indoor environments, would be greatly facilitated by the availability of databases of information on contaminant related model parameters. These databases need to include emission

rates for indoor sources (*e.g.*, consumer products, cooking, and combustion appliances), contaminant removal rates (*e.g.*, adsorptive sinks, deposition rates, *etc.*), representative occupant schedules, and effectiveness values for existing control technologies (*e.g.*, filter efficiencies, exhaust fan specifications, *etc.*). Much of this information exists in the literature; however, it is not readily available in a convenient form, thereby requiring users to furnish their own model input parameters. To streamline the contaminant modeling process, there is a need for well-documented and reliable databases of experimental data on contaminants.

In response to this need, the National Institute of Standards and Technology (NIST) has begun an effort to compile model input data needs into searchable databases and to define a format for users to enter data. To date, NIST has created a library of airflow leakage elements, wind pressure coefficients, and ventilation system schedules for use in its multizone IAQ and ventilation model, CONTAMW. The next phase of this work, and the focus of this paper, is the development of a VOC source emission rate database based on thousands of records that have been collected from published and unpublished data as well as existing source emission rate databases. As part of this effort, a standard data entry format has been developed as well as a computer program to search the database for specific records. As a result of this work, modelers will be able to have convenient access to available VOC source emission data as well as a format to enter new data. These modeling tools will allow HUD and others to continue intervention investigations beyond the initial scope of the HHI project.

SOURCE MODELS

The databases compiled as part of this effort can in fact be used in any multizone IAQ model. Multizone modeling 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 (HVAC ducts, doors, windows, cracks, *etc.*) between the zones of a building. The network nodes represent the zones, which are modeled with a single pressure, temperature, and pollutant concentration. After calculating the airflow between zones and ambient, zonal pollutant concentrations are calculated by applying mass balance equations to the well-mixed zones, which may contain pollutant sources or sinks. The following mass balance may be used to describe contaminant transport in a multizone building:

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

where:

- $m_{\alpha,i}$ = mass of contaminant α in zone i
- $R_{\alpha,i}$ = removal coefficient for contaminant α in zone i
- $C_{\alpha,i}$ = concentration mass fraction of contaminant α in zone i
- $F_{i,j}$ = rate of airflow from zone i to zone j
- $F_{j,i}$ = rate of airflow from zone j to zone i
- $\eta_{\alpha,j,i}$ = air flow leaving zone i
- $C_{\alpha,j}$ = concentration mass fraction of contaminant α in zone j
- m_i = mass of air in zone i
- $k_{\alpha,\beta}$ = kinetic reaction coefficient in zone i between species α and β
- $C_{\beta,i}$ = concentration mass fraction of contaminant β in zone i

$G_{\alpha,i}$ = generation rate of contaminant α in zone i .

There are several models available to solve the mass balance equations for a given indoor space. This paper will focus on NIST's multizone airflow and pollutant transport model CONTAMW. Detailed information regarding CONTAMW may be found elsewhere.^{1,2,3} The software and manual may be downloaded from the following website: <http://www.bfrl.nist.gov/IAQanalysis/>. In summary, CONTAMW 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. The resulting mass airflow rate values (F) are then used with contaminant information to calculate concentrations in each zone. The user must supply data regarding airflow paths, contaminant source emission rates, contaminant removal rates, chemical reaction coefficients, and occupant schedules.

To date, NIST has created a library of airflow leakage elements, wind pressure coefficients, and ventilation system schedules to aid the user when adding airflow path information.⁴ The next phase of the project is the compilation of source emission rates for use when adding the generation rate ($G_{\alpha,i}$) term in Equation 1. The generation rate of VOCs has been described with several different source models. A summary of the source models currently available in CONTAMW 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 VOC source emission rates in CONTAMW.

Source Model Name	Equation	Example Uses
Constant Coefficient Model	G G = generation rate	Dry sources (e.g., linoleum)
Pressure Driven Model	$G \cdot \Delta P^n$ 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 small closet)
Decaying Source Model	$G_0 \exp(-t/t_c)$	Wet 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	Sources characterized by a boundary layer (e.g., wall or flooring materials)
Burst Source Model	mass added to zone	Occupant activities (e.g., using air freshener)

As shown in Table 1, each model is more applicable for specific types of sources. For example, an exponential model may better describe VOC emissions from a “wet” source than a constant source model. The modeler may choose which source model to apply, however, use of the different source models requires knowledge of the specific coefficients. The constant coefficient and first-order decay 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 availability of mass transfer values is quite limited.

To determine the empirical model coefficients or to validate the physical models, source emission rates have been experimentally measured for hundreds of indoor materials and activities. Source emissions testing is typically completed in controlled laboratory chambers ranging in size from approximately $3.5 \times 10^{-5} \text{ m}^3$ (field and laboratory emission cells) to $> 10 \text{ m}^3$ (room size). Although no standard testing conditions for sources exists, there are several recommended guidelines including: ASTM,^{5,6} European Guidelines,⁷ and Matthews.⁸ A summary of the recommended testing conditions for each guide is provided in Table 2. In general, important testing parameters to consider include: the chamber physical characteristics, extent of chamber mixing, purity of inlet air, chamber air change rate, air velocity near the material surface, temperature, humidity, product loading ratio, sample preparation, sample age, and product history. In an attempt to standardize the information included in the database, data entry fields were created for each of these test parameters. By including this information for each record also allows the user to search for VOC emission rate experiments conducted at test conditions recommended in these guidelines.

SOURCE DATA

There is an abundance of VOC source emission rate data available in the literature. Although there is not a comprehensive database available, there are several abridged versions that can serve as starting places as well as provide a standard format for the database. For example, the Indoor Environment Management Branch of the U.S. Environmental Protection Agency (U.S. EPA) compiled measurements of emissions from different indoor sources into a single Excel spreadsheet named “Sources of Indoor Air Emissions (SIAE)”.⁹ The SIAE_599 version of the spreadsheet contains 8490 emission rate records from 72 references reviewed through May 1999. Records represent approximately 78 types of materials in 17 source categories. Table 3 lists the number of records for each category and type. Each record contains information regarding the emission source classification, emission testing conditions, chemical information and analytical methods, emission factors, emission modeling parameters if available, and any relevant comments. This database will serve as the focus of this paper.

A second source of VOC source emission rate data identified for this project is the material emission database assembled by the National Research Council of Canada (NRC).¹⁰ The NRC database includes VOC emissions data based on tests conducted in their Indoor Environment Program laboratory chambers. This database currently contains emission rates of 245 contaminants from 50 different types of materials (see Table 3).

In addition, source emission rate data is continuously being generated and added to the literature. While the goal of this project is to provide model users with as much emission rate data as possible, it will not be an ongoing process. Thus, a second outcome of this work is the creation of a standard data format and linking mechanism for future users to add to the databases.

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

Parameter	ASTM Full-Scale Chambers ⁵	ASTM Small-Scale Chambers ⁶	European Guideline ⁷	Matthews ⁸
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 measure 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 µg/m ³ for single VOC, < 10 µg/m ³ ΣVOCs	inlet conc. < 2 µg/m ³ for single VOC, < 10 µg/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

Table 3. Distribution of database entries for SIAE and NRC source emission rate databases.

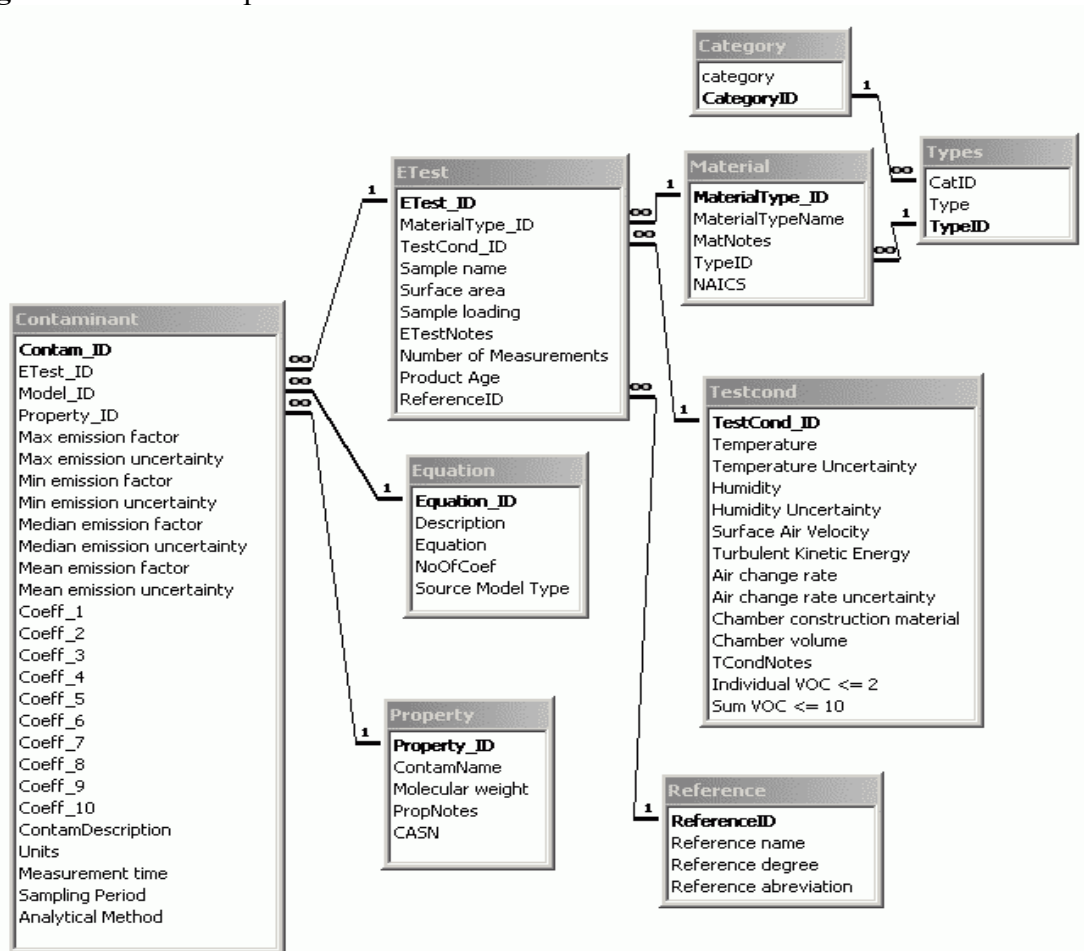
CATEGORY	TYPE	SIAE	NRC	
ADHESIVES	Carpet adhesive	21	0	
	Cove base adhesive	26	0	
	Flooring adhesive	95	3	
	Miscellaneous adhesive	8	0	
CABINETS	Composite wood cabinet	2	0	
	Kitchen cabinet	136	0	
CAULKS AND SEALANTS	Caulk, general	9	3	
	Sealant, general	4	0	
	Disinfectant	2	0	
	Misc. cleaning agents	9	0	
FLOOR MATERIALS	Carpet- synthetic fiber	1050	3	
	Nylon/Latex backing	0	3	
	Carpet cushion	195	3	
	Carpet seaming tape	14	0	
	Carpet system	5	0	
	Cork flooring	24	0	
	Cove base	60	0	
	Sheet vinyl flooring	1277	4	
	Tile vinyl flooring	10	0	
	Underlayment	14	0	
	Wood flooring	387	2	
	Other flooring	25	0	
	FURNISHINGS	Drapery	18	0
		Drapery lining	18	0
Furniture, wood		14	0	
Office furniture		22	0	
Office furniture – wood		3	0	
Residential furniture – wood		4	0	
HVAC SYSTEMS AND COMPONENTS	Air cleaning device	16	0	
	Air moving equipment	2	0	
	Ductwork	116	0	
INSULATION PRODUCTS	Fibrous insulation	7	0	
	Foam insulation	10	0	
MACHINES	Air cleaner, in-room	5	0	
	Office machine(s)	786	0	
	Photocopier, dry-process	77	0	
	Vacuum cleaner	3	0	
MISCELLANEOUS MATERIALS	Brick	4	0	
	Ceramic tile	4	0	
	Clothing	9	0	
	Concrete	2	0	
	Glass	7	0	
	Metal	4	0	
	Microbial culture	1	0	
	Mortar	9	0	
	Paper-based material	1	0	
	Stone	4	0	
	Smoking	38	0	
	PAINTS AND COATINGS	Lacquer	51	0
Finish, oil-based		64	0	
Polyurethane coating		22	0	

	Paint, solvent-based	1038	1
	Stain	551	3
	Unknown type of paint	30	0
	Varnish	42	0
	Finish, water-based	40	0
	Paint, water-based	1347	3
	Wax	183	3
PERSONAL CARE ITEMS	Dry cleaning	21	0
	Hair spray	2	0
PESTICIDES	Misc. cleaning agents	9	0
	Moth repellent	23	0
SPACE HEATING AND COOKING EQUIPMENT	Cooking burner, gas	1	0
	Space heater, gas-fueled	1	0
	Space heater, oil-fueled	10	0
WALL AND CEILING MATERIALS	Ceiling tile	39	3
	Gypsum board	35	3
	OSB	0	3
	Plaster	2	0
	Softwood	0	1
	Wall paneling	8	0
	Wallpaper	13	0
	Wallpaper/wallcovering	74	0
WOOD PRODUCTS	Chipboard	1	0
	Particleboard	99	3
	Plywood	55	3
	Solid natural wood product	96	0
	Veneer	42	0
	Wood product	1	0
	Other wood products	33	0

SOURCE EMISSION RATE DATABASE

The first step toward completing a source database/model link was to develop a database format in Access[®]. This format was based on fields from both the SIAE and NRC databases. 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 which 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 CONTAMW. The tables were 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.

Figure 1. Relationships for tables in database.

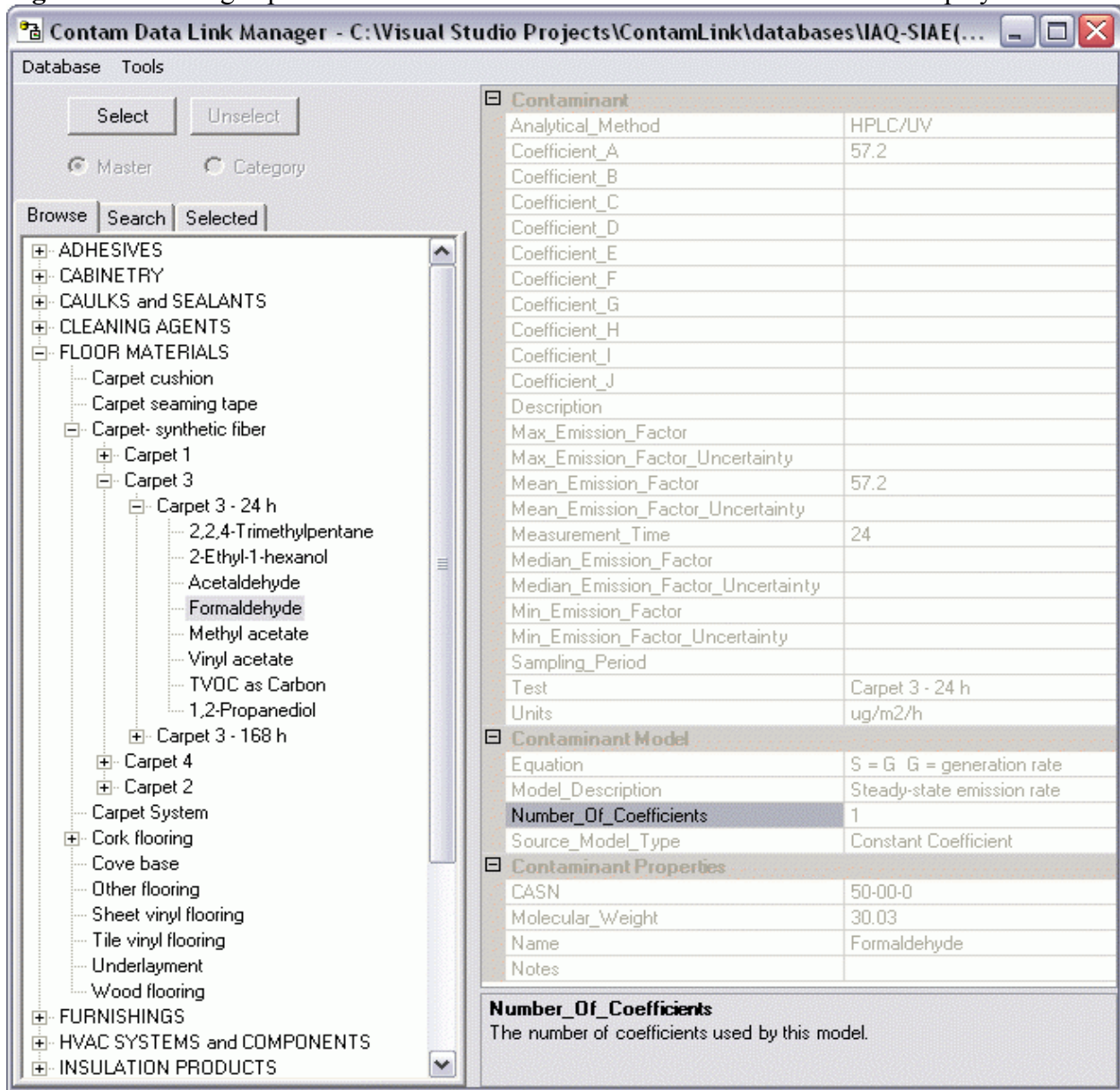


Based on these tables, data entry forms were created. Using these forms, the database was populated with records from the SIAE spreadsheet focusing on data from peer-reviewed journal articles (first degree references). The original papers were consulted for information not provided in the original spreadsheet. These forms may also be used for future data entry, thereby compiling consistent information from different testing facilities.

The NRC database was originally in Access[®] format and contained 15 tables linked by one-to-many relationships. Although this format is slightly different than that of the proposed source database, the NRC data will not need to be modified for use with CONTAMW.

To aid the user in navigating either the SIAE or NRC database, a computer program (CONTAMW Data Link Manager) was developed to allow the following capabilities: browsing, searching, and selecting data for use in CONTAMW. The user may look at all the available data in each category using the program's browse tool. Within each category/type, a list of specific materials tested is included. As shown in Figure 2, the user can see all the available information about testing conditions and contaminant results.

Figure 2. Browsing capabilities with CONTAM Link and contaminant results display.



If the user is looking for specific materials, certain test conditions or contaminants, the program may be used to search the database. A search may be based on the following criteria: name of a contaminant; air change rate, temperature, relative humidity, and surface air velocity of testing chamber; product loading ratio; age of the product at start of test; authors and peer-review degree of reference; and the type of source model used to predict emission rate (see Figure 3). It is possible to conduct a search based on a single parameter or multiple criteria. The relevant records are displayed where the user can see all the information related to the selected contaminant (see Figure 4) and test (see Figure 5).

Figure 3. Searching capabilities: a) single parameter search, and b) multiple criteria search.

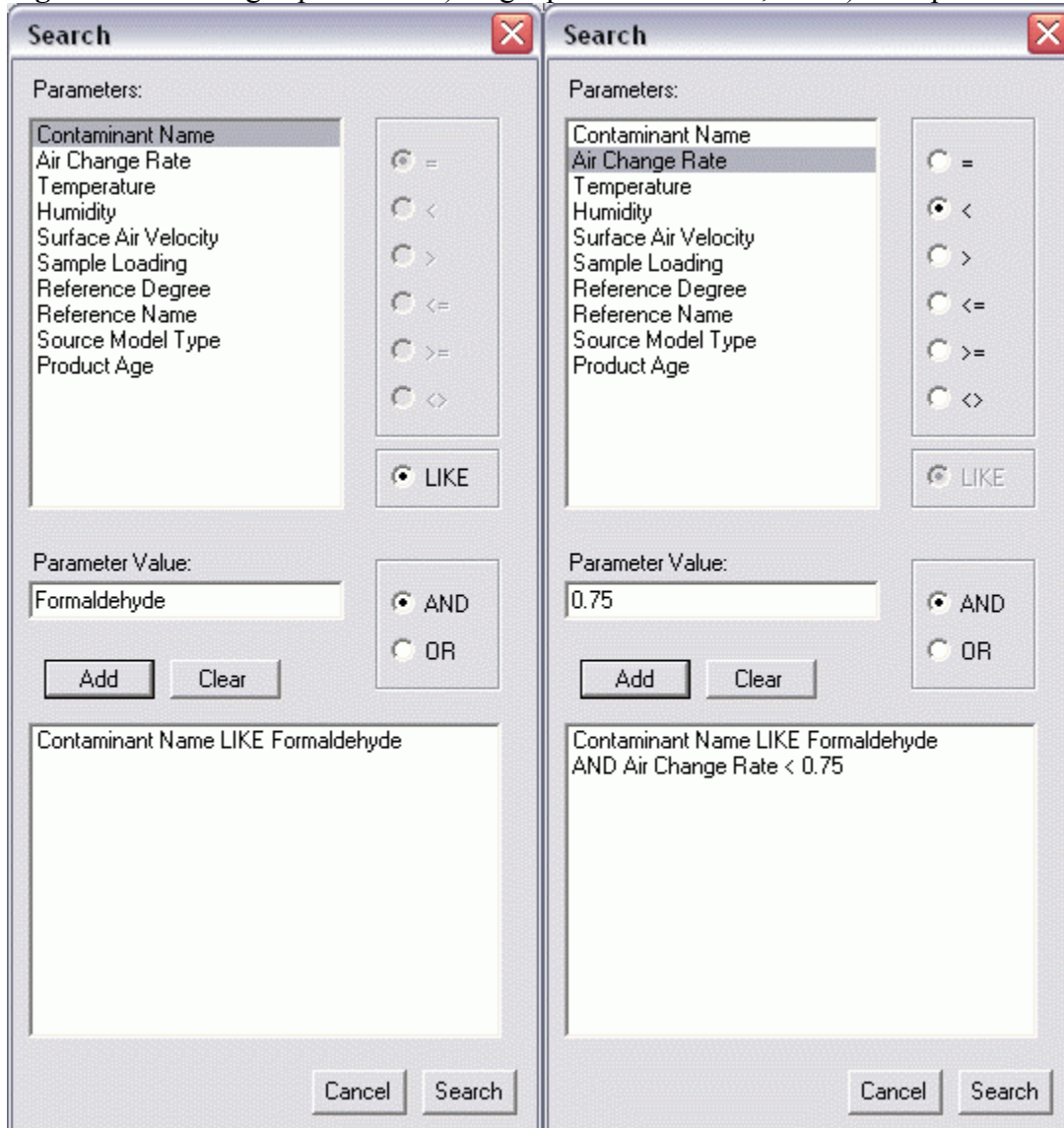


Figure 4. Search results for single parameter (contaminant = formaldehyde) and example of summary of contaminant results.

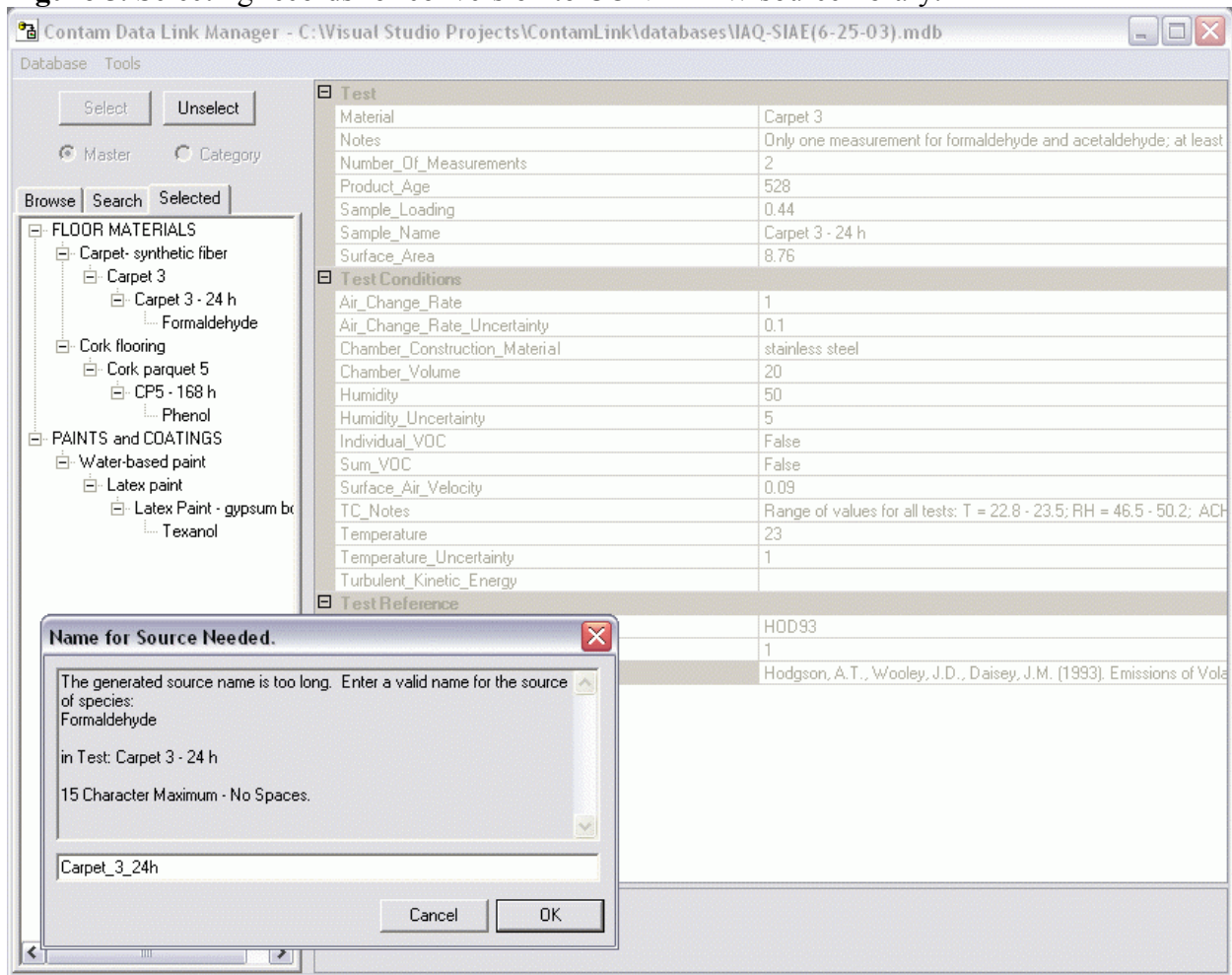
The screenshot shows the 'Contam Data Link Manager' application window. The left pane displays a hierarchical tree of 'FLOOR MATERIALS' with 'Formaldehyde' selected under 'Carpet 3 - 24 h'. The right pane shows a summary table for the selected contaminant.

Contaminant Summary Table:

Contaminant	
Analytical_Method	HPLC/UV
Coefficient_A	57.2
Coefficient_B	
Coefficient_C	
Coefficient_D	
Coefficient_E	
Coefficient_F	
Coefficient_G	
Coefficient_H	
Coefficient_I	
Coefficient_J	
Description	
Max_Emission_Factor	
Max_Emission_Factor_Uncertainty	
Mean_Emission_Factor	57.2
Mean_Emission_Factor_Uncertainty	
Measurement_Time	24
Median_Emission_Factor	
Median_Emission_Factor_Uncertainty	
Min_Emission_Factor	
Min_Emission_Factor_Uncertainty	
Sampling_Period	
Test	Carpet 3 - 24 h
Units	ug/m2/h
Contaminant Model	
Equation	S = G G = generation rate
Model_Description	Steady-state emission rate
Number_Of_Coefficients	1
Source_Model_Type	Constant Coefficient
Contaminant Properties	
CASN	50-00-0
Molecular_Weight	30.03
Name	Formaldehyde
Notes	

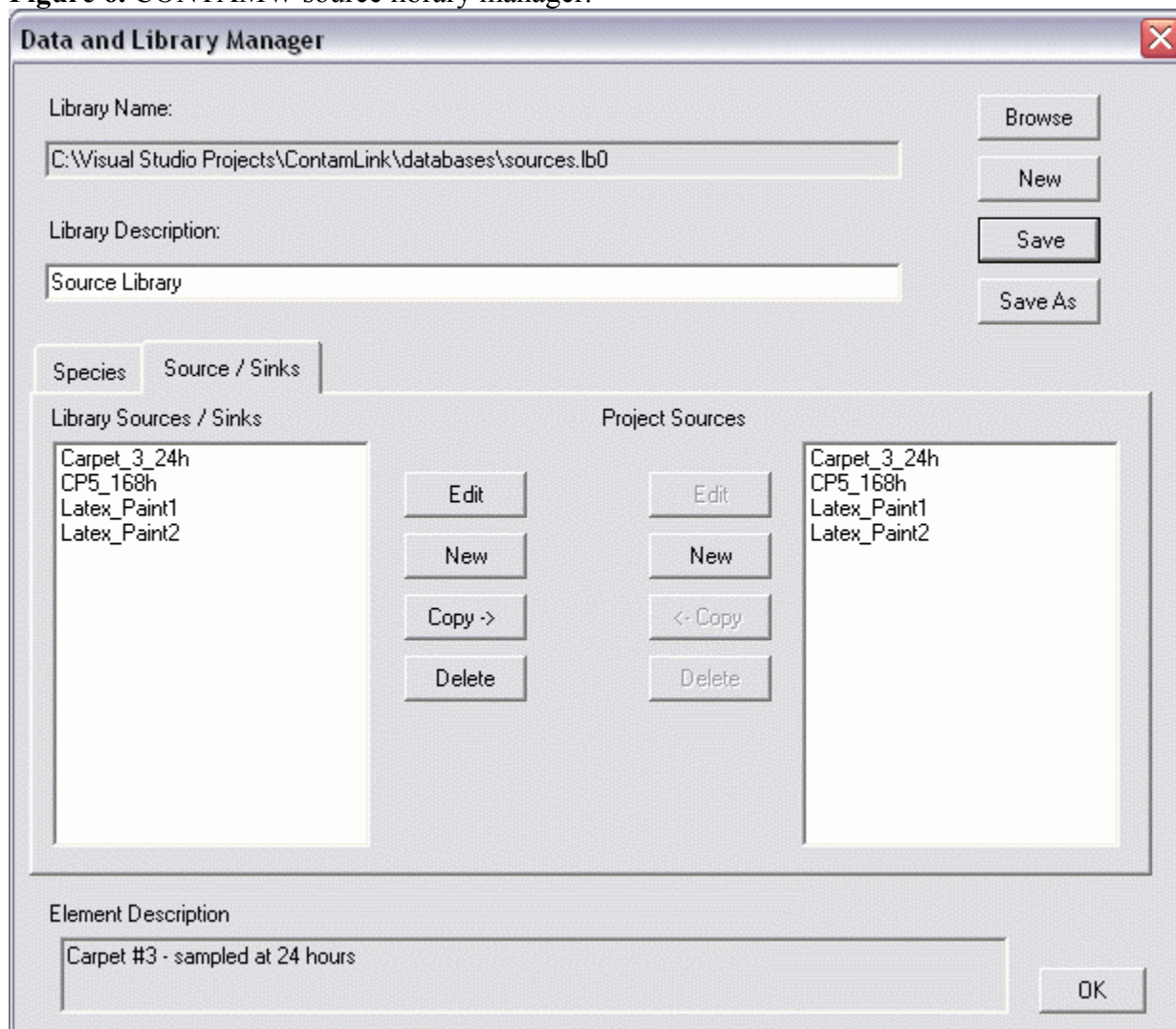
Number_Of_Coefficients
The number of coefficients used by this model.

Figure 5. Selecting records for conversion to CONTAMW source library.



Finally, the program allows the user to select which records to populate a library for use in CONTAMW. CONTAMW library files store data elements that may be shared between model project files. Once the records are selected based on browsing or searching the database, the program converts the source model information to the appropriate format for use in CONTAMW. The user now has a source library specific to their modeling needs (see Figure 6). Additional records can be added to the library using the CONTAMW Data Link Manager as needed, and the CONTAMW Library Manager is used to import library data into a CONTAMW project file.

Figure 6. CONTAMW source library manager.



SUMMARY AND FUTURE WORK

A standard VOC emission rate database format has been developed by the National Institute of Standards and Technology (NIST) for use with any indoor air quality models. The database is initially being populated with records from EPA's SIAE database. A second VOC emissions database that is being made available as part of this effort is NRC's material emissions database. A computer program was developed to search these databases based on contaminant, reference, and a variety of test conditions. The program also links the records in the databases to NIST's indoor air quality model CONTAMW. As a result, model users now have access to VOC emission rate data in a single location that has a user-friendly interface.

This project is still in its beginning stages, so there is additional work to be completed. For example, additional records may be added to the VOC emissions source database. Also, a statistical package may be added to the CONTAMW Data Link Manager to calculate the mean, maximum, minimum emission rate value for a selected group of records in the database. A source emission database for particles is also planned to be completed. Additional databases will

be developed that include contaminant loss rates, air cleaner removal efficiencies, and occupancy schedule information. These databases will be developed using a similar methodology to the VOCs database.

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DISCLAIMER

Certain commercial equipment, instruments, or materials are identified in this paper in order to specify the experimental procedure adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose.

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