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CONTAM96 User Manual

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George N. Walton

U.S. Department of Commerce National Institute of Standards and Technology Building and Fire Research Laboratory Gaithersburg, Maryland 20899

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ABSTRACT

This manual describes the use of a computer program, CONTAM96, for analyzing the air movement and indoor air quality in multizone buildings. The program is used to create and edit the building description including data for all features relating to airflow or to the generation and removal of contaminants. It uses a graphic interface to establish the spatial relationship of these features. These data along with weather data are used to calculate the airflows and dynamic levels of indoor contaminants. The results of the calculation may be reviewed graphically and printable files may be generated. This program is an extension of the earlier CONTAM93 program.

Key Words: airflow analysis; building technology; contaminant dispersal; indoor air quality; multizone analysis; user interface

DISCLAIMER

The Department of Commerce makes no warranty, expressed of implied, to users of the CONTAM96 computer program, and accepts no responsibility for its use. Users of CONTAM96 assume sole responsibility under Federal and State law for determining the appropriateness of its use in any particular application; for any conclusions drawn from the results of its use; and for any actions taken or not taken as a result of analyses performed using CONTAM96.

Users are warned that CONTAM96 is intended for use only by persons competent in the field of airflow and contaminant dispersal in buildings and is intended only to supplement the judgement of the qualified user. The computer program described in this report is a prototype methodology for computing the airflows and contaminant migration in a building. The calculations are based upon a simplified model of the complexity of real buildings. These simplifications must be understood and considered by the user.

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1. Introducing CONTAM96

1.1. What is CONTAM96

CONTAM96 is an *indoor air quality analysis* program designed to help you determine:

- (a) *airflows*: infiltration, exfiltration, and room-to-room airflows in building systems driven by mechanical means, wind pressures acting on the exterior of the building, and buoyancy effects induced by temperature differences between the building and the outside.
- (b) contaminant concentrations: the dispersal of airborne contaminants transported by these airflows; transformed by a variety of processes including chemical and radio-chemical transformation, adsorption and desorption to building materials, filtration, and deposition to building surfaces, etc.; and generated by a variety of source mechanisms, and/or
- (c) *personal exposure*: the predictions of exposure of occupants to airborne contaminants for eventual risk assessment.

CONTAM96 can be useful in a variety of applications. Its ability to calculate building airflows is useful to assess the adequacy of ventilation rates in a building, to determine the variation in ventilation rates over time and the distribution of ventilation air within a building, and to estimate the impact of envelope airtightening efforts on infiltration rates. The prediction of contaminant concentrations can be used to determine the indoor air quality performance of a building before it is constructed and occupied, to investigate the impacts of various design decisions related to ventilation system design and building material selection, and to assess the indoor air quality performance of an existing building. Predicted contaminant concentrations can also be used to estimate personal exposure based on occupancy patterns in the building being studied. Exposure estimates can be compared for different assumptions of ventilation rates and source strengths.

1.2. New Features

Users of earlier versions of CONTAM (Walton, 1994) will be interested in some of the following new features in CONTAM96. A method that draws and simulates a duct system is now available. You can now determine the exposure of occupants as they move among the different zones in the building as a function of time. Flow elements, schedules, and wind pressure profiles can now be saved to "library" files and called into other project files which should reduce the amount of numeric input as you develop your own personal libraries. CONTAM96 can now perform simulations for longer than one day -- actually, for up to one year. Since the detailed flow and concentration output files from such long runs could be very large, the program can produce summary statistics of these runs. These summaries consist of average, maximum, minimum, and standard deviations for age-of-air, contaminant concentrations, and exposures. The summaries can be used to determine critical days in the long simulation. A restart file is produced which allows the user to run individual days with the detailed output.

1.3. Overview of User Tasks

An analysis of airflow or contaminant migration in a building usually involves six distinct tasks:

- 1. Building Idealization: form an idealization or specific model of the building being considered,
- 2. SketchPad Representation: represent the building idealization using the diagrammatic SketchPad conventions of the program,
- 3. Data Entry: collect and input data associated with each of the SketchPad icons,
- 4. *Simulation*: select type of analysis to be conducted, set simulation parameters, and execute the simulation,
- 5. *Review & Record Results*: review the results of simulation and record selected portions of the results, and
- 6. *Project Documentation*: document the system idealization, input data, and simulation parameters.

Task 1 - *Building Idealization* - is an acquired skill that is gained through experience in airflow and indoor air quality analysis and familiarity with the theoretical principles and details upon which indoor air quality analysis is based. Building idealization is the process by which the user represents a building as a number of zones that exchange air with each other and the outdoors. A given building can be idealized in a number of ways depending on the building layout, the ventilation system configuration and the problem of interest. Regrettably, this task can be only indirectly supported by the CONTAM96. This is an area where engineering judgement will have to be used.

Task 2 - *SketchPad Representation* - will be the focus of your interaction with CONTAM96. With CONTAM96's SketchPad you will be able to draw a diagram - a *SketchPad diagram* - of your building idealization using drawing tools and libraries of icons to represent components of the building system. CONTAM96 will, in effect, translate that diagram into a system of equations that model the behavior of the building and solve these equations to complete analysis. In this chapter, we will introduce you to the basic aspects of SketchPad diagrams and establish the link between the types of building idealizations supported by the program and the diagrammatic conventions used to represent them. Chapter 3 provides an introduction to the SketchPad conventions, and Chapter 4 reference details on the use of all of CONTAM96 features, including SketchPad operations.

Task 3 - *Data Entry* - can be one of the more time-consuming parts of the process of using CONTAM96. It involves the determination and input of the numerical values of the parameters associated with each of the SketchPad icons. These icons represent the elements of the building model and include air leakage paths (windows, doors, cracks), ventilation system elements (fans, ducts, vents), contaminant sources, filters, and sinks. Each of these elements is associated with a number of parameters, and values of these parameters must be obtained by the user for entry into the model. Depending on the element and the application, these values can be obtained from building-specific data, engineering handbooks, and product literature. In many cases, a degree of engineering judgement will be involved. CONTAM96 allows the user to create libraries of these elements that are likely to be used frequently in the current and future modeling efforts.

Task 4 - *Simulation* - is the use of CONTAM96 to predict the airflow and contaminant concentrations of interest. This step involves determining the type of analysis that is needed, that is, steady-state or transient, and a number of simulation parameters. These parameters depend on the type of analysis, and

include convergence criteria and in the case of a transient analysis, time steps and the duration of the analysis. Once these simulation parameters have been specified, the simulation is executed.

Task 5 - *Review & Record Results* - CONTAM96 allows the user to view the simulation results on the screen and then to output them to a file for input to a spreadsheet program or a data analysis program developed by the user. Airflows and pressure differences at each flow element can be viewed directly on the SketchPad. Contaminant concentrations for a zone can also be plotted as a function of time directly from the SketchPad. The user can then decide which data they wish to examine more closely and export these to a file for later analysis.

Task 6 - *Project Documentation* - should occur throughout the process of using CONTAM96. It involves recording, in electronic form (such as a text file) or in a lab notebook, the details behind the simulation. These include a description of the building being studied, how it is being idealized within CONTAM96, the basis for the decisions regarding the idealization, and the sources of the input data.

1.4. Building Idealization

CONTAM96 supports the analysis of whole building systems *idealized* or *modeled* using collections of control volumes or *zones* linked by air flow paths - doors, windows, ventilation fans, cracks or leakage paths in the building construction, etc. These airflow paths are, in turn, modeled by so-called *flow elements*. As such, CONTAM96 is a *macroscopic* analysis tool - a term used to distinguish the modeling approach used from *microscopic* analysis based on computational fluid dynamics that are useful for modeling the details of flow and contaminant transport within individual rooms or connected spaces. CONTAM96 is the most recent member of a family of related macroscopic analysis programs developed at NIST. Its relation to other members of the NIST family of programs and its theoretical basis are briefly discussed in Chapters 5 and 6. At this point, we will skip the underlying mathematical and numerical intricacies of the program and address the problem of transforming a real building, existing or proposed, into an idealization suitable for macroscopic analysis with CONTAM96.

The manner in which a building is idealized as a number of zones depends on the layout of the building, the zoning of the ventilation system and the reason that the user is performing the analysis, that is the question to be answered. One could include every conceivable zone in a building idealization, down to every room and closet. Fortunately, it is unlikely that such a detailed idealization is necessary. Depending on the building and the purpose of the analysis, the zones may be building floors, groups of floors, or individual rooms. Floors may be grouped together if they are served by a common ventilation system, or are assumed to have common air leakage and pollutant source characteristics. For example, an office building with an underground garage could be modeled as two zones (the garage and the rest of the building. Instead, if they are trying to understand airflow between the floors of the building, a single zone idealization of all the occupied floors will not be appropriate, and the building will need to be divided into a number of zones.

To make the discussion more concrete consider the "real" building sketched in Figure 1 in plan and perspective - a four story apartment building with two units on each floor, an access stairway, and a four-story light shaft.

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To form an idealization of this real building suitable for macroscopic analysis we must represent it as a collection of zones. There are many ways to do this, some clearly reasonable and useful, and some that are not. For example, we could *model* the apartment building as a single zone. This might be appropriate if we need only to get a rough estimate of indoor air pollutant concentrations when air flows freely between all eight units within the building - not likely to be a common occurrence.

Alternatively, we could *model* each living unit in the building as a single control volume and the stairway shaft as an additional single control volume as sketched in Figure 2. This idealization would allow us to predict airflows into, out of, and between units and to estimate average air contaminant concentrations within units.



Finally, we could *model* each room in each living unit as separate zones and the stairway shaft as a vertical stack of zones as sketched in figure 3. This idealization would allow us to predict airflows into, out of, and between rooms and units, to estimate average air contaminant concentrations within rooms, and to account for vertical distributions of contaminants in the stair shaft.



1.5. SketchPad Representation

The SketchPad consists of an invisible array of small cells into which the user places various icons representing building features relevant to the calculation of airflow and contaminant dispersal. This produces a simple illustration which has been chosen intentionally to represent the simplicity of the underlying mathematical model. The SketchPad is used to establish the geometric relationships of the relevant building features. It is not intended to produce a scale drawing of the building. Instead, it is used to create a simplified model where the walls, zones, and airflow paths are topologically similar to the actual building. The SketchPad allows the entry and display of the data in an intuitive manner and provides context sensitive, on-screen help.

Once the user has decided how to represent the building as a multizone system and has determined appropriate input values, the building data is entered into the SketchPad. For each of the three building idealizations considered above a separate *SketchPad representation* could be made. As indicated in the sketches above, it seems natural to organize these zones by building level. Therefore, modeled zones are represented on the SketchPad using plan views of the zones on each building level. A level would typically be a building floor, but a suspended ceiling acting as a return air plenum or a raised floor acting as a supply plenum may also be treated as a level.

1.5.1. Walls The first step in creating a building representation is the draw the walls. Each level is divided by walls into zones. Walls include the building envelope and internal partitions with a significant resistance to air flow, and are drawn as either horizontal or vertical lines. Figure 4 shows the walls for the first level of the example building. This sketch includes the lightshaft (a), the stairwell (b), and the two apartments which are each divided into two individual rooms (c) and the well-mixed remainder (d).





1.5.2 Zones Once the walls of a zone have been drawn a zone icon can be placed within the wall boundary and the zone numeric parameters can be defined. The type (a) icon in figure 5 indicates an outdoor, or 'ambient' zone (there is an ambient zone around the outside of the building by de-The type (b) icons indicate 'normal' fault). There is also a 'phantom' zone icon (not zones. shown) which indicates that the area on the current level is actually part of the zone on the level immediately below. The data includes the name of the zone associated with the zone icon. the zone temperature, volume, and initial contaminant concentration if applicable.

1.5.3. Airflow Paths After the building is idealized as a collection of zones, the next step in the process of idealizing the building is to identify and idealize the airflow paths between the zones of the building and between the zones and outdoors. As was the case for zones, there are a number of different ways that the airflow paths in a given building can be idealized. And, again as in the case of zones, it is not generally necessary or desirable to include every conceivable airflow path in a building idealization. This step begins with identifying the airflow paths in a building. These include any location where air can flow between zones, either intentionally or unintentionally, including windows, doors, vents, and intersections between walls and floors, walls and roofs, and walls and foundations. Research has shown that many, if not most, air leakage sites in buildings are not in obvious locations, that is windows, doors and vents. Instead, air leakage is generally associated with unobvious, and sometimes hard-to-find, airflow paths in exterior walls and interior partitions. Therefore, identifying the airflow paths in a building involves developing a list of paths, which includes information on the zones that they connect, their height and some quantitative information on their leakage characteristics.

In figure 6 the icons labeled (a) represent leakage openings between the zones and ambient. It may be desirable to use several openings to represent the individual airflow features on each wall. The icons (b) indicate the closed doors between the stairwell and the apartments. The icons (c) indicate open doorways which can allow a two-way flow between zones with different temperatures. In association with the path icon, the user enters data describing the flow/pressure relationship, the height of the path relative to the current level, and wind pressure data which will be used to convert wind speed and angle to pressure on envelope openings. Additional information can include whether the path acts as a contaminant filter



and whether it "operates" on a schedule (like a window or vent that opens at certain times). A large number of flow/pressure formulations are provided which the user can choose for each flow path.



Figure 7 shows the second level in the building. It was created by a single command that copied the first level and then was modified by adding a few flow paths. The icons (a), which are not on walls, represent flow paths through the floor separating this level from the one below to allow an inter-level flow. Icon (b) in the stairwell has been set to indicate a large opening between levels to indicate a low resistance to airflow. The icons (c) represent exhaust fans which can move air from zones to ambient according to a schedule. These icons indicate the direction of air flow, in this example out of the building to ambient.

1.5.4 Simple Ventilation System After identifying the airflow paths in the building, the next step in the idealization process is the identification of any mechanical ventilation systems. These systems can be separated into those that can be idealized as single fans that simply force air from one zone to another, such as a kitchen exhaust fan as was shown in figure 7, and those that are more complex involving several different zones and a system of air distribution ductwork. The idealization process for each system involves obtaining information on the zones served by the system, the system airflow rates, and if needed fan curves, filtration efficiencies and schedules of operation.

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A simple model of an air handling system is available with supply and return point symbols placed within the appropriate zones. Icon (a) in figure 8 represents the implicit supply and return nodes (zones) in such an air handling system, which are placed independent of the building zones. The supply zone is implicitly connected to all the icon (b) supply points, and the icon (c) return points are connected to the return zone. At the return zone some air may be exhausted and some recirculated; at the supply zone some outdoor air enters the system. All supply and return airflows follow user defined schedules. In this example a separate system has been created for each apartment by using two (a) icons.





1.5.5. **Detailed Ventilation System** More detailed model of air handling systems is also available. In addition to the simple AHS model of figure 8, CONTAM96 now provides a detailed model of ductwork shown in figure 9. The duct lines are drawn in much the same way as walls Every duct line must terminate were drawn. either in a zone as indicated by icons (a) or at a junction with other ducts shown by icons (b). When the flow characteristics of the duct segment are defined, a small icon (c) is created which indicates the normal direction of flow (and the point at which the characteristics may be modified). The actual flow direction will be computed in the simulation. Special junction icons can be

created which indicate that a duct segment is connecting junctions on two building levels.

1.5.6. **Contaminants** The contaminants of interest may be obvious in some cases, but if the user is simulating a source which emits a number of contaminants, e.g. cigarette smoke or some building materials, they will have to decide which of the contaminants will be included in the simulation. If any of the contaminants are subject to radioactive decay, these decay constants will be needed for the simulation. The last step in the idealization process is identifying the contaminant sources and sinks in the building. This step involves identifying which sources and sinks are in which zones, which of the models supported by CONTAM96 is most appropriate for each source and sink, and the values of the quantitative pa-



rameters needed to describe them. Contaminant source (or sink) icons, (a) in figure 10, may be placed in any zone. These represent any feature which produces, removes, or adsorbs a contaminant. The basic model is the constant coefficient model, $S_{\alpha} = G_{\alpha} - R_{\alpha} \cdot C_{\alpha}$, where S_{α} is the contaminant α "source strength" computed from the generation rate, G_{α} , removal rate, R_{α} , and concentration in the zone, C_{α} . Other models include a pressure driven model, a cutoff concentration model, a decaying source model, and a boundary layer source/sink model. All source/sink icons include an optional schedule which can be used to vary the source strength as a function of time.

1.5.7. Occupant Exposure A significant addition to the capabilities of CONTAM96 has been exposure analysis represented by the icons (a) in Figure 11. In addition to just computing the transient contaminant concentrations in each zone, you can now determine the exposure of an individual as he or she moves to different zones as a function of time. You simply define the occupancy schedule which describes where the person is as a function of time. In some cases you will be interested in exposure to contaminants generated by the occupants, and the exposure icon can be used to ensure that the contaminant generation schedule matches the occupancy schedule.



2. Getting Started with CONTAM96

2.1 Requirements

CONTAM96 requires a 386 class (or higher) PC compatible computer with a math coprocessor, approximately 2 megabytes of RAM, VGA graphics, and MS-DOS (5.1 or higher). This level of CPU is necessary for the DOS extender because CONTAM96 requires more than the DOS standard 640 kilobytes of RAM to run. The use of a more advanced CPU chip (486DX or Pentium equivalent) is recommended for its faster computational performance. CONTAM96 is a DOS program which can also be run in a DOS window under Windows 3.1 and Windows 95.

2.2 Availability

CONTAM96 is available on diskette and by anonymous FTP on the Internet. For a diskette, contact the Indoor Air Quality & Ventilation Group
Building Research, Room A313
National Institute of Standards and Technology
Gaithersburg, MD 20899

It is faster and easier to get CONTAM96 by using the anonymous FTP process on the Internet. The FTP site is *ftp.nist.gov*. The latest upgrades will be posted here first. They will be described in the ASCII file CONTAM96.TXT which you should download occasionally to check for the latest modifications and fixes.

Source code is available from the NIST IAQ&V Group upon request.

2.3 Installation

It is recommended that the CONTAM96 programs be installed in a single directory and that project files be processed and saved in subdirectories of the CONTAM96 directory. The TREE structure would look something like this:



When you perform a study with CONTAM, it will probably require the creation of several project data files to simulate different variations or options of the building design. These data files should be grouped together below the CONTAM96 directory in a separate subdirectory for each study as shown above with *study1* and *study2*.

2.3.1 Installation from Diskette

The installation process is discussed in the README file on the distribution diskette. Be sure to read this file before installing or using the program. The README file will include the most current information on the installation and use of CONTAM96.

CONTAM96 can be installed on the hard disk by placing the distribution diskette in drive A: (or drive B: if appropriate). If you want CONTAM96 installed in the C:\CONTAM96 directory (the default) enter a command like:

A:INSTALL A:

where

A: is the drive where you have placed the CONTAM96 disk,

Or you may enter a command like:

A:INSTALL A: C: C:\CONTAM96

where

C: is the drive where CONTAM96 will be installed, and

C:\CONTAM96 is the full path to the CONTAM96 directory.

Replace these parameters with values appropriate for your computer. Then answer the questions that the program asks (by pressing Y or N) to install the selected programs and/or data files onto your hard disk.

2.3.2 Installation from the Internet

Details of the FTP transfer will depend on the software you have. It typically involves the following steps:

ftp ftp.nist.gov	connect to the NIST FTP site
user name: anonymous	signon as "anonymous"
password: guest	or use your internet address
cd contam	change to contam directory
bin	set binary transfer mode
get <file></file>	get file(s)
•••	
bye	signoff

The following files are available:

CONTAM96.ZIP	primary CONTAM96 files.
OTHER96.ZIP	other files including Rational Systems DOS extender.
TESTS96.ZIP	CONTAM96 test case project files.
CONTAM96.TXT	information about the above files.
REPORT96.ZIP	a copy of the CONTAM96 User Manual.
PKUNZIP.EXE	PKWARE program to unpack .ZIP files. Files are
	packed to minimize storage and transmission time.

Get all six files for an initial installation. Be sure to read the ASCII file CONTAM96.TXT which includes the latest installation information. Periodically get a copy of the CONTAM96.TXT file to keep track of the latest program fixes and upgrades. To upgrade, you will only need the CONTAM96.ZIP file.

Create a subdirectory and then make it the default. For example, to install on the C: drive enter the following three commands:

C:	(insures that you are on the C: drive)
MKDIR C:\CONTAM96	(creates subdirectory for CONTAM programs)
CHDIR C:\CONTAM96	(shifts to CONTAM96 subdirectory)

Copy the files PKUNZIP.EXE, CONTAM96.TXT, CONTAM96.ZIP, and OTHER96.ZIP to the CONTAM96 subdirectory. Then unpack the ZIPped files with two commands: PKUNZIP -0 CONTAM96 PKUNZIP -0 OTHER96

You may then delete both .ZIP files. Keep the PKUNZIP.EXE file to process future updates. You may either add the CONTAM96 directory to your path in the AUTOEXEC.BAT file or edit the C96.BAT file to include the full path you set for CONTAM96 and save it in a directory that is always in your path.

Create a subdirectory of CONTAM96 for the test case project files and unpack them there. From the CONTAM96 directory enter the following commands:

MD TESTS CD TESTS ..\PKUNZIP -o <path > TESTS96

2.3.3 CONTAM96 Files

The following files are installed into the CONTAM96 directory:

CONTAM.EXE	The CONTAM96 input/output processor.
CONTAM.HLP	Data entry and help screens for CONTAM.EXE.
CONTAMX.EXE	A CONTAM batch-mode simulation program.
WEATHER.EXE	A program to create weather files.
C94TOC96.EXE	A program to convert CONTAM94 project files.
W94TOW96.EXE	A program to convert CONTAM94 weather files.
PKUNZIP.EXE	PKWARE program to unpack files.
PATHCHK.EXE	A program to check and modify the path.
C96.BAT	A program for setting the path before a simulation session.
CONTAM.ICO	An icon that you may use with Windows95.
CONTAM96.TXT	General instructions and a list of program changes.
Files which will be added to th	e CONTAM96 directory during program execution:
CONTAM.CFG	User created configuration data.
And temporary files rewritten v	with every run:
PROJECT.BKP	Copy of most recent project file read by CONTAM.
WEATHER.BKP	Copy of most recent weather file read by CONTAM.
CONTAM.WDW	Used to save and restore screen images.

CONTAM.LOG	Log data (e.g. error messages) from latest CONTAM run.	
CONTAM.KEY	A copy of all keystrokes made during latest CONTAM run.	
CONTAMX.LOG	Log data (e.g. error messages) from latest CONTAMX run.	
Files that should be in a se	parate project subdirectory of the CONTAM96 directory:	
project.PRJ	The project data file; <i>project</i> is a user-defined name.	
weather.WTH	Weather file created by WEATHER.EXE.	
project.SIM, etc.	Plus any output files created by CONTAM.	

Access to the files can be significantly improved by using the DOS SMARTDrive disk-caching program. Add a line to your CONFIG.SYS file similar to:

DEVICE=C:\DOS\SMARTDRV.SYS 1024

Reserve at least 1 M-byte, if possible. See your MS-DOS manual for details.

It may be desirable to move the PKUNZIP.EXE file to a directory that is always in your path.

2.3.4 Completing the Installation

For running directly from DOS:

You may either add the CONTAM96 directory to your path in the AUTOEXEC.BAT file or process the C96.BAT file which would include the following steps. (1) Edit the line set c96=C:\CONTAM96 to include the full path you set for CONTAM96, and (2) copy C96.BAT your C:\DOS directory which insures that it is always in your path.

For running from the Windows MS-DOS prompt:

Process the C96.BAT file. (1) Edit the line set c96=C:\CONTAM96 to include the full path you set for CONTAM96, and (2) copy C96.BAT your C:\WINDOWS directory which insures that it is always in your path.

2.4 Running CONTAM96

Remember that CONTAM is a DOS program. It must be run either directly from DOS or from a DOS window. If you are in Windows, you may either exit Windows or execute a DOS window.

Once you are in the DOS mode, you must move to the directory which contains your project files, for example, C:\CONTAM96*study1*. There are two way to do this.

(1) If you have added the CONTAM96 directory to your path, use the standard DOS CHDIR commands to move to that directory.

(2) If you have properly modified and moved C96.BAT, just enter: C96 study1.

Once you are in the directory containing your project files, enter the word CONTAM to begin processing. If you plan to use an existing project file named *project*.PRJ, a shortcut is to enter CONTAM *project*. Context sensitive help is always available by pressing the F1 or F2 function keys. To exit CONTAM press the <Alt> and Q keys simultaneously.

If entering the word CONTAM did not start the program it is probably because the directory containing CONTAM.EXE and DOS4GW.EXE is not in your path. Check your directory structure and the location and contents of the C96.BAT file.

2.5 Upgrading CONTAM96

Obtain the updated CONTAM96.ZIP file on disk or, more quickly, from the Internet FTP site. From the CONTAM96 directory enter the command:

PKUNZIP - o < path > CONTAM96

where < path > is the path to the new CONTAM96.ZIP file. This is assuming that PKUNZIP.EXE is either still in the CONTAM96 directory or has been moved to a directory that is in your path.

2.6 Getting Help

If a problem that you cannot handle occurs while running CONTAM, exit CONTAM and immediately copy the CONTAM.LOG, CONTAM.KEY, PROJECT.BKP and (if available) WEATHER.BKP files to a diskette. If a problem occurs while running CONTAMX, also include a copy of the *project*.NDF file. These files should permit a recreation of the problem. E-mail these files to George Walton at: gwalton@nist.gov. Mr. Walton's phone number is 301-975-6421. If Mr. Walton is not available, contact the Indoor Air Quality & Ventilation Group at 301-975-6431.

2.7 Removing CONTAM96

CONTAM96 can be easily removed from your computer if all the data directories are subdirectories of the CONTAM96 directory and you have DOS 6.0 or higher. Then you simply go to the directory above CONTAM96 and enter DELTREE CONTAM96. If you have an older version of DOS, you must delete the files and directories individually. Remember to fix the PATH command in your AUTOEXEC.BAT file by removing the path to CONTAM96 and/or delete the C96.BAT file.

3. The CONTAM96 Graphical User Interface

3.1. Screen Layout

The screen is divided into three areas as shown in Figure 12.

The main portion of the screen is occupied by the SketchPad Area. This is used to display building sketches, data entry screens, or help screens. The Options Area includes, from top to bottom, the name of the current project file, a list of **Alt** key shortcuts, a list of menus activated by the function keys, and a list of SketchPad icon processing and creation keys. The Status Area displays information such as error messages, task execution instructions, and summary information on a currently



Figure 12. Areas on the CONTAM96 Screen

highlighted icon. The status area also serves as an input line for the CONTAM calculator.

3.2. User Input

Most interaction with CONTAM occurs within the SketchPad area either by drawing or manipulating the schematic or entering data and making menu selections within data entry screens. The options and status areas are not directly accessible with the cursor keys or mouse.

3.2.1. Keyboard Data input is primarily via the keyboard. In the discussion in this manual some of the keys are described by special symbols:

↑ ↓ → ←	cursor keys
Insert Delete	
Home End	<pre>} editing keys</pre>
PgUp (page up)	
PgDn (page down)	J
<u>ب</u>	the enter (or return) key
Escape	the escape key
Tab	the tab key
<ctrl></ctrl>	the control key
< Alt >	the alt key
F #	the numbered function keys F1 through F9
	- J J

3.2.2. Mouse The mouse may be used in place of a few of these keys. The left button corresponds to the \leftarrow key; the right button to the Esc key. Vertical motion corresponds to the \uparrow and \downarrow cursor keys, and horizontal motion corresponds to the \rightarrow and \leftarrow cursor keys. In general, the mouse is best used for reviewing the SketchPad and data screens, while the keyboard is best for creating or revising the SketchPad and data.

3.3. Options Area

The options area indicates the various keys that can be pressed while the user is processing the SketchPad.

3.3.1. < Alt > Key Shortcuts and Modes

The top line in the options area gives the name of the current project and a reminder that you can always exit the program by pressing the <Alt>Q key combination. Also shown are eight other <Alt>key shortcuts which can be invoked from the SketchPad:

< Alt > N	Normal sketchpad display mode;
< Alt > W	Wind pressure display mode;
< Alt > R	Results display mode (user may not alter sketch);
<alt>Z</alt>	Zoom out to display the entire SketchPad;
< Alt > B	display (in gray) the icons on the level Below this one;
< Alt > C	Check the completeness of the description of this level;
<alt>S</alt>	Save the current building description to the project file;
< Alt > A	compute Age-of-air for zones (while in results mode only).

When a mode is in effect, the background color changes from green to red.

3.3.2. Function Key Menus

Pressing the function keys allows access to data and program features not directly related to the SketchPad icons, but which allow the user to perform project-related tasks such as accessing help, setting simulation parameters, configuring display options, etc. The following is a list of the function keys and their associated uses.

- F1 help for the meaning of the information of the screen;
- F2 help for how to use the program;
- F3 specify the project file and modify the user interface;
- **F4** set up the simulation controls and begin simulation;
- F5 prepare various output reports;
- **F6** access to libraries of component models;
- **F7** set up steady state and transient weather data;
- F8 actions (e.g., create) related to an entire building level;
- **F9** navigate the SketchPad and change the SketchPad display.

When a menu is in effect, the background color changes from green to red.

3.3.3. Icon Editing Keys

The next four keys in the options section (\leftarrow C M Del) are used to operate on existing icons on the SketchPad. Move the cursor to the icon and press \leftarrow (or the left mouse button) to present the data entry screen for the icon. This will let you define or redefine the description of the feature represented by the icon. Note that undefined icons are displayed in dark red.

You may copy (C) or move (M) many (but not all) of the icons. Copying makes it easy to create many instances of identical or similar building features. It is sometimes necessary to move an icon in order to fit other features properly on the SketchPad. When a move cannot be done, try a copy and delete (Del). See section 4.2 for details.

3.3.4. Icon Creation Keys

The remaining keys in the options section (W B Z P A F S, etc.) are used to place icons on the SketchPad. In the case of walls (W), box-shaped walls (B), and ducts (D) these icons form lines which are drawn with the mouse or cursor keys as described in section 3.4.2.5. The other key commands place individual icons at the current cursor location. When data must be entered to complete the definition of the icon, the icon is displayed in dark red.

Note that when the background color for one of the function keys or icon keys is highlighted in red, that action must be completed before any other actions (except F1 and F2 help) indicated in the options area are available.

3.4. SketchPad

The SketchPad consists of an array of small cells into which the user places various icons representing building features relevant to the calculation of contaminant dispersal. This produces a simple illustration resembling floor plans. This method of representation has been chosen intentionally to portray the simplicity of the underlying mathematical model. The SketchPad is used to establish the geometric relationships of the relevant building features. It is not intended to produce a scale drawing of the building. It is used to create a simplified model where the walls, zones, and air flow paths are topologically similar to the actual building. The SketchPad enables the entry and display of the data in an intuitive manner. Through user interaction with items on the SketchPad, the program provides access to various data entry screens needed to define the mathematical characteristics of the various building features.

3.4.1. Icons

The building description is created on the SketchPad by processing various building elements which are represented by icons. Everything that appears on the SketchPad is either an individual icon or, in the case of walls and ducts, is made up of a set of icons. Figure 13 shows the various icons used on the SketchPad.

walls:	_	I	r	٦	2	Ŀ	ŀ	Ŧ	4	ـله	+
zones:		D									
ducts:	=	11	F	จ	리	Ľ	₩	¢	atta	Ħ	¥
junctions:	0	₿	#	#		8	Ø				
simple AHS:	雪	X	Ø								
flow paths:	•	¢	Φ	0	٠	•	¢	¢			
source:	E										
exposure:	۲										

3.4.2. Icon Operations

The following is a list of basic operations that can be performed on the SketchPad icons:

> Create an icon (in a single cell). Delete an icon. Copy an icon. Move an icon. Create a line (series of icons). Delete a line. Define an icon (enter the data).

Figure 14. SketchPad Icons

Each of these operations is explained in more detail in the following sections. Instructions appear in the Status Area during several of the operations. There are no options for copying or moving a line.

3.4.2.1. Create an icon: Move the cursor to the position desired for the icon; press the key associated with the icon (as shown in the options area). The icon appears in a dark red color to indicate that it has not been defined, that is, the associated numerical data has not been entered.

3.4.2.2. Delete an icon: Move the cursor to the icon; press the **Del** key; respond to the alert displayed in the Status Area (a guard against accidental deletions). Undefined icons can be deleted without the alert.

3.4.2.3. Copy an icon: Move the cursor to the icon; press C; move the cursor to the new location; press \leftarrow to copy the icon or Esc to abort the move. Copy mode continues with move and \leftarrow , until Esc is pressed, allowing the user to make several copies of an icon. The word "Copy" is highlighted in the options area. Pressing \leftarrow while at the copied icon brings up the data entry screen to confirm/revise icon data. Some types of icons may not be copied.

3.4.2.4. Move an icon: Move the cursor to the icon; press M; move the cursor to the new location; press \leftarrow to complete the move or Esc to abort the move. The word "Move" is highlighted in the options area. The movement of icons is often restricted. For example, the icon representing a zone may not be moved across the walls defining that zone.

3.4.2.5. Create a line: Press the appropriate key to enter line creation mode; move the cursor to the place where the line starts; press \leftarrow to start the line; move the cursor to trace the path of the line; then press \leftarrow to indicate the line is done. The user may then repeat this process (\leftarrow , move, \leftarrow) or press Esc (at any time to abort) and return to normal mode. Line creation is used for walls, boxes (walls in the shape of a rectangle) and ducts.

The cursor moves two cells at a time (which automatically prevents the creation of several invalid configurations). Backing up over a previously drawn line generally removes it. There is a check for valid line placement, e.g., not over another icon. The options area indicates that the line creation mode is in effect by highlighting the wall, box, or duct options. Note that a line is a set of related icons placed in contiguous cells on the SketchPad. These contiguous icons are always processed as a group.

3.4.2.6. Delete a line: Move the cursor to the line; press Del; respond to the alert for the highlighted line. Lines are deleted between junctions with other lines. If the cursor is at a junction of walls, the program will automatically indicate each possibility until a deletion is made.

3.4.2.7. Define an icon: Move the cursor to the icon; press \leftarrow . (In the case of a duct line, this means a single icon on the line.) This will invoke the data entry form which covers the SketchPad. The word "data" is highlighted in the options area. Fill out the data form as described in section 3.5. Quit or done on the data form returns the user to the SketchPad.

3.5 Data Entry Screens

In addition to the relationships established on the SketchPad, numeric data is required to define the mathematical model for the simulation. This data is prepared in the data entry screens. A data entry screen consists of one or more control buttons and data entry fields (designated by a special color: light gray on the blue background) and accompanying text. The data entry fields are generally organized with the most important data toward the top of the screen. A more detailed explanation of the data entries is available by pressing F1. If you are unsure about a value, you should generally leave the default. A detailed explanation of how to use each control button or data entry field is available by pressing F2.

Each data entry screen is numbered. The number appears within brackets, e.g., [100], in the upper right corner of the screen. These numbers allow a means to refer to individual screens and how on secreen refers to another as in Appendices A and C.

Keyboard or mouse input is required from the user whenever the cursor is in a data entry field. The field may be blank or it may present a default response. The contents of a data entry field may be edited. That is, characters may be overwritten, deleted, or inserted. Overwrite and insertion modes are shown by the shape of the cursor. Press the Insert key to toggle between modes.

3.5.1. Navigating the Screen There are usually several data entry fields on a single screen. These fields are ordered from top to bottom and left to right in a linear and circular manner. That is, the last field on the screen can be accessed as if it were above the first field and the first field as if it were below the last field. Movement between fields is done with the mouse or the \uparrow and \downarrow keys. Use the PgUp and PgDn keys to move directly to the first and last fields. The Esc key can also be used to reach the last field. It may or may not be necessary to make an entry in a field depending on context. When an entry is required but has not been made, you will be notified by an error message.

3.5.2. Control Buttons are used to initiate screen actions or set program switches.

3.5.2.1. **IDENTIFY and SET UP:** The pushbutton: A pushbutton allows the user to initiate the action indicated in the adjacent text. If the text is followed by an ellipsis (...) the pushbutton causes another data entry screen to be displayed. A mouse click or an \leftarrow activates the pushbutton.

3.5.2.2. **I** radio button - off;

radio button - on: Radio buttons come in groups, only one of which is activated at a time. A mouse click or an \leftarrow turns on the highlighted radio button and simultaneously turns off all other radio buttons in the group.

3.5.2.3. $\| \mathcal{I} \|$ check box: A check box button acts like an on/off (toggle) switch: when it is checked, it is turned on and when it is not checked, it is turned off. A left mouse button click or an \leftarrow toggles the check box.

3.5.2.4. ∎↑scroll button - up;

scroll button - down: Scroll buttons allow the user to move through a long list. Move to the scroll button and click or \leftarrow .

3.5.2.5. indicating that action described is either currently not applicable or not available (i.e. it is to be included in a future release of CONTAM).

3.5.2.6. Quit At the bottom of most data entry screens are the options "done" and "quit". Press \leftarrow at "done" to save the entries you have made; \leftarrow at "quit" (or Esc at "done" or "quit") to not save them. If you entered this screen only to review the data, note that by pressing Esc (or the right mouse button) twice you will return to the prior screen without changing any data.

3.5.3. Data Entry Fields are used to provide alphanumeric data to the program.

3.5.3.1. Editing Options The size of the field indicates the maximum number of characters which may be entered. Data entry begins in the overwrite mode, i.e. the value of the key pressed replaces the character at the cursor. Pressing Ins will toggle between the insert and overwrite modes. These modes are indicated by the shape of the blinking cursor. Pressing Del will remove the character at the cursor. Pressing $\langle Ctrl \rangle \in End$ will clear the data entry field to the right of the cursor. Move the cursor to the right with the \rightarrow , $\langle Ctrl \rangle \rightarrow$, or End keys. Move the cursor left with the \leftarrow , $\langle Ctrl \rangle \leftarrow$, or Home keys. When the edited data is satisfactory, press \leftarrow or Tab which accepts the data and passes you to the next data field. $\langle Ctrl \rangle \leftarrow$ accepts the data and passes you to the prior field. The use of any command causing a move between fields before pressing \leftarrow , $\langle Ctrl \rangle \leftarrow$, or Tab will restore the field to its original value. The mouse equivalents of the \leftarrow , Esc, \uparrow , or \checkmark keys may be used within the data field,.

3.5.3.2. Numeric Data When numerical data is required, a proper number must be entered. In some cases the value must be an integer (e.g. 1000). In other cases a real value with a decimal point (1000.0) and/or scientific notation (1.0e3) is acceptable. If the characters you type are not a valid number, or if the number is physically impossible, an error message results. The error must be resolved before proceeding to another field.

3.5.3.3. Units Data entries representing physical values also have the units displayed in brackets, e.g. $[m^2]$. Press < Alt > U to change the units by selecting from among the units presented on the screen. After the units have been selected, the original value in the data entry field will be converted and displayed in the new units.

3.5.3.4. Calculator If the desired input value is some arithmetic combination of known values, press < Alt > V to activate an on-screen calculator in the status area. Enter a mathematical expression as described in section 3.7.5. When you press \leftarrow to complete the calculation, it will enter the results directly into the field.

3.5.3.5. Named Data Features In order to minimize the amount of numerical data entered, data representing a single building feature, such as a doorway, is grouped together and given a name by the user. When that feature is needed at another place in the building, it can be referred to by name instead of re-entering all the numeric data. Such a *name field* is indicated by <...> within it. Whether an entry is required or what no entry would mean is indicated within the <...>. For example, the following entries appear for defining an airflow path:

Flow element name: strep/d>

These indicate that a flow element name is required but that a filter name is not. Failure to enter a filter name will simply mean there is no filter in this particular path, whereas if you do not enter a valid flow element name you will not be permitted to exit the data entry screen except via the "quit".

When a named feature is required, and the feature has not been previously defined or you do not remember the name, put a blank (press the space bar) in the first column of the field and then click or press \leftarrow to define the feature. This will allow you to select a previously defined feature or create an entirely new one. Pressing \leftarrow with a name already present, displays the completed data entry screen for the feature. Blanks are not permitted in feature names.

3.6. Help Screens

Context sensitive help is available from most points in the program by pressing the F1 key or the F2 key.

3.6.1. Help1 Pressing F1 provides a screen of text which tells what the various options / data input fields mean. F1 gives information about *what* the program is requesting from the user, e.g., the physical description of a flow element and its input parameters.

3.6.2. Help2 Pressing F2 provides a screen of text which tells how the currently active procedure is used, e.g. how a wall is drawn or how radio buttons work. F2 gives information about *how* to perform the current operation, e.g., how to enter a flow element name or copy an icon.

3.6.3. Navigating Help Screens The help screen will completely cover the SketchPad or data entry screen. Press Esc to exit help and return to the SketchPad or data entry screen. Occasionally the help message is more than one page (screen) long in which case the status area will indicate that cursor commands (\uparrow \downarrow) are available to switch to other pages.

3.7. Status Area

The status area displays information about the SketchPad or data entry screen, and provides an area for some special user inputs.

3.7.1. Icon Status As you move the cursor across the SketchPad icons, summary data is displayed on the status line. The actual data depends on the icon and the SketchPad mode: normal, wind pressure, or results.

3.7.2. Building Status The lower right corner of the screen usually displays some building status information including the name of the building level displayed on the SketchPad. Additional information is displayed in the wind pressure and results modes, such as a scaling factor for displayed wind pressures, scaling factors for the simulated airflows and pressure drops, and time data for the results of a transient simulation.

3.7.3. Error Messages are also displayed in the status area. They appear with a red background color, and they have a pushbutton indicator (3.5.2.1) at the right side of the status area. The pushbutton indicates that you will have to press \leftarrow or **Esc** to clear the error message and continue interacting with the program. Error messages may be only informational, or they may require corrective action, or they may indicate the occurrence of a fatal error which then terminates the program.

3.7.4. Inquiries Occasionally the program will ask you a question in the status area. Questions appear with a red background and include a 1-character wide data entry field for your response to the question. If the field is blank, make your response by pressing either the Y or the N key. If the field contains a Y or N default response and that is the response you want, press \leftarrow . If you do not want the default, press Y or N as desired.

3.7.5. Calculator When a numerical data entry field is highlighted, you may invoke the calculator to compute a real number (see section 3.5.3.4.). If the calculator is available, it will be so indicated in the Status Area. You will then enter a mathematical expression in the status area and then press \leftarrow . The result of evaluating the expression is placed in the data entry field. An error message will appear if the expression cannot be evaluated and you may then correct the expression.

Numbers may include a sign (-3), a decimal point (0.001), and scientific notation (2.4e4 or 1.56e-3). Two shortcut characters are provided to represent special numbers: V is the current value in the data entry field, and P is π (3.1416).

The expression may use these five mathematical operators:

+ - * / ^ (^ is exponentiation: $2^{0.5} = 1.4142$).

The expression is evaluated from left to right:

3 + 4 * 2 is equal to (3 + 4) * 2, not 3 + (4 * 2).

Use parentheses to explicitly order the evaluation.

Press Esc to return to the data entry field without evaluating the expression.

4. Using CONTAM96

4.1. Strategies for Developing CONTAM Projects

The building descriptions created with CONTAM are saved in project data files which are identified by a .PRJ file name extension. These files must be saved to keep a record of what was simulated because the various reports provide only the results of simulation, not the building description. A research or design study will usually involve several different project files describing different conditions from which comparisons and choices will be made. A project data file is created or updated (i.e., overwritten) by CONTAM whenever the project save command (shortcut < Alt > S) is issued. It is useful to keep a backup of the most recent version of the project file under a different name. The user does not directly access the data files describing the building. All access is done through the CONTAM program and its graphic interface.

The description of the building is created or modified via the SketchPad. The SketchPad consists of an array of small cells into which the user places various icons representing building features relevant to the calculation of contaminant dispersal. This produces a simple illustration resembling floor plans which has been chosen intentionally to represent the simplicity of the underlying mathematical model. The SketchPad is used to establish the geometric relationships of the relevant building features. It is not intended to produce a scale drawing of the building. It is used to create a simplified model where the walls, zones, and air flow paths are topologically similar to the actual building. Engineering judgement must be used to define this model of the building. The SketchPad allows the entry and display of the data in an intuitive manner. The SketchPad provides access to various data entry screens needed to define the mathematical characteristics of the various building features.

Building data is organized by "levels". A level would typically be a building floor, but a suspended ceiling acting as a return air plenum or a raised floor acting as a supply plenum may also be treated as a level leading to multiple levels per building floor. Levels are created under the F8 menu option. The SketchPad display includes features on the current level in dark colors, and, optionally, features on the level below in light colors. When the levels are similar, most of the lower level features are hidden by the features on the current level. You may need to define a roof level which has no zones but does include openings from ambient to the level below.

The first step in defining the building on the SketchPad is to define the walls on a given level which are used to separate regions of uniform air temperature and contaminant concentration, called zones. Such walls include the building envelope and internal partitions with a significant resistance to air flow. Walls must be drawn to create enclosed regions (zones). There is a set of implicit walls (actually floors) separating the zones on different levels. The walls will determine the size of the SketchPad — you can make the SketchPad larger than the screen and scroll to different areas. When dong a multi-level building it can be useful to define the largest level first.

If you are also planning to simulate the air handling system in detail, lay out the ductwork next because the ducts are created with a line drawing algorithm and are not permitted to cross any other features except walls. It is therefore easiest to draw the ducts first and then place the other icons as convenient. The next step is to name and define the numerical properties of the zones, such as temperature and volume, by placing a single zone icon in each of regions which have been defined by the walls and completing the zone data entry screens. Every zone region must be so identified. A default ambient zone surrounds the building.

An airflow path indicates some building feature by which air can move from one zone to another. Such features include cracks in the building envelope, open doorways, and exhaust fans. Path icons placed on the walls are used to represent openings between zones or to ambient; any other placement represents an opening in the floor to the zone on the level below. At this point it is probably reasonable to complete the definition of the airflow properties of the ducts. A simple model of an air handling system is also available with supply and return point icons placed within the appropriate zones. Once the complete set of zones and flow paths have been defined, it is helpful to do some steady state airflow simulations to check for possible errors in the building description.

Contaminant source (or sink) icons may be placed in any zone. These represent any feature (within the list of available models) which produces or removes a contaminant. Exposure icons are used to represent a person who may move to different zones according to a schedule. With this icon you may compute contaminant exposure and potential dose, and you can also create a simple contaminant source that moves between zones in time. These icons may be placed anywhere on the SketchPad.

4.2. Working with CONTAM Project Files

All data describing the airflow and contaminant source/sink characteristics of the building are stored in a "project" file. This is an ASCII file, for ease of transmission over a network, but the file is intended to be "read" only by the CONTAM program. This is similar to the relationship between a word processing program and the files it can create and edit; such files usually cannot be understood when viewed by another program.

While working on a building description, you will establish a *project name*. When you save the description to this disk, it will be stored as a *project file* named < project name > .PRJ. Therefore, a project name is limited by the characteristics of a DOS file name: it may be up to 8 character long and the name may not include periods, colons, back-slashes, or blanks. This project name is displayed at the top of the options area in the upper right corner of the screen.

You must keep track of the project/file names to avoid over-writing files and losing data. Project files can become rather large, but they are very compressible. A single design project will require many project files. When the design project is completed, archive the files to floppy disk using a file compression program, and remove the files from the local directory. This will simplify the search for a particular project file.

Project file operations are found under the F3 (project) menu option. The following things can be done from screen [040].

4.2.1. Saving a Project File This option saves the building description to the project file on disk. Note there is a shortcut, $\langle Alt \rangle S$, which can be used directly from the SketchPad. There are two minimum requirements that must be met before the project data can be saved: (1) a building level must be defined (4.6) and (2) the project must have a name (4.2.4). Whenever the project file is saved, the current

version of the file is copied to CONTAM.BKP before a revised project file is written. You may be able to use this file to restore a project file that has been corrupted in some way.

4.2.2. Clearing the SketchPad If you already have any part of a building description on the SketchPad, opening a new project would cause the loss of that data. This option lets you clear the SketchPad and clear the program memory for a new project.

4.2.3. Opening an Existing Project File You may retrieve previously prepared project data by entering an existing project name, i.e. the name of an existing project file in the local directory. If you do not know the name, press \leftarrow with the default field (or cleared field) to bring up a list of all project files in the local directory. As you move the cursor through the list, the description which you gave the file and the date the file was last updated appear in the status area.

4.2.4. (Re)naming a Project The name displayed here determines the file which will store the new data or changes you make in this work session. If the new project name is the same as the old project name, the data in the old project file will be over-written. You may or may not want that to happen. If you specify the name of an existing file, you will be warned that saving the file will overwrite the existing file.

4.2.5. Set Project Description Use the project description to give a very brief summary of the contents of the project file, for example how it varies from the base case. This line of data, up to 66 characters long, will later help you search through old project files.

4.2.6. Execute DOS Command You can also execute DOS commands from within CONTAM. This is particularly useful to change the default directory, or to copy files.

4.2.7. Quitting CONTAM Exiting the program is the final option on the project screen. Note there is a shortcut, $\langle Alt \rangle Q$, which can be used directly from the SketchPad. If you have made any changes to the building since the project file was last saved, a warning will be given allowing you save the project before exiting.

4.3. Configuring CONTAM96

Options to configure CONTAM are also found under the F3 (project) menu option. The following things can be done from screen [040].

4.3.1. SketchPad Size The SketchPad consists of an array of cells which can hold the various icons which CONTAM uses to describe the building. The SketchPad is displayed in a window which is 66 cells wide and 58 cells high. This array may be too small to conveniently display some buildings. Although you cannot change the size of the window, you can increase the width and/or height of the underlying SketchPad by up to a factor of eight.

The graphic display of pressures and flows makes it desirable to have a margin at least 5 cells wide around the building. The margins on all four sides are displayed at the top of the screen. These margins change as the SketchPad size is changed. You may also shift the entire pattern of icons representing the building in order to adjust the margins.

The following actions, (4.3.2) to (4.3.7), are accessed through the "set defaults" button which brings up screen [044] which has a series of options that takes you to other screens.

4.3.2. Default Display Units Most of the world, including NIST, uses S.I. units. However, in the United States it is still necessary to allow for other units. CONTAM permits a great deal of flexibility in units. Screen [050] lets you specify the defaults. "I-P" means "inch-pound". Most data entry screens allow you to make local changes in the units of an individual parameter.

Note that CONTAM always uses mass flow units when reporting flows - e.g., kg/s. When flows are expressed in volumetric units, these values are simply the mass flow divided by the density of air at standard conditions. Therefore, sL/s means "standard liters per second" which is a volumetric flow of dry air at standard conditions - 1 atm. & 20 C. Similarly, scfm means "standard cubic feet per minute" which refers to a volumetric flow at the same conditions - 1 atm. & 68 F.

4.3.3. Default Zone Temperature Most building zones will probably be at the same temperature. That value may also be entered on screen [050]. Changes for individual zones can be made later. You will also have the opportunity to reset all zone temperatures to the value you have entered here.

4.3.4. Keyboard and Mouse sensitivity may be adjusted at screen [052]. When you hold a key down, the keystroke is repeated to the screen. The repeating is controlled by two parameters: the delay before the first repeat is generated and the repeat rate. Valid delay values are 0 (0.25 s) through 3 (1.00 s). Valid repeat rates are 0 (30 char/s) through 31 (2 char/s). This keyboard sensitivity persists after exiting CONTAM.

Mouse sensitivity is given in terms of the distance (measured in 10ths of a millimeter) the mouse must travel to move the cursor between data entry fields or between cells on the SketchPad. Smaller values give greater sensitivity.

Normally, the left button corresponds to the Enter key and the right button to Escape. Specify a left-handed mouse to reverse that association.

4.3.5. Display Colors may be adjusted by the user at screen [054]. This is intended primarily as an aid for persons with color perception problems. You may recover the default colors at any time. The 14 modifiable colors (not including black and white) are described in terms of the amount of red, green, and blue displayed. Modify these numbers (0 to 63) to change the colors. It is especially useful to use <Alt> + and <Alt> - to incrementally change and display the colors.

4.3.6. External Libraries You may set the default library file names at screen [056]. There are four types of data elements which can be saved in library files:

weekly and daily schedules, wind pressure profiles, airflow elements, and duct elements.

You may create more than one of each class of library. These library files are stored in the directory containing the CONTAM.EXE file.

4.3.7. Saving the Configuration The configuration options (4.3.2) through (4.3.6) may be saved at your discretion. They will be stored in a file named CONTAM.CFG, which is stored in the same directory as the CONTAM.EXE file. Whenever the CONTAM program is started, it looks for this file and, if it exists, resets the program configuration from the default to the values you have saved.

4.4. Named Data Elements

Named data elements are used to minimize the amount of numerical data entered. Their use is described in section (3.5.3.5). This section describes the various types of named data.

4.4.1. Schedules are used to control or modify various simulation features as a function of time.

A week-schedule is made up of day-schedules where the numeric values are entered. There are 12 day-schedules: 1 (Sunday) through 7 (Saturday) plus five special schedules - 8 through 12 - which allow for holidays, etc. A weather file includes the day schedule number with each day's data.

Each day-schedule consists of a set of data points, each point consisting of a time and a schedule value, from 00:00:00 through 24:00:00. You may specify whether a value between the data points t_1 and t_2 will be computed by linear interpolation or is equal to the value at time t_1 .

4.4.2. Wind Pressure Profiles are used to account for the wind direction effects. See section (4.14) for a discussion of the wind pressure calculation.

You may enter up to 16 angle/pressure coefficient points. Values are in the range -1 to 1. The first value must be at angle 0 which is for a wind blowing directly toward the surface on which the opening lies. An identical value at angle 360 is automatically assumed. 90 degrees indicates a wind blowing parallel to the wall from the right, and 270 degrees would be from the left. By making these angles relative to the wall containing the opening, the same profile might be usable on different openings around the building.

4.4.3. Airflow Elements describe the mathematical relationship between the flow through some feature and the pressure drop across that feature. Several different models are available.

The powerlaw model permits airflow in only one direction through the path based on the direction of the pressure drop. There are three forms of the powerlaw equation, $Q = C (\Delta P)^n$, $F = C (\Delta P)^n$, and $F = C \sqrt{\rho} (\Delta P)^n$, where Q = volume flow rate, F = mass flow rate, ΔP = pressure drop, and ρ = air density. You may directly enter the values of C and n for these models.

CONTAM also allows you to create a powerlaw model from a physical description of some types of flow path, or from measured or tabulated data. The physical features include an orifice described in terms of an area and a discharge coefficient, a crack described by its length and width, a stairwell, and other large (e.g. elevator) shafts. The C and n coefficients of the powerlaw model can be computed from two measured (ΔP , F) data points or from a single data point if the value of n is assumed. The powerlaw model can also be created from the "connection" model used by the ASCOS program (Klote, 1981) or the "leakage area" data in Chapter 25, Ventilation and Infiltration, of the Handbook of Fundamentals (ASHRAE, 1997).

An alternative to the powerlaw model is the quadratic model (Baker, Sharples & Ward, 1987), which has two forms: $\Delta P = aQ + bQ^2$ and $\Delta P = aF + bF^2$. You may enter the coefficients, a and b, directly or let the program compute them from a detailed crack description or two measured data points.

The two-way flow models may be used to represent tall openings where the difference in air temperature on either side of the opening might cause two-way flows induced by the stack effect.

The backdraft damper flow models allow you to model a feature which has different flow resistances depending on the direction of the pressure drop. These models use the volume and mass flow [Q = C $(\Delta P)^n$ and F = C $(\Delta P)^n$] versions of the powerlaw model.

The "fan" models will be used to describe known or mechanically forced flows. Models provide for constant volume flow, constant mass flow, and the use of a fan performance curve (pressure versus flow rate).

4.4.4. Duct Elements describe, in addition to the flow-pressure relationship, the geometry of the duct and its leakage characteristics.

The most common duct model uses the Darcy-Weisbach relation and Colebrook's natural roughness function together with the geometry and roughness of the duct to compute the airflow resistance. See chapter 32, Duct Design, in the *Handbook of Fundamentals* (ASHRAE, 1997) and the duct database for more information. Other duct elements use some of the same flow-pressure models described in (4.4.3) for airflow elements. These include all three version of the powerlaw equation, all three fan models, and both backdraft damper models.

4.4.5. Filters are described in terms of the single pass filter efficiency for each contaminant. Efficiency is the fraction of contaminant (between 0.0 and 1.0) removed in a single pass through the filter.

4.4.6. Kinetic Reactions are a description of linear chemical reactions among the contaminants. The production or destruction of a contaminant α is given by $R_{\alpha} = \sum K_{\alpha,\beta} C_{\beta}$, where $K_{\alpha,\beta}$ are the reaction rate coefficients and C_{β} is the concentration of another contaminant β . CONTAM96 uses the convention that positive reaction coefficients produce an increase in contaminant concentration. The units of concentration are kg contaminant / kg air. The reaction coefficients are displayed in matrix form with the matrix displayed in two sections to fit it on the screen.

4.4.7. Contaminant Sources & Sinks represent any feature which produces, removes, or adsorbs a contaminant. Since the contaminants are specific to a given project file, source/sinks cannot be stored in library files.

The basic model is the constant coefficient model, $S_{\alpha} = G_{\alpha} - R_{\alpha} \cdot C_{\alpha}$, where S_{α} is the contaminant α "source strength" computed from the generation rate, G_{α} , removal rate, R_{α} , and concentration in the zone, C_{α} . Other models include a pressure driven model for contaminant sources which are governed by the inside-outside pressure difference, a cutoff-concentration model which may be appropriate for some volatile organic compound sources, a decaying source model which may be appropriate for other volatile organic compound sources, and a boundary layer source/sink model which may be used to model a reversible source/sink.
4.4.8. Occupancy Schedules are used to define where a person is as a function of time. Since the zones are specific to a given building, occupancy schedules cannot be stored in library files.

This occupancy schedule is made up of 12 occupancy day-schedules: 1 (Sunday) through 7 (Saturday) plus five special schedules - 8 through 12 - which allow for holidays, etc.

Each occupancy day-schedule consists of a set of data points, each point consisting of the time a person enters a zone and a pointer to the zone, from 00:00:00 through 24:00:00. The occupancy schedule may be defined by tracking the sequence of zones on the SketchPad.

4.4.9. Deleting Named Elements Unused elements accumulate in local lists of elements - they take up space and make it harder to look for the elements currently used. Unused elements can be deleted through the library menu, F6.

4.5. Using Library Files

Access to the lists and libraries of named data elements is through the F6 Library menu option which brings up screen [070]. There are four types of data elements which can be saved in library files: weekly and daily schedules, wind pressure profiles, airflow elements, and duct elements. You may create more than one of each class of library. These library files are stored in the directory containing the CONTAM.EXE file. You can select an existing library file or search a list of available library files. You can enter the name of a new file to create a new library. Each library is given a description that can be used to distinguish between various library files.

Library element data is used or revised through screen [072]. The body of the screen consists of the data elements arranged in alphabetical order in two columns, the library elements on the left and the local elements on the right. For each element there are buttons allowing you to:

- (a) delete the library element,
- (b) copy from the library to the local list,
- (c) copy from the local list to the library, or
- (d) delete the local element.

When the data for the local element is identical to the data for the library, an = sign is displayed between the two columns. You may not delete a local element that is referenced somewhere in the project file.

Saving the modifications you have made to the library is a separate operation which you must remember to do if you want to modify the library file. This separate operation does make it a little harder to accidentally modify the file.

Some data elements are stored in a list local to each project file and not in libraries. Screen [070] also lets you check these elements and delete those that are not used.

4.6. Working with Building Levels

The definition of and access to building levels is done by pressing the F8 key and processing the appropriate items on screen [080]. Each level is required to have a name, elevation, and height. When you create a new level, you may copy to it all the icons from another level. This is very useful for tall buildings where successive floors are very similar. You may also remove a building level. One

command allows you to move to another building level. Another command checks the completeness of the description of the current level.

4.7. Working with Walls

"Walls" are used to separate regions of uniform air temperature and contaminant concentration on a given level. Such walls include the building envelope and internal partitions with a significant resistance to air flow. Walls must be drawn to create enclosed regions -- zones. There is a set of



implicit walls (actually floors) separating the zones on different levels.

4.7.1. Drawing Walls may be done in two ways. Press **B** to draw a box — a rectangular enclosure. Move the cursor to the place where you want a box to start and press \leftarrow . Then move the cursor to position the opposite corner of the box. When you reach the correct size and shape, press \leftarrow .

Press W to draw almost any shape wall using the line drawing method described above. The broad colored line will be converted into a wall after pressing \leftarrow . The walls must always form complete enclosures (zones). Therefore, a wall cannot have an open or dangling end. It also may not be drawn across other building features except walls and ducts. An invalid wall shape or placement will be indicated by a warning message.

When you press B or W, the appropriate option will be highlighted in red to indicate that a line drawing mode is in effect. Press Esc at any time to exit the box or wall drawing mode.

Note: Walls are drawn on the odd numbered rows and columns of the SketchPad to avoid conflicts with the duct lines which are drawn on the even rows and columns. Therefore, the cursor may shift when you invoke a line drawing mode.

4.7.2. Deleting Walls A wall can be deleted by moving the cursor to the wall pressing Del. The section of wall to be deleted is highlighted for confirmation.

4.7.3. Modifying Walls Modify the positions or shapes of walls by adding and deleting. For example, if you want to modify figure (a) to figure (b), add line 1 and then delete line 2.



Modifying walls may require other icons to be moved. For example, in the modification above, if there is a zone icon within both the original area (a) and the expansion area (1), eliminating line (2) would put two zone icons within the same area. This is not permitted and will be indicated with an error message requiring that one of the zone icons be deleted.

4.8. Working with Zones

A "zone" indicates a volume of air with uniform temperature and contaminant concentration. Zones are defined on the SketchPad as a region surrounded by walls. Every zone must be identified with a single defined zone icon. A zone is defined by moving the cursor to the desired position in the walled region, adding the desired zone icon, and completing the zone data entry screen.

Zone Icons	

4.8.1. Zone Types - normal, phantom, ambient A "normal" zone icon, \square , is used to represent a zone which is separated by a floor from the zone below. A "phantom" zone icon, \square , is used to indicate that there is no floor to a particular region. That is, the region on this level is actually part of the zone below, and it, therefore, has the same temperature and contaminant concentrations. (Such a zone may be used to reprint a multi-story atrium.) An "ambient" zone icon, \square , represents the outdoor air. Such a feature is required to represent a courtyard. The ambient zone which surrounds the building has already been identified by the icon at the upper-left corner of the SketchPad.

4.8.2. Zone Icon Operations Move the cursor to the place in the walled region where you want the zone icon. Press Z to create a normal zone icon; press P to create a phantom zone icon; and press A for an ambient zone icon. You may not place two zone icons in the same region as defined by the walls. A zone icon may not be copied. You may move (3.4.2.7) a zone icon to any other blank cell in the walled region, i.e., you may not cross a wall.

4.8.3. Defining Zones You may define or revise the zone data by pressing \leftarrow while the cursor is on the zone icon and processing the zone data entry screen [90].

The zone must be given a name. All the zones on a single level must have unique names. The zone name is displayed in the status area and on reports as a reminder to you of what the zone represents. Specify a name accordingly. The zone temperature will be used in determining stack effects. A default zone temperature can be set in the project, F3, menu.

The zone air pressure relative to ambient can be specified as a constant. This option can be used to simulate a fan pressurization (blower door) test of a building. This process is described in section (4.18.3). It has also been useful in the development of analytic test cases. Otherwise, it probably should not be used in most simulations.

Zone volume is used in the dynamic contaminant calculations. Instead of the volume, you may enter a floor area which is multiplied by the height of the current building level to compute a volume. This area is not used for any other purpose by CONTAM. For phantom zones, the zone volume is set at the normal zone icon on the lowest level for the entire zone including the phantom zones on the levels above.

Enter the initial contaminant concentrations for dynamic simulations. The defaults are set in the project, F3, menu. Values can be reset in the simulation, F4, menu. The name of a kinetic reaction can be specified, if needed.

4.9. Working with Flow Paths

An airflow path indicates some building feature by which air can move from one zone to another. Such features include cracks in the building envelope, open doorways, and exhaust fans. The flow through most of these paths is determined by the air pressures in the adjacent zones and the flow characteristics of the path itself. The two zones that are connected by a path are determined by where the path icon is placed on the SketchPad. If the path icon is placed over a wall icon, it connects the zones on opposite sides of the wall. If it is placed in a blank cell (the "floor"), it connects the zone on this level with the zone on the level below. Therefore, there are several restrictions on the placement of flow paths: they may not



be placed on a wall corner, or connecting to a level that does not exist, or connecting a zone to itself.

4.9.1. Path Icon Operations To create a path icon, move the cursor to the position where you want the path and press the \mathbf{F} key. If the position is invalid, you will get a warning sound or message. Otherwise, this will create a red path icon of type (a).

Path icon deletion, copying, and moving proceeds according to the instructions in sections (3.4.2.2-4) with some special placement restrictions. A path that is on a wall may only be copied to another wall, and a path that is on a floor may only be copied to another floor.

4.9.2. Defining Paths You may define or revise the path data by pressing \leftarrow while the cursor is on the path icon and processing the path data entry screen [100]. Included in the path data is the elevation of the path above the elevation of the current building level, an optional named schedule which varies the resistance or flow as a function of time, an optional named contaminant filter, a wind pressure description for paths in the building envelope, and optional flow or pressure limits which can be useful in the design of a smoke control system.

The only required entry is the name of the airflow data element. Airflow elements can be stored in the external libraries (4.4.3). The type of flow element will determine the shape of the path icon. One-way flows are represented by path icon types (a) and (b). Two-way flows are represented by path icon types (c) and (d). The user selects between these pairs of icons to visually differentiate between small and large openings. The mathematical characteristics of the opening are determined by parameters of the flow element being used. Flow elements which represent fans use icon types (e) through (h) which indicate the normal direction of flow.

4.10. Working with a Simple AHS

The simple air handling system (AHS) provides a means of approximating the operation of most air handling systems without going into the details of describing the duct network. It consists of 2 implicit airflow nodes (return and supply), 3 implicit flow paths (recirculation, outdoor, and exhaust air), and multiple supply and return points in the



building zones. The implicit nodes and flow paths do not appear on the SketchPad, but are represented in the AHS model depicted below:



A filter can be placed in the outdoor air path or in the recirculation air path. It is not necessary to have both supply and return points in a system. That is, you may create a system that only supplies air into or exhausts air from the building. It is also not necessary to exchange air with the ambient zone, i.e., you can use an AHS to move air from one or more zones to other zones in a different part of the building.

4.10.1. The AHS Algorithm The system algorithm operates by summing all the supply flows, $\sum F_s$, and all the return flows, $\sum F_r$. These are the flows from the supply node and to the return node of the AHS. The amount of outdoor air that gets mixed with the recirculated air is determined in the following manner:

 $F_o = max(f_o \cdot \sum F_s, min(\sum F_s, m_o)),$ where

 F_{o} = the "outdoor air needed",

 f_{\circ} = the "fraction outdoor air" input parameter, and

 $m_o =$ the "minimum outdoor air flow" input parameter. The amount of recirculated air is: $F_R = min(\sum F_r, \sum F_s - F_o)$. The actual outdoor air delivered is: $F_O = \sum F_s - F_R$. The amount of exhaust air is: $F_X = \sum F_r - F_R$.

Note that when the sum of the supply flows exceeds the sum of the return flows, the balance is made up with outdoor air. Also note that any excess return air is exhausted. That is, a mass balance is always maintained within the AHS.

4.10.2. AHS Icon Operations The implicit nodes and paths are part of the AHS icon (a) which may be placed in any blank cell on the SketchPad. Move the cursor to the desired location and press **H** to create an AHS icon. Supply (b) and return (c) point icons must be placed within the appropriate zones. Move the cursor to the desired location and press **I** to create a supply icon or **O** to create a return icon. The AHS must be defined before any related supply/return points may be defined. The supply and return points may be copied to any valid position or they may be moved within the walls defining a zone. The AHS icon may not be copied but may be moved to any valid position, including outside the building.

4.10.3. Defining AHS Icons A unique name is required for each system so it can be referenced by the supply and return points as they are defined later. Optional data includes the fraction outdoor air, f_o , which is entered as scheduled data, the minimum outdoor air flow, m_o , the filter name(s) if present, the volumes of the supply and return zones (for contaminant calculation), and the initial contaminant concentrations in those zones.

Each supply or return point refers to the name of a previously defined system. The data for each supply/return point includes the design, i.e. maximum, airflow rate and an optional schedule to modify that flow as a function of time. A filter may also be specified and is placed in the implicit flow path between the supply/return point and the supply/return node.

4.11. Working with Ducts

The AHS provides a simple means for moving a specified, perhaps scheduled, amount of air between zones. It provides a reasonable model of an air handling system that is providing the specified flows, i.e., one where the system is properly balanced and the fan is overwhelming any other pressurizing effects in the building. You may want a more detailed model handling a broader range of conditions. For example, when the fan is off, the ductwork may provide flow paths between zones which are significant in relation to the normal construction cracks or openings. The duct model is designed for these more detailed cases.



Ductwork consists of duct segments (paths) and junctions or terminal points (nodes). Every duct segment begins and ends at either a *junction* with other ducts (icons a-d) or a *terminal point* where air goes from the ductwork to the surrounding zone (icons e-g) and *vice versa*.

4.11.1 Drawing Ducts Press D to enter the duct drawing mode. Move the cursor to the place where you want a duct segment to start and press \leftarrow . Then move the cursor to trace the path of the new duct segment which is shown as a special color. When you reach the spot where you want the duct segment to end, press \leftarrow . The broad colored line will then be converted into an undefined (dark red color) duct - a line of duct icons.

The junction/terminal icons (types a or e) at the end of each duct segment are created automatically as you press \leftarrow . Therefore, to split a single duct segment into two segments, press \leftarrow twice at the point where you want the junction. You can also create a terminal point that is isolated from the ducts on this

level but connected either up or down to ductwork on the next level by pressing \leftarrow twice at the desired location. Press Esc at any time to exit the duct drawing mode.

4.11.2 Deleting and Modifying Ducts Deletion of ducts is a two-step process. Pressing the Del key at a defined duct or junction will undefine it, converting the color from blue to red. Pressing the Del key at a undefined duct or junction will then delete it. The duct layout can only be modified at undefined duct icons. Therefore it is strongly recommended that you lay out the walls and the ducts before defining any icons -- modifications can be made without losing the duct definition data.

4.11.3 Defining Junction and Terminal Points Press \leftarrow while on the undefined junction or terminal point to start the definition process. Because of the way the SketchPad displays one level at a time, it cannot directly show ducts connecting junctions / terminals on different levels as ducts. Such connections are indicated on the SketchPad by distinctive icons. You may select:

icon (a) which represents a junction connected to ducts only on the same level;

icon (b) for a junction connected by a vertical duct to a junction on the level above;

icon (c) for a junction connected to a junction on the level below;

icon (d) for a junction connected to junctions both above and below;

icon (e) for a terminal point connected dy a duct to a junction on the same level;

icon (f) for a terminal point connected to a junction on the level above;

icon (g) for a terminal point connected to a junction on the level below.

The junction temperature and elevation will be used to determine how duct flows respond to, and influence, the building stack effect. When a duct terminal point is placed in the ambient zone, it represents a supply or exhaust point. These points are subject to wind pressure in a manner just like flow paths in the building envelope. When a connection to the level below is selected, the characteristics of the connecting duct will also be specified.

4.11.4 Defining Ducts Press \leftarrow while on the undefined duct to start the definition process. In addition to the red-to-blue color change, the defined duct icons will be modified into an arrow shape which indicates the direction of "positive" flow. The volume of a junction is determined from the volumes of the related duct segments.

The name of the duct data element is required. Duct elements can be stored in the external libraries (4.4.4). The duct element data includes the flow resistance (or forced flow) characterics of the duct, its cross-sectional geometry, and an optional leakage per unit length. This information is combined with segment specific data such as length and dynamic losses to determine the frictional resistance, volume, and leakiness of the duct segment.

The presence of a filter can be specified by entering a filter element name. The schedule is a special multiplier which can change the flow characteristics of the duct as a function of time. This is probably appropriate only for a fan element. In the cases of fans it is necessary to know which direction is defined as positive. The arrows indicate the positive direction for pressure rise and flow.

The duct leaks are merged into a single point at each junction -- for a duct segment that means half of the leakage to one junction and half to the other. The leakage between the junction and the zone containing that junction (as determined on the sketchpad) is a function of the leakage characteristics and the pressure difference between the junction and the zone. Put at least one junction in each zone that the duct passes through.

4.12. Working with Contaminants is best done after the building and all airflow paths (including ducts) have been defined and then tested with a steady state simulation.

4.12.1. Define Contaminants under the F3 (project) menu option. Transfer to screen [042] and define each contaminant by a name, molecular weight, decay constant, default concentration, and the units used to report the concentration. The default concentrations will be used as the initial zone concentrations and the ambient concentrations for steady state simulations. The initial zone concentrations can be modified either at the zone icon (4.8.3) or before a simulation under the F4 menu option. The units may be redefined at any time -- this is useful especially when you want different units when viewing or printing the simulation results.

4.12.2 Contaminant Sources and Sinks represent any feature which produces or removes a contaminant within the list of available models. They are indicated by icons which may be placed in any zone except ambient. A contaminant icon is defined by moving the cursor to the desired position in the walled region, pressing the S key, and then completing the contaminant data entry screen.



You may move a contaminant source icon as long as the icon remains

in the zone where it started. You may copy a contaminant source icon to any blank cell except one in the ambient zone.

Define or redefine any source sink icon by moving the cursor to the icon and pressing the \leftarrow key. This will open data screen [110] which requires you to name a source/sink element and lets you specify a schedule and multiplier. Creation of, and access to, the named elements is similar to the method used for all other named elements, except source/sink elements are not stored in an external library.

4.13. Working with Occupant Exposures

The exposure icon is used to represent a person who may move to different zones according to a schedule. With this icon you may compute contaminant exposure and potential dose, and/or you can create a simple contaminant source that moves in time.

4.13.1 Exposure Icon Operations This icon will be created at the current cursor position by pressing the X key while in either the *normal* or the *results presentation* mode. In the latter case the exposure is computed from the contaminant concentrations previously simulated. When the icon already exists at simulation, exposure values are computed during the simulation. Since the person moves through the building, the location of this icon is not significant. That is, it may be placed in any open SketchPad cell. The icon may be moved but not copied.

4.13.2 Defining Exposure begins with a description for each personal exposure icon using screen [190]. This description will accompany any reports generated and it will appear in the status area when the SketchPad cursor is at the personal exposure icon.

You must define (screen [170] and [172]) the occupancy schedule which tells where the person is. This can be done graphically (screen [176]) by tracking the person's position on the SketchPad. The schedule can also be reviewed graphically but must be modified by text input through screen [178]. Two special zone names are provided: "ambt" indicates the person is in the ambient zone and, therefore, exposed to the ambient concentrations, while "null" indicates the person is not in any zone in the model and, thus, not exposed to any contaminants.

In some cases you may be interested to contaminants generated by the occupants, or you may want to represent a contaminant source which moves through the building. You can specify contaminant generation rates and schedules which will assigned to zones according to the occupancy schedule using the exposure icon.

Body weight and inhalation rates are used to compute potential dose. Inhalation is defined in terms of a peak rate and a schedule. Body weights for typical persons and inhalation values $[m^3/h]$ for different activity levels are available in the *Exposure Factors Handbook* (EPA, 1989).

4.14. Working with Wind

Wind pressure can be a significant driving force for infiltration. It is a *complicated* function of wind speed, direction, building configuration, and surroundings. For a general introduction see Chapter 15, Airflow Around Buildings, in the *Handbook of Fundamentals* (ASHRAE, 1997, pp 15.1 - 15.8).

The equation for wind pressure (ASHRAE, 1997, p 15.3) is

$$P_{w} = \frac{\rho V_{H}^{2}}{2} \cdot C_{p} \tag{1}$$

where V_H is the wind speed at the top of the upwind wall (usually the height of the building). A general method of specifying wind pressures has been implemented in CONTAM96, but it does require a significant amount of effort from the user. A method is provided to check for input errors by reviewing the computed wind pressures. Wind pressures may be entered as constant values or may be computed by the program from

$$P_{w} = \frac{\rho V^{2}}{2} C_{h} f(\theta)$$
⁽²⁾

where

 ρ = ambient air density,

V = reported wind velocity,

 C_h = a coefficient accounting for terrain and elevation effects, and

 $f(\theta)$ = a function of the relative wind direction.

The relative wind direction is given by

$$\Theta \equiv \Theta_w - \Theta_s \tag{3}$$

where

 θ_{w} = wind azimuth angle (N = 0, E = 90, etc.), and

 θ_{s} = surface azimuth angle.

The $\rho V^2/2$ term in equation (2) is computed by CONTAM from the steady state or weather file temperature, pressure and wind speed data. The C_h term, which accounts for the difference between V and V_H , is entered by the user. The pressure coefficient, C_p , used by ASHRAE is equivalent to $f(\theta)$ in the CONTAM formulation. See Swami and Chandra (1988) for pressure coefficient data.

4.14.1 Defining Wind Pressures in CONTAM Wind pressures may be defined only for flow paths which connect building zones to the ambient "zone", and for duct terminal points which are in the ambient zone. You may select how the wind pressure will be computed. The first choice is no wind pressure. The second choice will transfer you to data entry screen [140] to set a constant wind pressure, i.e., one which is independent of wind speed and direction. The third choice will transfer you to data entry screen [142] to set the coefficients for equation (2) for a variable wind pressure.

Screen [142] calls for three inputs. The "wind pressure modifier" represents the value C_h in equation (2). The "wall azimuth angle" and "wind pressure profile" are used to define $f(\theta)$. The profile is displayed at the bottom of this screen.

Use the following formula for the wind pressure modifier, C_h :

$$C_h = A_o^2 \left(\frac{H}{10}\right)^{2a} \tag{4}$$

where H is the wall height and A_o and a depend on the terrain around the building (ASHRAE, 1989, p 14.3):

urban-- $A_o = 0.35$,a = 0.40.suburban-- $A_o = 0.60$,a = 0.28;airport-- $A_o = 1.00$,a = 0.15.

The wind speed, V, is usually measured at an airport (open terrain) at an elevation, $H_m = 10m$, above the ground. The wind speed, V_o , at that same elevation at the building site is given by

$$V_o = A_o V \tag{5}$$

The wind speed, V_H , at the top of the wall, elevation H, is then given by

$$V_{H} = V_{o} \left(\frac{H}{H_{m}}\right)^{a} \tag{6}$$

Equation (4) is obtained by substituting equations (5) and (6) into (1) and then comparing to equation (2).

Note: The value for C_h will typically be constant for all openings on a given building. You can modify the default value for C_h by F7 weather \rightarrow set building wind-related values. Data entry screen, [058], sets the values of H, A_o , and a in equation (4) and even allows you to reset previously defined values for C_h .

The "wall azimuth angle" is defined as the direction the wall faces with north being 0°, east 90°, south 180°, and west 270°. A default azimuth angle is provided based on the orientation of the wall on the SketchPad with the top of the SketchPad being north. You will have to change the azimuth angle for walls on non-rectangular buildings. For a rectangular building which is rotated from the cardinal directions, you can modify the default orientation of screen north by F7 weather \rightarrow set building wind-related values \rightarrow relative north. Changing this default can also change the azimuths of walls already defined.

The wind direction as used with the steady-state or transient weather data must be defined in a similar manner. When the wind blows from the north, its angle is 0° ; from the east is 90° , etc. The angle of the wind is the direction it is blowing from. The angle of the wall is the direction it is facing toward.

The wind pressure profile is defined with data screen [144]. The profile is named so a single profile may be used for multiple flow paths. This screen allows the definition of $f(\theta)$ at up to 16 values of θ . It is critical to understand the meaning of θ , the *relative* wind direction. An angle of 0 means the wind is blowing directly toward the surface. An angle of 180 means it is blowing directly away from the surface. To figure out 90 and 270 think of yourself standing on the outside the building with your back against the wall/opening. When the wind blows from the right, that is 90; and when it blows from the left, that is 270.

4.14.2 Checking Wind Pressure Data Because of the complexity of the wind pressure data, CONTAM offers a simple visual check of how you have defined the wind pressure. While viewing the SketchPad, press < Alt > W to get into the wind pressure checking mode. Press F7 (weather) to set a wind speed and a wind direction using the entries in the middle of data screen [074].

When you return to the SketchPad, it will graphically display the wind pressures for all the paths for the conditions you have defined. As you move the cursor across a flow path, the computed wind pressure will also be shown. Remember that the wind pressures computed during the simulation will be based on either the steady-state or weather file conditions and not the wind pressure display conditions.

4.15. Working with Weather

Weather parameters (ambient temperature, barometric pressure, wind speed and wind direction) are important factors influencing building airflows. Depending on the type of simulation selected, you may need steady state or transient weather data.

4.15.1. Steady State Weather Data is specified on data screen [078] which is accessed from the F7 (weather) menu option via screen [074]. Be sure to use absolute barometric pressure instead of pressure corrected to sea level. If you do not know the absolute pressure, then enter the altitude of the building site on screen [076] (site data) and a default pressure will be computed. A type of day (1-12) is specified to determine which day is used when the simulation accesses any schedules.

4.15.2 Transient Weather Data is stored in files with a .WTH file name extension. This file contains time-dependent information on ambient temperature, wind speed and direction, and ambient contaminant concentrations. The weather file must be in the local directory. It is prepared external to CONTAM: the WEATHER.EXE program is provided to create a weather file, and W94TOW96.EXE is provided to convert a CONTAM93/94 weather file to the new 96 format.

4.15.3 Weather File Format (ASCII text) is described below because it may be necessary for the user to create a weather file from sources not already provided. In the listing below I1 indicates a character string, I2 indicates a short integer, I4 indicates a long integer, and R4 indicates a four-byte real number. The variable names refer to names used in the CONTAM code. Individual lines of data are separated by dashes.

```
HEADER DATA:
               /* weather file description (up to 78 characters long) */
I1 descr[];
               /* number of contaminants */
I2 nc;
for each contaminant:
              /* contaminant name (each on a separate line; in order) */
  I1 name[];
I2 start date; /* day of year */
I2 end date;
DAILY WEATHER DATA:
for each day:
                 /* day of year (1-365) */
  I2 dayofy;
                 /* month (1-12) */
  I2 month;
  I2 dayofm;
                 /* day of month (1-31) */
  I2 dayofw;
                 /* day of week (1-7) */
                 /* type of day (1-12) for schedules */
  I2 daytyp;
 I2 DSTind; /* daylight savings time indicator */
R4 suncos[3]; /* solar direction cosines */
  for each time:
                   /* from 00:00:00 through 24:00:00; step may be variable */
                   /* time-of-day [s] */
    I4 time;
   R4 tmpambt;
                   /* ambient temperature [K] */
                   /* barometric pressure (Pa) NOT corrected to sea level */
   R4 barpres;
                   /* wind speed (m/s); */
   R4 windspd;
   R4 winddir;
                   /* wind direction: 0 = N, 90 = E, 180 = S, ...; */
   R4 solhtot;
                   /* total solar flux on horizontal surface [W/m^2] */
   R4 solhdif;
                   /* diffuse solar flux on horizontal surface [W/m^2] */
   R4 tskyeff;
                   /* effective sky temperature [K] */
    for each contaminant; in order:
      R4 CC;
                     /* mass fraction [kg/kg] */
```

The solar and sky values are not used in CONTAM96. They are reserved for a future version of the program with thermal analysis.

4.16. Controlling a Simulation

Menu option F4 (simulate) lets you define the type of simulation to be performed and then start the simulation from data screen [060].

4.16.1. Run Control options on screen [062] let you define the type of simulation to be performed. You may specify either a steady-state or transient calculation of the airflows. A steady-state contaminant simulation may only use steady airflows. Transient and cyclic contaminant simulations may use steady or transient airflow simulation with certain restrictions. A cyclic simulation repeats a 24-hour cycle until steady-periodic conditions are achieved, i.e., the contaminant concentrations at the end of the day match those at the beginning. A transient simulation may run for all or some days of the weather file, or for a single day with steady-state airflows.

If you have specified a steady-state airflow simulation, you can reset the steady-state weather data through screen [078] as described in section (4.15.1). Transient flow simulation requires a weather file which is specified by name. If you do not know the name, press \leftarrow with a blank name to search the list of weather files in the local directory.

A steady flow simulation uses the date and time to select control schedule values for any controlled elements. A transient flow and contaminant simulation begins at the initial date/time and ends at the final date/time.

A transient or cyclic simulation produces a "restart file" (< project > .RST) which records the complete simulation status at midnight of each day. You may use the restart file from a previous simulation to run a short (one or a few days) transient simulation and produce more output than is practical for a long transient simulation.

The "simulation time step" is the constant time step for the transient or cyclic simulation. Shorter time steps are more accurate but require more computation time. During the simulation the screen is updated at every "display time step".

4.16.2. Simulation Outputs are saved to binary files as the simulation proceeds. Data screen [064] lets you define the type of outputs generated. Reviewing the results will be described in section (4.17).

Detailed results for airflows and/or zone contaminant concentrations are saved to the < project > .SIM file. These data will be used to display airflow results on the SketchPad or as graphs of transient values. Output is created at every "listing time step" which must be an even multiple of the simulation time step shown in parentheses. Shorter steps allow you to see the results in more detail, but they create a larger simulation results file.

For long transient simulations it may be better to request the "summary data" for flows, contaminants, and exposures. These results will be presented graphically as "box-whisker data" which shows the average value, maximum and minimum values, and standard deviation of the values for all simulation time steps. For multi-day runs, daily displays are available in addition to the final summary.

4.16.3. Numeric Parameters on screen [066] allow you to reset several parameters that control the computational process. These are options for the advanced user. They are described in the on-screen help.

4.16.4. Other Run Control Parameters include an opportunity to easily reset all the initial zone contaminant concentrations. They can be reset to zero or to their default values (see 4.8.3). Resetting to current results is especially useful for cyclic simulation, where you may (1) continue a simulation that has been interrupted before convergence, (2) continue simulation with tighter convergence criteria, or (3) create a project file for archive which can be rerun as a one-day transient to quickly compute cyclic results.

You can create an input file for the batch simulation program CONTAMX. This would be useful if you find that you want to do several simulations which are too long for convenient interactive processing. You can create a batch file to execute several CONTAMX runs at consecutively. You can also create an input file for use with the TRNSYS program. There are restrictions on the features which can be simulated by TRNSYS.

The final option on screen [060] is to start the simulation. If this would result in replacing some results files, you will be given a warning with the option to not proceed with the simulation, in which case you would probably rename the project file of the prior results files before doing the simulation.

4.16.5. Running the Simulation The current simulation date and time are displayed while the simulation is running. You may press <Alt>P to pause the program and initiate a proper termination of the simulation.

Warning! Pressing $\langle Alt \rangle Q$ would terminate program execution and return to DOS, but this will leave invalid $\langle project \rangle$.SIM, .SUM, etc. files in the directory which must be deleted before the project can be processed by CONTAM.

4.17. Reviewing Simulation Results

The results available for review will depend upon the selections made in section (4.16.2) before the simulation was run. Viewing results requires that CONTAM be in the "results mode" initiated with the <Alt>R command. At the end of a simulation the program is automatically put in results mode. This also happens when a project file that has matching results files is opened. While in results mode you may not make substantial revisions to the SketchPad — that requires the normal, <Alt>N, mode.

While in the results mode, the simulation time and important scaling information will be displayed in the lower right corner of the screen. You may use the home and end keys to move the results display ahead and back through time. Use < Ctrl> End to advance to the end of the day and < Ctrl> Home to return to the start of the day.

4.17.1 Path and duct results are based on saving the "detailed results for airflows." This will provide an on-screen display of the flow and pressure drop for every flow path plus flows to or from the ducts. Moving the cursor to a path or duct icon will cause the display of the flow and pressure drop values in the status area. If you have set flow or pressure limits (4.9.2) that have been exceeded, there will be a red warning signal at the path icon. For a transient simulation results move the cursor to the path icon and press \leftarrow which will lead through screen [106] to a graphic display of the flow and pressure drop for the entire day.

4.17.2 Zone results include age-of-air and contaminant concentrations. The "age-of-air" refers to mean time since the air molecules in the zone entered the building. Short values indicate high ventilation rates. In CONTAM age-of-air is computed from a formula (see Roulet and Vandaele, 1991) assuming steady state conditions. If you have saved the detailed results for airflows, press < Alt> A and the age-of-air will be computed using the flow values for the current time. This value will be displayed when you move the cursor to the zone icon. (Note: calculating the age-of-air involves inverting a matrix. This can be time-consuming for building with many zone and duct junctions.)

Press \leftarrow at the zone icon to bring up screen [092] which allows access to a screen showing the transient contaminant concentrations for the day, a summary of contaminant concentrations for the run, and a summary of age-of-air values for the run, depending on the simulation results that have been saved.

4.17.4 Exposure results can be computed while in the results mode, and more accurate results can be computed during the simulation for summary results display. If detailed contaminant concentrations have been saved, you can create an exposure icon (4.13) and use it to display transient exposures for each contaminant. When the icon exists before the simulation and exposure summaries have been requested, the summary values are computed at the simulation time step (4.16.1) rather than the (usually longer) listing time step (4.16.2).

4.17.5 Report and export files may be created to save the simulation results in a more permanent form. Menu option F5 (output) lists several options for writing different types of results to files. "Report files" are simple ASCII files; "export files" are comma/quote delimited files suitable for import into spreadsheet programs. In addition, summary results in (4.17.3) and (4.17.4) may also be written to report files. When you specify the name of an existing output file, you have the option of replacing the file or appending the current output to the end of the file.

4.18. Special Simulation Features

This section includes instructions, or considerations, for using CONTAM to simulate several different building features.

4.18.1. Shafts

Buildings contain several architectural features which offer very low resistance to airflow between building levels. These features include atria, elevator shafts, and stairwells. CONTAM provides two ways of modeling such a low resistance path: the phantom zone and the low-resistance (or large) opening. Select the most appropriate model based on how this path interacts with the rest of the model.

This interaction can be understood by using three flow resistances in series to model a shaft between two levels. There is a resistance to flow through the shaft and resistances representing the paths (doors) connecting the shaft to the two different levels. Using the powerlaw relationship, $Q = C(\Delta P)^{1/2}$, and assuming C = 3.10 for the shaft, 1.55 for an open door, and 0.01 for a closed door, the following equivalent flow coefficients, $C_e = (\Sigma C_i^{-2})^{-1/2}$, are computed for four different assumptions:

- (1) both doors closed, ignore shaft resistance: $C_e = 0.007070$
- (2) both doors closed, include shaft resistance: $C_e = 0.007066$
- (3) both doors open, ignore shaft resistance:
- $C_{e} = 1.096$ (4) both doors open, include shaft resistance: $C_{e} = 0.984$

Cases (1) and (2) show that when flow resistance is dominated by the closed doors, it is not necessary to include the shaft flow resistance. Cases (3) and (4) show that when the resistances at the (open) doors is of the same order as the shaft resistance, it is important to include the shaft resistance in the model. For a quick estimate of relative flow coefficients, remember that the flow coefficient is usually roughly proportional to the opening area.

4.18.1.1 Atria

If an atrium were modeled as individual zones on each level, the inter-level flow resistances would be very low. A cursory comparison of the inter-level opening areas to the sum of all openings from the atrium to other zones will usually indicate that an atrium should be modeled using CONTAM's phantom zone procedure. This is done by placing a standard zone icon at the atrium's lowest level. This icon will define the atrium temperature and total volume. Place a phantom zone icon at all higher levels which contain parts of the atrium. A phantom zone icon indicates that the region within the walls on this level are actually part of the zone on the level below the icon. The volume of a space defined by phantom zones is entered at the standard zone icon which represents that space on its lowest level. Enter the volume of the entire space; ignore the floor area value. If it is necessary to have different temperature or contaminant concentrations at the different levels in an atrium, then those levels must be modeled as individual(normal) zones connected by very large openings.

4.18.1.2 Stairwells

Achakji and Tamura (1988) provided data to describe the airflow characteristics of a stairwell in terms of an equivalent orifice. This is a perfect representation for CONTAM, which allows you to create a powerlaw flow element from the physical characteristics of the stairwell. These include the cross-sectional (horizontal) area of the stairwell shaft, whether the fronts of the stair treads are open or closed, and the number of people on the stairs. This last item might be important in an evacuation scenario. Since the equivalent orifice area of the shaft is on the same order as it's cross-sectional area, and this area is likely to be smaller than the sum of the areas of the doors entering the stairwell, it is generally best to model a stairwell as individual zones on each level connected by openings which have been defined CONTAM's Achakji/Tamura model.

4.18.1.3 Elevator Shafts

Elevator shafts (hoistways) will generally lie in some modeling regime intermediate between stairwells and atria. Measured data for the flow resistance of an elevator shaft have not yet been identified. CONTAM provides a powerlaw flow element based on flow resistance from the Darcy/Colebrook model of a conduit or duct. A significant difference between an elevator shaft and a stairwell is that the door between the shaft and the building is never fully open because, when it is open, air must flow through openings in the elevator car to pass between the building and the shaft. In several computational examples, Klote and Milke (1992) indicate the equivalent orifice area for closed elevator doors is about 0.15 m². This is fairly small compared to the cross-sectional area of the shaft, especially for hoistways with multiple cars, so it is likely that the airflow in most elevator shafts can be modeled with sufficient accuracy by phantom zones. However, it may be necessary to split the shaft into several sections to achieve sufficient accuracy in modeling contaminant transport.

4.18.1.4 Convergence

The relative magnitudes of the flow coefficients have some effect on the convergence of CONTAM's nonlinear equation solver (Wray & Yuill, 1993). Airflow networks containing paths whose resistances differ by many orders of magnitude will typically require more iterations than networks with paths of similar resistances. Convergence of these more difficult cases can often be helped by reducing the relaxation coefficient from its default value of 0.75 to a value nearer one-half. The maximum number of iterations can also be increased. However, the most effective way to improve convergence is to remove those very low resistance paths that are not likely to effect the computed airflow rates. That is, replace the zones and large openings model of a shaft with the phantom zones model.

4.18.1.5 Shaft Report

Because of the importance of shafts for some smoke control systems (Klote & Milke, 1992), CONTAM provides a special reporting feature for shafts. The shaft report is created in three phases while the program is in results mode. The shaft is defined in the first phase, displayed in the second phase, and written to a file in the third. To begin the shaft, press S. Then move to the icon of the zone representing the shaft and press \leftarrow . If there is a zone icon in the same position on the level above or below the current level, those zones will be part of the shaft. The shaft consists of all contiguous levels having a zone icon in the same location on the SketchPad. Then move the cursor to the primary path of interest, e.g. the one representing the stairwell door, and press \leftarrow . The shaft report will display pressure drop and flow information on every level of the shaft where there is a path icon in the same location on the

SketchPad. This is displayed on the left side of the report. A secondary path can be defined in the same manner which will be displayed on the right side of the report. As soon as the secondary path is defined, the shaft report is displayed on the screen. You can scroll to view all of a tall shaft. You can save the shaft report to a report file by entering the name of the file.

Because of the way the elements of the shaft report are defined, it is important to place the icons correctly as the sketch is created. The level-copy (from F8) command automatically creates icons in the same positions on different levels. The zone and path icons can also be moved from their original placement to customize the shaft definition. For a stairwell pressurization system, you may want to record the pressurization flows by creating a simple AHS model with supply points in the shaft. Make these supply points the secondary path. You may use supply point icons aligned on every level with some or most of the flows set to zero, or you may use icons only on those levels with a pressurization flow. Alternatively, for shafts on an exterior wall of the building, you may wish to use the constant flow rate path elements through the exterior wall to provide the pressurization air. This type of flow path will also report the pressure difference between the shaft and ambient. You may want to align these constant flow paths above the open doorway on the first level.

4.18.2. Chimneys

A duct can be used to create a simple chimney model. At its simplest this will involve only a single duct connecting the inside of the building to the outside with the Darcy-Weisbach element used to model the flow resistance of the chimney. The height of the duct terminal points must reflect the height of the chimney and a special high temperature zone must be created around the inside terminal point so that the proper stack effect will result. Be sure to allow an appropriate low resistance path from this special zone to the rest of the building.

4.18.3. Building Pressurization Test

The building pressurization test (often implemented as a "blower door test") is a common way of determining the airtightness of a building's envelope. "Fan pressurization is relatively quick and inexpensive and it characterizes building envelope airtightness independent of weather conditions. In this procedure, a large fan or blower is mounted in a door or window and induces a large and roughly uniform pressure difference across the building shell." (ASHRAE, 1997, p 25.15; CGSB 1986; ASTM Standard E 779) A common airtightness rating is the airflow rate at 50 Pa divided by the building volume to give units of air changes per hour.

You may wish to do a simulated pressurization test to determine the airtightness rating of the building as described by CONTAM. This is easily done by setting one of the zones on the zero elevation level to a constant pressure of 50 Pa, running the simulation, and then observing the total airflow out of that zone. (Don't forget flows to other building levels.) Use standard m^3/h flow units and divide by the building volume to get the air change rate at 50 Pa. The flow rate at 4 Pa can be converted to ELA using equations in Chapter 25 of the *Handbook of Fundamentals* (ASHRAE, pp 25.15-16). Use the CONTAM results display to check that the building has been properly pressurized by moving the cursor to each path on the envelope to get the pressure drop reported on the status line. You can use the report of all flows (under F5) to get a listing of all flow and pressure drops. The pressure drop on every path to the ambient zone should be close to -50 Pa. The value is negative because of the default direction assigned for positive flow.

The reported pressure drop across various flow paths will not be exactly 50 Pa because of density effects. Minimize these differences by running all zones and ambient at the same (standard) temperature and no wind. Differences in pressure due to elevation make it critical that the constant pressure zone be on the level with zero elevation.

In a multizone building the effects of partitioning (internal walls and floors) usually are significant. There are two solutions depending on the goal of the simulation. If the goal is only to achieve a uniform pressure difference across the entire building shell, add some very large openings across each partition. If the goal is to reproduce a field test, simulate the internal doors as being open to get a relatively uniform pressure inside the building. Do either of these tests with a renamed copy of the project file so you do not have to reverse the changes to restore the original project file.

5. Contaminant Analysis

The CONTAM96 contaminant dispersal model is an implementation of Axley's (1987, 1988) methods. He states: "The central concern of indoor air quality analysis is the prediction of airborne contaminant dispersal in buildings. Airborne contaminants disperse throughout buildings in a complex manner that depends on the nature of air movements in-to, out-of, and within the building system; the influence of the heating, ventilating, and air-conditioning (HVAC) systems; the possibility of removal, by filtration, or contribution, by generation, of contaminants; and the possibility of chemical reaction, radio-chemical decay, settling, or sorption of contaminants. In indoor air quality analysis we seek to comprehensively model all of these phenomena."

The mass of contaminant α in zone i is

$$m_{\alpha,i} = m_i \cdot C_{\alpha,i} \tag{7}$$

where m_i is the mass of air in zone i and $C_{\alpha,i}$ is the concentration mass fraction of α . As previously stated, a zone is a region of uniform contaminant concentration which may correspond to a single room, a portion of a room, or several well-coupled rooms. Selection of the zones is a matter of engineering judgement. In CONTAM96 the contaminant concentration must be low enough so as not to significantly change the density of the air-contaminant mixture.

5.1 Solution of the Equations

Contaminant is removed from the zone i by:

(a) outward airflows at the rate $\sum_{i} F_{i,i} C_{\alpha,i}$ where $F_{i,j}$ rate of air flow from zone i to zone j,

(b) removal at the rate $C_{\alpha,i} R_{\alpha,i}$ where $R_{\alpha,i}$ is a removal coefficient, and

(c) first-order chemical reactions with other contaminants $C_{\beta,i}$ at the rate $m_i \sum_{\beta} \kappa_{\alpha,\beta} C_{\beta,i}$ where $\kappa_{\alpha,\beta}$ is the kinetic reaction coefficient in zone i between species α and β . (Sign convention: positive κ for generation and negative κ for removal)

Contaminant is added to the zone by:

(a) inward airflows at the rate $\sum_{j} (1 - \eta_{\alpha,j,i}) F_{j,i} C_{\alpha,j}$ where $\eta_{\alpha,j,i}$ is the filter efficiency in the path from zone j to zone i,

- (b) generation at the rate $G_{\alpha,i}$, and
- (c) reactions of other contaminants.

Conservation of contaminant mass for each species (and assuming trace dispersal - $m_{\alpha,i} \ll m_i$) produces the following basic equation for contaminant dispersal in a building:

$$\frac{dm_{\alpha,i}}{dt} = -R_{\alpha,i}C_{\alpha,i} - \sum_{j}F_{i,j}C_{\alpha,i} + \sum_{j}F_{j,i}(1-\eta_{\alpha,j,i})C_{\alpha,j} + m_{i}\sum_{\beta}\kappa_{\alpha,\beta}C_{\beta,i} + G_{\alpha,i}$$
(8)

This differential equation is approximated by a difference equation:

$$m_{\alpha,i}^{*} \approx m_{\alpha,i} + \Delta t \left[\sum_{j} F_{j,i} (1 - \eta_{\alpha,j,i}) C_{\alpha,j} + m_{i} \sum_{\beta} \kappa_{\alpha,\beta} C_{\beta,i} + G_{\alpha,i} - \left(R_{\alpha,i} + \sum_{j} F_{i,j} \right) C_{\alpha,i} \right]$$
(9)

where the * indicates a value at time $t + \Delta t$.

Instead of the generalized trapezoidal method used by Axley, CONTAM96 uses a fully implicit numerical approximation to solve equation (3):

$$\left[m_{i} + \Delta t \left(R_{\alpha,i} + \sum_{j} F_{i,j}\right)\right] C_{\alpha,i}^{*} - \Delta t \sum_{j} \left(1 - \eta_{\alpha,j,i}\right) F_{j,i} C_{\alpha,j}^{*} - m_{i} \Delta t \sum_{\beta} \kappa_{\alpha,\beta} C_{\beta,i}^{*} \approx m_{i} C_{\alpha,i} + G_{\alpha,i} \Delta t$$

$$(4)$$

 m_i is considered to be constant. Some special cases are handled by variants of the above equation. If zone i is specified as having no mass (e.g. in the ductwork), equation (4) becomes:

$$(R_{\alpha,i} + \sum_{j} F_{ij})C_{\alpha,i}^* - \sum_{j} (1 - \eta_{\alpha,j,i})F_{j,i}C_{\alpha,j}^* \approx G_{\alpha,n}$$

$$\tag{11}$$

Note that the kinetic reactions cannot be considered in this case. If a steady state solution is desired, equation (4) becomes:

$$(R_{\alpha,n} + \sum from j F_{i,j})C_{\alpha,i} - \sum_{j} (1 - \eta_{\alpha,j,i})F_{j,i}C_{\alpha,j} - m_i \sum_{\beta} \kappa_{\alpha,\beta}C_{\beta,i} \approx G_{\alpha,i}$$
(12)

If the mass flows and $R_{\alpha,i}$ should happen to be zero in equations (5) or (6), they cannot be solved. This case is handled by the simple expedient of letting $C_{\alpha,i}$ remain at its default value. These equations must be solved simultaneously for all zones and contaminants.

There are two major limitations in the equations presented above. First is constant zone air mass. This is consistent with the zone temperatures being constant and contaminant mass fractions being low. Second is the use of linear analysis which limits the kinds of kinetic reactions which can be modeled.

CONTAM96 maintains the same equation ordering for the contaminant equations as is used for airflows except that for each zone there is an equation for each contaminant species. These simultaneous linear equations for the implicit calculation of contaminant concentrations may be solved by any of three methods: a direct skyline algorithm, an the iterative biconjugate gradient (BCG) algorithm, or an iterative successive over-relaxation (SOR) algorithm (Press, *et.al.*, 1992). The skyline algorithm is the most reliable solution, and it is very fast for small problems but can be slow for large problems. The SOR algorithm requires much less memory and is faster unless there are convergence problems. In that case try the BCG solution. Before doing a long simulation, it may be useful to test the different methods to determine which will give optimum performance.

5.2 Contaminant Source/Sink Elements

CONTAM96 allows the user to define the generation, G_{α} , and removal, R_{α} , coefficients for some simple cases.

The general source/sink model (see data entry screen [270]) uses the following equation:

$$S_{\alpha} = G_{\alpha} - R_{\alpha} \cdot C_{\alpha} \tag{13}$$

where S_{α} is called the contaminant α "source strength". The CONTAM internal units for the terms in equation (7) are: $C_{\alpha} [kg_{\alpha} / kg_{air}]$, G_{α} , $S_{\alpha} [kg_{\alpha} / s]$, and $R_{\alpha} [kg_{air} / s]$. The user may express these values in a large number of units with automatic conversion to the internal values.

For a room air filtering device, G = 0.0 and $R = f \cdot e$ where f is the flow rate of the room air passing through the filter and e is the single pass removal efficiency of the device.

The pressure source/sink model (screen [272]) is intended to model contaminant sources which are governed by the inside-outside pressure difference, such as radon or soil gas entry into a basement. In this case the source equation is:

$$S_{\alpha} = G_{\alpha} \cdot (P_{ambt} - P_{i})^{n} \tag{14}$$

For volatile organic compounds the source equation is sometimes expressed in the form

$$S_{\alpha} = G_{\alpha} \left(1 - \frac{C_{\alpha}}{C_{cutoff}} \right)$$
(15)

where C_{cutoff} is the cutoff concentration (screen [274]) at which emission ceases.

Another source equation for volatile organic compounds is the exponentially decaying source (screen [274]) which is expressed in the form

$$S = G e^{-t/tc} \tag{16}$$

where:

S = the contaminant source strength,

G = the initial emission rate,

t = the time since the start of emission, and

 t_c = the decay time constant.

The boundary layer diffusion controlled reversible source/sink model (screen [278]) follows the descriptions presented by Axley (1991). The rate at which a contaminant is transferred into the sink is

$$h\,dA\,(C_i - \frac{C_s}{k})\tag{17}$$

where:

h = average film mass transfer coefficient over the sink,

d = film density of air, average of bulk & surface densities,

A = surface area of the adsorbent,

 C_i = concentration in the air,

 $C_s = concentration in the adsorbent, and$

k = Henry adsorption constant or partition coefficient.

6. Airflow Analysis

Over the years many methods have been developed to compute the building airflows which are necessary for the contaminant analysis. Feustel and Dieris (1992) report 50 different computer programs for multizone airflow analysis. Note than "zones" go by many other names in these programs, e.g., nodes, cells, and rooms are common alternatives. The airflow calculations in CONTAM96 are based on the algorithms developed in AIRNET (Walton, 1989a,b).

6.1 Basic Equations

The air flow rate from zone j to zone i, $F_{j,i}$ [kg/s], is some function of the pressure drop along the flow path, $P_i - P_i$:

$$F_{j,i} = f(P_j - P_i) \tag{18}$$

The mass of air, m_i [kg], in zone i is given by the ideal gas law

$$m_i = \rho_i V_i = \frac{P_i V_i}{RT_i} \tag{19}$$

where

 V_i = zone volume [m³], P_i = zone pressure [Pa], T_i = zone temperature [K], and R = 287.055 [J/kgK] (gas constant for air).

For a transient solution the principle of conservation of mass states that:

$$\frac{\partial m_i}{\partial t} = \rho_i \frac{\partial V_i}{\partial t} + V_i \frac{\partial \rho_i}{\partial t} = \sum_j F_{j,i} + F_i$$
(20)

where

 $m_i = mass of air in zone i,$

 $F_{j,i}$ = airflow rate [kg/s] between zones j and zone i: positive values indicate flows from

j to i and negative values indicate flows from i to j, and

 F_i = non-flow processes that could add or remove significant quantities of air from the zone.

Such non-flow processes are not considered in CONTAM and flows are evaluated by assuming quasisteady conditions leading to:

$$\sum_{j} F_{j,i} = 0 \tag{21}$$

6.2 Solving the Equations

The steady-state airflow analysis for multiple zones requires the simultaneous solution of equation (4) for all zones. Since the function in equation (1) may be, and usually is, nonlinear, a method is needed for the solution of simultaneous nonlinear algebraic equations. The Newton-Raphson (N-R) method (Conte & de Boor, 1972, p 86) solves the nonlinear problem by an iteration of the solutions of linear equations. In the N-R method a new estimate of the vector of all zone pressures, $\{P\}^*$, is computed from the current estimate of pressures, $\{P\}$, by

$$\{P\}^* = \{P\} - \{C\}$$
(22)

where the correction vector, $\{C\}$, is computed by the matrix relationship

$$[J] \{C\} = \{B\}$$

$$(23)$$

where $\{B\}$ is a column vector with each element given by

$$B_i = \sum_j F_{j,i} \tag{24}$$

and [J] is the square (i.e. N by N for a network of N zones) Jacobian matrix whose elements are given by

$$J_{i,j} = \sum_{i} \frac{\partial F_{j,i}}{\partial P_{j}}$$
(25)

In equations (7) and (8) $F_{j,i}$ and $\partial F_{j,i}/\partial P_m$ are evaluated using the current estimate of pressure $\{P\}$. The CONTAM program contains subroutines for each airflow element which return the mass flow rates and the partial derivative values for a given pressure difference input.

Equation (6) represents a set of linear equations which must be set up and solved for each iteration until a convergent solution of the set of zone pressures is achieved. In its full form [J] requires computer memory for N^2 values, and a standard Gauss elimination solution has execution time proportional to N^3 . Sparse matrix methods can be used to reduce both the storage and execution time requirements. A skyline solution process following the method of Dhatt (1984, pp. 282-192) was chosen. This method can be used to solve equations with symmetric or nonsymmetric matrices. It stores no zero values above the highest nonzero element in the columns above the diagonal and no zero values to the left of the first nonzero value in each row below the diagonal. In this case the Jacobian matrix is symmetric.

Analysis of the element models will show that

$$|J_{i,i}| = \sum_{j \neq i} |J_{i,j}|$$
(26)

This condition allows a solution without pivoting, although scaling may be useful. Note that the degree of sparsity of the Jacobian matrix after factoring is dependent on the ordering of the zones. Ordering can be improved by various algorithms or rules-of-thumb. In AIRNET it was easy to define an airflow network which has no unique solution. The CONTAM graphic input makes it difficult to incorrectly connect the airflow elements in the network.

CONTAM allows zones with either known or unknown pressures. The constant pressure zones are included in the system of equations and equation (6) is processed so as to not change those zone pressures. This gives flexibility in defining the airflow network while maintaining the symmetric set of equations. A sufficient condition for the Jacobian to be nonsingular (Axley, 1987) is that all of the unknown pressure zones be linked by pressure dependent flow paths to (a) constant pressure zone(s). In

CONTAM the ambient (or outdoor) air is treated as a constant pressure zone. The ambient zone pressure is assumed to be zero for the flow calculation causing the computed zone pressures to be values relative to the true ambient pressure and helping to maintain numerical significance in calculating ΔP .

Conservation of mass at each zone provides the convergence criterion for the N-R iterations. That is, when equation (4) is satisfied for all zones for the current system pressure estimate, the solution has converged. Sufficient accuracy attained by testing for relative convergence at each zone:

$$\frac{|\Sigma_j F_{j,i}|}{|\Sigma_j|F_{j,i}|} < \epsilon \tag{27}$$

with a test $(\sum |F_{j,i}| < \epsilon_1)$ to prevent division by zero. The magnitude of ϵ can be established by considering the use of the calculated airflows, such as in an energy balance. In any case, round-off errors may prevent perfect convergence ($\epsilon = 0$).

Numerical tests of the N-R method solution indicated occasional instances of very slow convergence as the iterations almost oscillate between two different sets of values. In AIRNET, this was handled by a Steffensen acceleration process. More recent tests by the author and by Wray (1993) indicate that the use of a simpler constant under-relaxation coefficient produces a faster, reliable convergence acceleration process. Equation (5) for the iteration process becomes

$$\{\boldsymbol{P}\}^* = \{\boldsymbol{P}\} - \boldsymbol{\omega}\{\boldsymbol{C}\}$$
⁽²⁸⁾

where ω is the relaxation coefficient. A relaxation coefficient of 0.75 has been found to be usable for a broad range of airflow networks. This value is not a true optimum but appears to work quite well without the computational cost of finding the theoretically optimum value.

When convergence is progressing rapidly, under-relaxation ($\omega < 1$) slows convergence compared to no relaxation. To prevent this a global convergence value is computed:

$$\gamma = \frac{\sum_{i} |\Sigma_{j} F_{j,i}|}{\sum_{i} \sum_{j} |F_{j,i}|}$$
(29)

When $\gamma^* < \alpha \gamma$, ω is set to 1. Currently CONTAM uses $\alpha = 30\%$. This often reduces the number of iterations.

Newton's method requires an initial set of values for the zone pressures. These may be obtained by including in each airflow element model a linear approximation relating the flow to the pressure drop:

$$F_{j,i} = c_{j,i} + b_{j,i}(P_j - P_i)$$
(30)

Conservation of mass at each zone leads to a set of linear equations of the form

$$[\mathbf{A}] \{\mathbf{P}\} = \{\mathbf{B}\}$$
(31)

Matrix [A] in equation (14) has the same sparsity pattern as [J] in equation (6) allowing use of the same sparse matrix solution process for both equations. This initialization handles stack effects very well and tends to establish the proper directions for the flows. The linear approximation is conveniently provided by the laminar regime of the element models used by CONTAM. When solving a set of similar problems, as when approximating a transient solution by successive steady-state solutions, it tends to be preferable to use the previous solution for the zone pressures as the initial values for the new problem.

6.3 Airflow Elements

Infiltration is the result of air flowing through openings, large and small, intentional and accidental, in the building envelope. Simulation programs require a mathematical model of the flow characteristics of the openings. For a general introduction see Chapter 25, Ventilation and Infiltration, of the *Handbook* of *Fundamentals* (ASHRAE, 1997) and section 2.2 of *COMIS Fundamentals* (LBL report 28560, 1990).

Flow within each airflow element is assumed to be governed by Bernoulli's equation:

$$\Delta P = (P_1 + \frac{\rho V_1^2}{2}) - (P_2 + \frac{\rho V_2^2}{2}) + \rho g(z_1 - z_2)$$
(32)

where

The following parameters apply to the zones: pressure, temperature (to compute density and viscosity), and elevation. The zone elevation values are used to determine stack effect pressures. When the zone represents a room, the airflow elements may connect with the room at other than its reference elevation. The hydrostatic equation is used to relate the pressure difference across a flow element to the elevations of the element ends and the zone elevations, assuming the air in the room is at constant temperature. Pressure terms can be rearranged and a possible wind pressure for building envelope openings added to give

$$\Delta P = P_i - P_i + P_s + P_w \tag{33}$$

where

 $P_i, P_j = \text{total pressures at zones i and j}$ $P_s = \text{pressure difference due to density and elevation differences, and}$ $P_w = \text{pressure difference due to wind.}$

Equation (16) establishes a sign convention for direction of flow: positive is from zone j to zone i. Since the airflow elements will be described by a relationship of the form $w = f(\Delta P)$, the partial derivatives needed for [J] in equation (8) are related by $\partial w/\partial P_j = -\partial w/\partial P_i$ which establishes the relation in equation (9). Many forms of airflow elements are available in CONTAM through data entry screen [104].

6.3.1 Powerlaw Flow Elements

Most infiltration models are based on the following empirical (powerlaw) relationship between the flow and the pressure difference across a crack or opening in the building envelope:

$$Q = C \left(\Delta P\right)^n \tag{34}$$

The volumetric flow rate, Q [m³/s], is a simple function of the pressure drop, ΔP [Pa], across the opening. A common variation of the powerlaw equation is:

$$F = C \left(\Delta P\right)^n \tag{35}$$

where the mass flow rate, F [kg/s], is a simple function of the pressure drop. A third variation is related to the orifice equation:

$$Q = C_d A \sqrt{\frac{2\Delta P}{\rho}}$$
(36)

where C_d = discharge coefficient, and A = orifice opening area.

Theoretically, the value of the flow exponent should lie between 0.5 and 1.0. Large openings are characterized by values very close to 0.5, while values near 0.65 have been found for small crack-like openings.

The primary advantage of equations (17-19) for describing airflow components is the simple calculation of the partial derivatives for the Newton's method solution of the simultaneous equations:

$$\frac{\partial F_{j,i}}{\partial P_i} = \frac{n F_{j,i}}{\Delta P} \quad \text{and} \quad \frac{\partial F_{j,i}}{\partial P_i} = \frac{-n F_{j,i}}{\Delta P}$$
(37)

The sign in equation (20) will agree with the sign of F. However, there is also a problem with equations (20): the derivatives become unbounded as the pressure drop (and the flow) go to zero. A simple way to avoid this problem is suggested by what physically happens at low flow rates: the physical character of the flow (and the form of the equation) changes. It goes from turbulent to laminar. Equations (17-19) can be replaced by

$$F = \frac{C_k \rho \Delta P}{\mu} \tag{38}$$

where C_k = laminar flow coefficient, and μ = viscosity. The partial derivatives are simple constants:

$$\frac{\partial F_{j,i}}{\partial P_j} = \frac{C_k \rho}{\mu} \quad \text{and} \quad \frac{\partial F_{j,i}}{\partial P_i} = \frac{-C_k \rho}{\mu}$$
(39)

The origin of this laminar relationship is shown by the duct equations in the next section. This technique has been independently discovered and used by several researchers (e.g., Axley, 1987; Isaacs, 1980). Although there is physical reason for using equation (21) at low pressure drops, its purpose here is to assure convergence of the equations when ΔP approaches zero for one of the many flow paths in a complex network, instead of accurately representing airflows which are too small to be of interest. Because the linear flow expression is not used as a true flow model but as a mathematical artifice, it is not necessary to adjust its flow coefficient. Given the uncertainty in estimating the temperature of the air as it flows through an opening, especially a crack, this additional detail is of debatable usefullness.

The CONTAM functions for powerlaw elements calculate flows using both the laminar and the turbulent models and select the method giving the smaller magnitude flow. There is a discontinuity in the derivative of the $F(\Delta P)$ curve where the two equations intersect. This discontinuity is a violation of one of the sufficient conditions for convergence of Newton's method (Conte & de Boor, 1972, p 86). However, numerical tests conducted by the author for flows at that point using a small airflow network have shown no convergence problem.

Separate data entry screens are provided for each of the three powerlaw forms. The volume flow form (17) uses screen [232]; the mass flow form (18) uses screen [208]; and the orifice equation form (19) uses screen [200].

6.3.1.1 Temperature Dependence

It is useful to think of the coefficient C as a simple constant, C_{α} , evaluated at a particular set of conditions (μ_0 , ρ_0 and $\nu_0 = \mu_0/\rho_0$) multiplied by a correction factor to account for actual air properties. Equations (17-19) are converted to a common form and summarized below with their appropriate temperature correction factors.

$$\Delta P > 0 \qquad \Delta P < 0 \qquad \text{correction factor}$$

$$F_{j,i} = K_a C_a \rho_j (\Delta P)^n \qquad F_{j,i} = -K_a C_a \rho_i (-\Delta P)^n \qquad K_a = (\rho_o / \rho)^n (\nu_o / \nu)^{2n-1}$$

$$F_{j,i} = K_b C_b \sqrt{\rho_j} (\Delta P)^n \qquad F_{j,i} = -K_b C_b \sqrt{\rho_i} (-\Delta P)^n \qquad K_b = (\rho_0 / \rho)^{n-1/2} (\nu_o / \nu)^{2n-1} \qquad (40)$$

$$F_{i,i} = K_c C_c (\Delta P)^n \qquad F_{i,i} = -K_c C_c (-\Delta P)^n \qquad K_c = (\rho_o / \rho)^{n-1} (\nu_o / \nu)^{2n-1}$$

CONTAM uses the following formulae for computing ρ and ν :

 $\rho = P / (287.055 T)$ $\mu = 3.7143 \cdot 10^{-6} + 4.9286 \cdot 10^{-8} T$ $\nu = \mu / \rho$

Using reference conditions of standard atmospheric pressure and 20C gives $\rho_o = 1.2041 \text{ kg/m}^3$ and $\nu_o = 1.5083 \cdot 10^{-5} \text{ m}^2/\text{s}$ Temperature adjustment is set in the run control (F4) screen [066].

6.3.1.2 Fitting Powerlaw Coefficients

Experimental data can be used to determine the coefficients in the orifice form of the powerlaw equation:

$$F = \pm C_b \sqrt{\rho_0} (\pm \Delta P)^n \qquad (K_b = 1)$$
⁽⁴¹⁾

If n is known or can be assumed, C_b can be computed from the inverse of equation (24)

$$C_b = \frac{F}{\sqrt{\rho_0} \left(\Delta P\right)^n} \tag{42}$$

This form is available with data entry screen [210].

When two points $(F_1, \Delta P_1)$ and $(F_2, \Delta P_2)$, are known, n can be computed from:

$$n = \frac{\ln(F_1) - \ln(F_2)}{\ln(\Delta P_1) - \ln(\Delta P_2)}$$
(43)

with C_b then computed from equation (25). This form is available with data entry screen [212].

6.3.1.3 Leakage Areas

The powerlaw model can be used with the component leakage area formulation which has been used to characterize openings for infiltrations calculations (ASHRAE, 1997, pp 25.18,19). The leakage area is based on a series of pressurization tests where the airflow rate is measured at a series of pressure differences ranging from about 10 to 75 Pa. The effective leakage area is based on a rearrangement of equation (19)

$$L = \frac{Q_r \sqrt{\rho/2\Delta P_r}}{C_d} \tag{44}$$

where

L = equivalent or effective leakage area [m²],

 ΔP_r = reference pressure difference [Pa],

 Q_r = predicted airflow rate at ΔP_r (from curve fit to pressurization test data) [m³/s], and

 C_d = discharge coefficient.

There are two common sets of reference conditions:

 $C_d = 1.0$ and $\Delta P_r = 4$ Pa or $C_d = 0.6$ and $\Delta P_r = 10$ Pa.

A leakage area can be converted to the flow coefficient in the orifice equation (19) by

$$C_{h} = L C_{d} \sqrt{2} (\Delta P_{p})^{1/2 - n}$$
(45)

This equation requires a value for n. If it is not reported with the test results, a value between 0.6 and 0.7 is reasonable.

Data entry for leakage areas is done through screen [202].

6.3.1.4 Stairwells

A stairwell will normally be modeled as a vertical series of zones connected by low resistance openings through the floors. The CONTAM model for airflow in stairwells is based on a fit to experimental data presented by Achakji & Tamura (1988). They expressed the airflow resistance per floor as an effective area A_e in the orifice equation (19) with a 0.6 discharge coefficient. The effective area is expressed in terms of the area of the shaft A_s , the distance between floors h, the density of people on the stairs d, and whether the treads are open or closed. A large number of people on the stairs, as in an evacuation scenario, influences the flow resistance. The experiment used densities of 0, 1, and 2 persons/m². For open treads the effective area is approximately

$$A_{e} \approx A_{e}(0.089h)(1.0 - 0.14\sqrt{d})$$
⁽⁴⁶⁾

and for closed treads

$$A_{e} \approx A_{s}(0.083h)(1.0 - 0.24\sqrt{d})$$
⁽⁴⁷⁾

The coefficients for the powerlaw equation are

$$n = 0.5$$
 and $C_0 = 0.6 \cdot \sqrt{2} \cdot A_e$ (48)

The data entry for a stairwell is done in screen [206].

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6.3.1.5 Cracks

Clarke (1985, p 204) indicates a relationship for flow through cracks that can be converted directly into a powerlaw airflow element:

$$Q = ka(\Delta P)^n \tag{49}$$

where

$$n = 0.5 + 0.5 \exp(-W/2) \tag{50}$$

and

$$k = 0.0097 \cdot (0.0092)^n \tag{(51)}$$

with

W = crack width (mm), and a = crack length (m).

Therefore, n is in equation (20c) given by (33) and

$$C_b = \sqrt{\rho_0} \ a \ 0.0097 (0.0092)^n \tag{52}$$

The data entry for this form of crack is done in screen [230].

6.3.2 Quadratic Flow Elements

Baker, Sharples, and Ward (1987) indicate that infiltration openings can be more accurately modeled by a quadratic relationship of the form

$$Q,\Delta P > 0 \qquad Q,\Delta P < 0$$

$$\Delta P = A Q + B Q^{2} \qquad \Delta P = A Q - B Q^{2} \qquad (53)$$

This form can be used as an airflow element by solving the quadratic equation for $F (= \rho Q)$. Letting $a = A/\rho$ and $b = B/\rho^2$ allows equations (36) to be rewritten as

$$\Delta P = aF + bF^2 \qquad \Delta P = aF - aF^2 \qquad (54)$$

These quadratic equations solve as

$$F = \frac{\sqrt{a^2 + 4b\Delta P} - a}{2b} \quad \text{and} \quad F = \frac{a - \sqrt{a^2 - 4b\Delta P}}{2b}$$
(55)

with the partial derivatives given by

$$\frac{\partial F_{j,i}}{\partial P_j} = \frac{1}{a+2b|F_{j,i}|} \quad \text{and} \quad \frac{\partial F_{j,i}}{\partial P_i} = \frac{-1}{a+2b|F_{j,i}|}$$
(56)

Equations (38) require that b be nonzero to prevent a division by zero and equations (39) requires that a be nonzero to prevent a division by zero as F goes to zero. Data for the volumetric quadratic flow element is entered through screen [236], and data for the mass flow form uses screen [238]. There are contrary opinions that the powerlaw relationship is better.

6.3.2.1 Temperature Dependence

It is useful to think of the coefficients a and b as simple constants evaluated at a particular set of conditions (μ_0 , ρ_0 and $\nu_0 = \mu_0/\rho_0$) multiplied by correction factors to account for actual air properties as was done for the powerlaw equations. That is

$$A = \left(\frac{v}{v_0}\right) A_0$$
 and $a = \left(\frac{v}{v_0}\right) a_0$ (57)

and

 $B = \left(\frac{\rho_0}{\rho}\right) B_0 \quad \text{and} \quad b = \left(\frac{\rho_0}{\rho}\right) b_0 \tag{58}$

Note that $\rho_0/\rho = T/T_0$ for a perfect gas of constant composition.

6.3.2.2 Fitting Quadratic Coefficients

The quadratic coefficients can also be computed from measured flow and pressure data. Given two points $(F_1, \Delta P_1)$ and $(F_2, \Delta P_2)$, the values of a_0 and b_0 are:

$$b_{0} = \frac{\left(\frac{\Delta P_{1}}{F_{1}} - \frac{\Delta P_{2}}{F_{2}}\right)}{F_{1} - F_{2}}$$
(59)

and

$$a_0 = \frac{\Delta P_1}{F_1} - b_0 F_1 \tag{60}$$

The main advantage of the quadratic model over the powerlaw model is computation speed achieved by avoiding the slow power function. (Tests have shown pow(x) four to eight times slower than sqrt(x). This performance is hardware and software dependent.) It must still be determined which model is the most accurate representation for a particular airflow element. For example, it has been found that the powerlaw model is a better approximation for smooth ducts while the quadratic model is a better approximation for very large openings the derivatives (39) can become quite large leading to slow convergence of the simulatneous mass balance equations.

6.3.2.2 Crack Description

Baker, Sharples, and Ward (1987) give theoretical relationships between A and B and the physical characteristics of the openings. These are

$$A_0 = 12 \mu_0 z / L d^3$$
 and $B_0 = \rho_0 C / 2 d^2 L^2$ (61)

where μ = viscosity, ρ = density, z = distance along the direction of flow, d = crack width, L = crack length, and C = 1.5 + number of bends in the flow path. For the mass flow form of the equations (37) the coefficients are

$$a_0 = 12 \mu_0 z / \rho_0 L d^3$$
 and $b_0 = C / 2 \rho_0 d^2 L^2$ (62)

The data for this relationship is entered through screen [230].

6.3.3 Ducts

The theory of flows in ducts (and pipes) is well established and summarized in chapter 32 of the *Handbook of Fundamentals* (ASHRAE, 1997). More extensive treatment is given by Blevins (1984) in a long chapter on pipe and duct flow. See the *Duct Fitting Database* (ASHRAE, 1994) for extensive data on dynamic losses in duct fittings. Analysis is based on Bernoulli's equation and its assumptions. The friction losses in a section of duct or pipe are given by

$$\Delta P_f = f \frac{L}{D} \frac{\rho V^2}{2} \tag{63}$$

where f = friction factor, L = duct length, and D = hydraulic diameter. The dynamic losses due to fittings and so forth are given by

$$\Delta P_d = C_d \frac{\rho V^2}{2} \tag{64}$$

where C_d = dynamic loss coefficient. Total pressure losses are given by

$$\Delta P = \Delta P_f + \sum \Delta P_d \tag{65}$$

Since $F = \rho VA$, where A is the cross section (or flow) area,

$$F = \sqrt{\frac{2\rho A^2 \Delta P}{f L/D + \Sigma C_d}}$$
(66)

The friction factor can be computed using the nonlinear Colebrook equation (ASHRAE, 1997, p 2.9, eqn. 29b)

$$\frac{1}{\sqrt{f}} = 1.44 + 2 \cdot \log(D/\epsilon) - 2 \cdot \log\left(1 + \frac{9.3}{Re \cdot \epsilon/D \cdot \sqrt{f}}\right)$$
(67)

where ϵ = roughness dimension, and Re = Reynolds number = $\rho VD/\mu = FD/\mu A$. This nonlinear equation may be readily solved using the following iterative expression derived from equation (50) by Newton's method:

$$g^* = g - \frac{g - \alpha + \gamma \ln(1 + g\beta)}{1 + \gamma \beta/(1 + g\beta)}$$
(68)

where

g = f^{-1/2}, α = 1.14 - $\gamma \ln(\epsilon/D)$, β = 9.3/(Re $\cdot \epsilon/D$), and γ = 2 $\cdot \log(e)$ = 0.868589.

The convergent solution is achieved in 2 or 3 iterations of equation (51) using $g = \alpha$ as a starting value. If the value of g has been saved from the previous time it was computed for a particular duct element, and the flow rate has not changed greatly, only one iteration of equation (51) will be needed to compute the friction factor.

The exact derivatives of equation (49) are difficult to compute, so CONTAM uses a secant approximation. The derivatives suffer the standard problem of powerlaw equations — they go undefined as ΔP approaches zero. This is solved in CONTAM by the linear approximation (21) with the coefficient computed to give the same flow as equation (49) at the user specified transition Reynolds number (default = 2000). A more detailed description of the flow in the laminar region could be developed, but that would probably exceed the level of detail with which the rest of the problem is described in CONTAM.

Data describing a duct flow element is entered through screen [250].

6.3.4 Fans

6.3.4.1 Constant Flow Fans

One particularly simple but useful airflow element sets a constant flow between two nodes. Since the flow is constant, the partial derivatives of flow with respect to the node pressures must be zero. The constant flow element element does not contribute to the Jacobian, [A], but it does add to the right side vector, {B}.

Constant flow elements do not mathematically link the pressures of the adjacent nodes. It is necessary that all node in the network be linked to constant pressure nodes in order to have a unique solution. Violation of this restriction will produce a division by zero somewhere in the solution of the equations. Consider the following simple network:



where P_1 and P_6 are known pressures, and F_1 and F_2 are known flows. Since the flow through C_2 is determined by $P_3 - P_4$, and no other flow is related to those pressures, there are not enough equations to determine P_3 and P_4 uniquely. This is a mathematical expression of the fact that it is possible for F_1 and F_2 to be assigned different flows, which produces a physically impossible condition.

CONTAM provides two constant flow elements: one for constant mass flow (data entry screen [222]) and one for constant volumetric flow (screen [224]).

6.3.4.2 Variable Flow Fans

The theory of flows induced by fans is summarized in *HVAC Systems and Equipment* (ASHRAE, 1996, chapter 18). More extensive treatment is given by Osborne (1977). Fan performance is normally characterized by a performance curve which relates the total pressure *rise* to the flow rate for a given fan speed and air density. Conversion to another fan speed or density is done with the fan laws.

$$Q/Q_0 = N/N_0 \tag{69}$$

or

$$F/F_0 = N\rho/N_0\rho_0 \tag{70}$$

and

$$P/P_0 = N^2 \rho / N_0^2 \rho_0 \tag{71}$$

where Q = volume flow rate, F = mass flow rate, P = total pressure rise, ρ = density, N = rotational speed, and subscript 0 indicates values at rating conditions.

These laws are valid if all flow conditions at the two speeds are similar. In particular, they will not apply at very low flows where fully turbulent conditions have not been developed.

In CONTAM the fan performance curve is represented by a cubic polynomial:

$$P = a_0 + a_1 F + a_2 F^2 + a_3 F^3 \tag{72}$$

with

$$P' = \frac{dP}{dF} = a_1 + 2a_2F + 3a_3F^2$$
(73)

The polynomial coefficients are developed with air density and fan speed at the rating conditions. Therefore, when N and ρ are not at the rating conditions, convert the actual pressure rise P to P₀.

$$P_{0} = P N_{0}^{2} \rho_{0} / N^{2} \rho$$
(74)

Solve (55) for F_0 and (56) for P_0' . Convert these values to current conditions.

$$F = F_0 N \rho / N_0 \rho_0 \tag{75}$$

and

$$P' = P_0' N / N_0 \tag{(76)}$$

The derivative for flow with respect to pressure *drop* is given by

$$\frac{dF}{dP} = -\frac{1}{P'} \tag{77}$$

There are two important factors to note on the shape of the fan performance curve. First, it is described by a relationship of the form P(F) instead of F(P) which would be more appropriate for the calculation of flow and partial derivatives for the Jacobian. The basic shape of the performance curve cannot be well represented by a simple polynomial with P as the independent variable. CONTAM uses an analytic solution of the cubic polynomial (55) to determine F as a function of P.

Second, it is common for the performance curve to contain points of contraflecture (where P' = 0) creating up to three different flow rates at certain values of fan pressure rise. This causes difficulty in solving for the flow rate and has points where dF/dP goes to infinity. However, it is usually not recommended that the fan operate in the region of the contraflecture points. Therefore, the fan can be modeled with a performance curve that does not include the contraflecture so long as the user then checks that the air distribution system has not operated in that region.

It is easy to identify the points of contraflecture from the coefficients of the polynomial. Solving equation (55) for F gives:

$$F = \frac{-2a_2 \pm \sqrt{4a_2^2 - 12a_1a_3}}{6a_3} \tag{78}$$

If $4a_2^2 > 12a_1a_3$, there are two real points of contraflecture; if $4a_2^2 = 12a_1a_3$, there is a point of inflection which still has the derivative problem; and if $4a_2^2 < 12a_1a_3$, the fan performance curve is monotonic and well-behaved for computing the derivatives for the Jacobian.

6.3.5 Doorways (Large Openings)

The powerlaw and quadratic models allow flow in only one direction at a time. Flows through large openings (e.g. doorways) tend to be more complex with the possibility of flows in opposite directions in different parts of the opening. The temperature and resulting density differences between two rooms may mean that the stack effect causes a positive pressure difference at the top of the doorway and a negative pressure difference at the bottom (or vice versa) allowing a two-way flow in the opening. A summary of research on heat transfer through doorways is presented by Barakat (1987). Most research has attempted to develop dimensionless correlations (using Nusselt, Prandlt, and Grashoff numbers) of the form

$$N_d / Pr = C \cdot Gr_p^{\ b} \tag{79}$$

where b is approximately 0.5 and C lies between 0.22 and 0.33 depending on the temperature difference used for the correlation. It has been shown that such a heat transfer is equivalent to an airflow which can be modeled by powerlaw elements (Walton, 1982) by dividing the total opening into several smaller openings having the same total area but configured to properly account for the magnitude and direction of airflows at different heights in the opening.

An alternative approach is to create a single airflow element which accounts for the flow over the entire opening. A simple theory which estimates the stack induced air flow through a large opening in a vertical partition is given by Brown and Solvason (1962). This model of a doorway tends to be faster that the multiple opening approach. However, it also complicates the assembly process for the Jacobian matrix because one or two flows may exist. More importantly, development of the doorway element model requires knowledge of the vertical temperature profile used in the node model (here assumed to be constant) in order to compute the pressure difference as a function of height across the opening. This requirement compromises the independence of the modularity of airflow network program.

6.3.5.1 Multiple Opening Model

By assuming that the air density in each room is constant, the hydrostatic equation is used to relate pressures at various heights in each room:

$$P_{0j} = P_j + \rho_j g(h_j - h_0)$$
 and $P_{0i} = P_i + \rho_i g(h_i - h_0)$ (80)

$$P_{j}(y) = P_{0j} - \rho_{j}gy$$
 and $P_{i}(y) = P_{0i} - \rho_{i}gy$ (81)

where

P_{0j}, P_{0i}	pressure in zones j and i at $y = 0$, the reference elevation of the opening,
$\rho_{\rm i}, \rho_{\rm i}$	air densities of zones j and i,
P _i , P _i	reference pressures of zones j and i,
h _i , h _i	reference elevations of zones j and i, and
h ₀	elevation of the center of the opening.

Following Brown & Solvason (1962) it is assumed that the velocity of the airflow as a function of height is given by the orifice equation:

$$V(y) = C_d \left(\frac{2(P_j(y) - P_i(y))}{\rho}\right)^{1/2}$$
(82)

where

 C_d = discharge coefficient, and ρ = density of the air going through the opening.

The opening, H high by W wide, may be divied into multiple openings each representing a thin horizontal strip Δy high and W wide. The mass flow through each strip would be

$$F_{y} = C_{d} \sqrt{2\rho \Delta P} W \Delta y \tag{83}$$

The coefficient for the powerlaw model (19) for each sub-opening is thus given by

$$C_0 = \sqrt{2} C_d W \Delta y \tag{84}$$

6.3.5.2 Two Opening Model

An approximate model can be constructed by considering an opening between two zones which have no flow paths to any other zones. Then the flow in each direction must be equal and $P_{0j} = P_{0j}$. Integration of equation (65) from y=0 to y=H/2 using (64) to compute ΔP gives the flow through the top half of the opening.

$$w = \int_{y=0}^{y=H/2} \rho V W dy = \frac{C_d}{3} W \sqrt{\rho g \Delta \rho H^3}$$
(85)

This is equivalent to a simple powerlaw model with

$$C_0 = C_d \sqrt{2} \left(\frac{WH}{2} \right) \tag{86}$$

(a simple orifice with one half the total opening area) placed at y = 2H/9 elevation. The two opening model is completed with an identical opening at y = -2H/9 elevation allowing an equal flow in the opposite direction. Since the orifice is being modeled with simple orifice openings, any additional pressure drop between the zones due to other forces is included in the two opening model. The model becomes less accurate as the neutral plane shifts from the center of the opening. This model is available through data entry screen [220].

6.3.5.3 Single Opening Model

An third approach is to create a single airflow element which accounts for the flow over the entire opening. Begin by defining the neutral height, Y, where the velocity of the air is zero. From equation (65) this must occur when $P_i(y) = P_i(y)$. From equations (64) this must be

$$Y = \frac{P_{0j} - P_{0i}}{g(\rho_j - \rho_i)} \quad \left(= \frac{P_{0i} - P_{0j}}{g(\rho_i - \rho_j)} \right)$$
(87)

If |Y| < H/2, there is a two-way airflow through the opening. If $\rho_j = \rho_i$, the neutral height cannot be computed, but, since there is no possibility of two-way flow, the opening can be considered a simple orifice opening.

Define $\Delta \rho \equiv \rho_j - \rho_i$ and a transformed height coordinate $z \equiv y - Y$. Then the pressure difference across the opening is given by

$$P_{i}(z) - P_{i}(z) = -gz\Delta\rho \tag{88}$$

The mass flow through the opening above the neutral height is given by

$$F_a = W \int_{z=0}^{z=\frac{H}{2}-Y} \rho_m V dz \qquad m = j \text{ or } i$$
(89)

and the mass flow below the neutral height by

$$F_b = W \int_{z=-\frac{H}{2}-Y}^{z=0} \rho_m V dz \qquad m = j \text{ or } i$$
(90)

Whether the subscript m should be j or i depends on the direction of flow. Integration of equations (72) and (73) gives several different solutions for the airflow depending on the value of Y and the sign of $\Delta \rho$. Defining:

$$G = \frac{2}{3} W C_d (2g |\Delta P|)^{1/2}, \qquad f_a = |\frac{H}{2} - Y|^{3/2}, \qquad f_b = |\frac{H}{2} + Y|^{3/2}$$
(91)

gives the following equations for flows.

Case 1:
$$Y \le -H/2$$

$$F = -G\sqrt{\rho_i} |f_a - f_b| \qquad F = G\sqrt{\rho_j} |f_a - f_b| \qquad (92)$$

Case 2: $Y \ge H/2$

$$F = G_{\sqrt{\rho_j}} |f_a - f_b| \qquad F = -G_{\sqrt{\rho_i}} |f_a - f_b|$$
⁽⁹³⁾

Case 3: -H/2 < Y < H/2

$$F_{a} = -G\sqrt{\rho_{i}}f_{a} \qquad F_{a} = G\sqrt{\rho_{j}}f_{a}$$

$$F_{b} = G\sqrt{\rho_{j}}f_{b} \qquad F_{b} = -G\sqrt{\rho_{i}}f_{b}$$
(94)

The partial derivatives are computed numerically in CONTAM. This model is available through data entry screen [218].
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Appendix A. Summary of Menu Actions

Menu items are grouped together in the options area at the right edge of the screen, and each is activated by pressing a *function key* while at the SketchPad. Menus operate on data not directly related to the SketchPad icons. Pressing the designated function key, will bring up the appropriate data entry screen. Exiting the menu item returns the user to the SketchPad.

- F1 help1
- F2 help2
- F3 project
- F4 simulate
- F5 output
- F6 library
- F7 weather
- F8 level or results
- F9 sketch

In the following description of CONTAM96 menu items indentation indicates operations on another data entry screen. Most of the data entry screens are numbered, e.g. [040], and are explained in more detail in the Reference section of this report. [...] indicates an unnumbered screen.

F1 - *Help1* Help as it currently exists telling what the various options / data input fields mean. F1 gives information about *what* the program is requesting from the user, e.g., the physical description of a flow element and its input parameters.

F2 - Help2 This would tell how the currently active procedure is used, e.g. how a wall is drawn or how radio buttons work. This is help for the novice or a reminder for the casual user. F2 gives information about *how* to perform the current operation, e.g., how to enter a flow element name or copy an icon.

F3 - Project Project and file related operations \rightarrow [040] Save project file; SketchPad shortcut: $\langle Alt \rangle S$. Clear the SketchPad. Open an existing project file \rightarrow [...] Select from list of all project files in local directory. Give the project file a new name. Revise the project file description. Define contaminants \rightarrow [042] Delete all contaminants and related building features - for a new project. Name, mol wt, decay rate, default, units for each contaminant. Set defaults and user preferences \rightarrow [044]. Set units and default values \rightarrow [050]. Set keyboard & mouse sensitivity \rightarrow [052]. Redefine display colors \rightarrow [054]. Set default library files \rightarrow [056]. Save preferences to .CFG file. Set SketchPad size and positioning \rightarrow [046].

Summary of Menu Actions

Shell out to DOS for simple DOS commands \rightarrow [048]. Quit CONTAM; shortcut: $\langle Alt \rangle Q$. **F4** - *Simulate* Simulation control \rightarrow [060] Set run control parameters \rightarrow [062] Type of simulation: steady, transient, cyclic. Set steady-state weather data \rightarrow screen [078]. Set ambient temperature, pressure, wind speed and direction. Select weather file for transient simulation. Set simulation start and stop times. Select restart option. Set simulation and display time steps. Set simulation outputs \rightarrow [064] Select detailed results for airflows or contaminants. Select summary results for age of air, contaminants or exposure. Set numeric parameters \rightarrow [066] Select calculations methods and convergence criteria. Reset initial contaminant concentrations. Prepare input file for a CONTAMX simulation. Prepare input file for a TRNSYS simulation. Save project file. Quit (return to SketchPad) or begin simulation \rightarrow [294]. F5 - Output menu of various reporting options \rightarrow [068]. Copy SketchPad graphic to printer. Copy SketchPad graphic to a PCX format file. Copy annotated project data to a file. Report flows - all zones / this time to a file. Export flows - all zones / this time to a file. Export flows - all zones / averaged to a file. Export flows - this path / all times to a file. Report contaminants - all zones / this time to a file. Report contaminants - all zones / all times to a file. Export contaminants - all zones / all times to a file. Export contaminants - this zone / all times to a file. F6 - Library library operations - [070]. Determine type of elements to be processed. Set the library file name. Reset the library file description. Process library elements \rightarrow [072]. Delete unused elements from project. Copy elements from project to library. Copy elements from library to project. Delete elements from library. Save modified library file. Set default library files for each element type \rightarrow [056]

Summary of Menu Actions

F7 - Weather define weather data \rightarrow [074]. Set site data \rightarrow [076] Location and elevation. Set steady-state weather data \rightarrow [078]. Set ambient temperature, pressure, wind speed and direction. Set building wind related values \rightarrow [058] Relative north, roof height, local terrain, velocity exponent. Set wind speed and direction for wind pressure display. **F8** - *Level* define/access building levels \rightarrow [080]. (F8 while in normal or wind pressure display modes) Check completeness of the description of the current level; shortcut: $\langle Alt \rangle C$ Remove the current level. Create a new level, possibly copying data from another level. Set/revise level name, elevation, and height. **F8** - *Results* results time navigation \rightarrow [084]. (F8 while in results display mode) Move to different time. Note shortcuts: ahead 1 time step - End back 1 time step - Home end of day - < Ctrl > End start of day - < Ctrl > Home Set calculation and display of age of air; shortcut: $\langle Alt \rangle A$ **F9** - *Sketch* settings and normal mode navigation \rightarrow [082]. Select normal, wind pressure, or results display modes. Note shortcuts: normal display - < Alt > Nwind pressure display - $\langle Alt \rangle W$ results display - < Alt > RAdd sublevel displays; shortcut: $\langle Alt \rangle B$ Zoom to view SketchPad larger than sketch window; shortcut: < Alt>Z Move to different building level. Note shortcuts: up 1 level - PgUp down 1 level - PgDn highest level - < Ctrl > PgUp lowest level - < Ctrl > PgDn.

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Appendix B. Shortcuts

Reminders for several $\langle Alt \rangle$ key shortcuts are displayed at the top of the options section of the screen. The actions they invoke are all accessible through the menu screens, but the experienced user should quickly learn to use these little shortcuts from the SketchPad. The most important is probably the command for quitting CONTAM.

< Alt > Q	Quit CONTAM; you are presented with the option of saving changes to the project file.
< Alt $>$ S	Save the current building description to the project file.
< Alt $>$ N	Switch to normal display mode where the building sketch can be changed.
< Alt $>$ W	Switch to wind pressure display mode to check this critical input.
< Alt $>$ R	Switch to the results display mode after a simulation.
< Alt $>$ Z	Zoom out to see a SketchPad larger than the normal screen display.
< Alt $>$ C	Check the completeness of the building description on the current level.
< Alt $>$ B	Display in gray the features on the level below the current one.
< Alt $>$ A	Compute and display the age of air for the zones.
Other shortcuts are provided for navigating the SketchPad:	
PgUp	Move up 1 level.
PgDn	Move down 1 level.
< Ctrl > PgUp	Move to highest level.
< Ctrl > PgDn	Move to lowest level.
And for reviewing the results of a transient simulation:	
End	Move ahead 1 time step.
Home	Move back 1 time step.
< Ctrl > End	Move to end of day.
< Ctrl > Home	Move to start of day.

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Appendix C. CONTAM96 Reference

Appendix C shows the data entry forms and associated help screens used by CONTAM96. Because of its length, 95 pages, it is not included in this printed report. It is included in the electronic copy of the report, file REPORT96.ZIP, available at the NIST FTP site as described in section (2.3.2) of this report.

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