

# IAQPC: AN INDOOR AIR QUALITY SIMULATOR

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## ABSTRACT

*An Indoor Air Quality Simulator for Personal Computers (IAQPC) has been developed in response to the growing need for quick, accurate predictions of indoor air contamination levels. Heating, ventilating, and air-conditioning (HVAC) system designers need ways to determine if a planned system will ensure the health of building occupants. Scientists will find this program useful as an experimental design aid. Building maintenance personnel will be able to use it to determine approaches that will alleviate contamination problems.*

*Version 2 of the Indoor Air Quality Simulator has been developed at a research institute under a cooperative agreement with the U.S. Environmental Protection Agency. This program extends Version 1 with more extensive input menus and output options. Improved algorithms for contaminant transport and flow have been incorporated. The program runs in a fraction of the time necessary for other current models.*

*This program models up to six pollutants concurrently for buildings of up to 20 rooms. It allows inclusion of sources, sinks, and air cleaners and can be adapted to a wide range of structures. The algorithms used to determine the concentrations have been tested against experimental data and found to yield accurate predictions. This paper describes the model's inputs, calculations, and outputs and presents a case study performed with the model.*

## INTRODUCTION

As the awareness of the potential health and air quality control problems resulting from indoor air contamination has increased, research has begun to determine the concentrations of pollutants in indoor air. Many potential sources have been studied in experimental studies; some have been studied in actual buildings. Work has begun in testing air-cleaning devices both in laboratories and in buildings. Some studies have been done to determine actual contaminant levels in occupied spaces. However, for this information to be used by building designers, HVAC system operators, and occupants, an easy-to-use, readily accessible, and quick method is necessary to disseminate the information and to apply the relevant data to any given situation. IAQPC is one answer to these needs.

IAQPC is an indoor air quality simulator for use on personal computers. Menus are used to enter data, describe the specific building, run the program, and output the results. This edition of the model, Version 2, has been developed at a research institute under a cooperative agreement with the U.S. Environmental Protection Agency. This program extends Version 1 (Sparks et al. 1988) with more extensive input menus and output options. Improved, faster algorithms for contaminant transport and flow have been incorporated. The algorithms that are used in this program run approximately

10 times as fast as the CONTAM program developed by the National Bureau of Standards (now the National Institute of Standards and Technology) (CONTAM 1987).

## DESCRIPTION OF THE PROGRAM

This program is easy to use in spite of the multiplicity of inputs required. Menus provide easy access to data input, run program, and output options. The main menu (Figure 1) gives the user access to the data entry, calculation, and data output options of this program. This approach makes it simple to enter the basic building design, HVAC system design, pollutant descriptions, and the source and sink locations (a sink is anything that removes a pollutant from the air).

Through the basic design menu (Figure 2) the user specifies the building floor plan, room volumes, and interconnections. This model is for use with any single-story building with an HVAC system. The floor plan to simulate the structure need not match the actual layout. The important consideration is to match function.

There are six possible basic layouts for the building, as shown in Figure 3. Each has a minimum number of rooms and expansion rooms. The total number of rooms may range from 2 to 20. The interconnections between the rooms, outside, and the HVAC system are specified as total connecting areas. These areas provide a relative measure of flow resistance and are not necessarily equal to the physical area. For example, if a room has an open 3 ft by 8 ft door connecting to the hall, the approximate hall interconnection value will be 24. If the door is to be shut during the run, a small value for the crack under the door, possibly 0.25 (for 1 in by 3 ft), would be specified. A summary of the room volumes and connecting areas for all the rooms in the building can be viewed in a convenient table in a window that opens up on the screen.

Values directly related to the HVAC system are entered in the HVAC system design menu. Required data include the total flow when the system is on, flow when the HVAC system is off, pressure head, and fraction of makeup air. A sub-menu allows selection of up to eight on/off changes in the HVAC system status for every 24 hours of simulated time. The HVAC system is assumed to be off until the first time specified.

Several options, besides data input, are available through this menu. The airflows may be balanced and displayed while in this menu, allowing the user to check the values before running the simulator. This is especially useful if a building has been experimentally characterized. The user may check to see that the calculated values reflect the real values and change the input data, such as the interconnecting areas, to achieve precise results.

The pollutant characteristics menu allows the user to choose which pollutants will be modeled and to enter source rates, air cleaner efficiencies, concentration averaging periods, acceptable limits, and outdoor concentrations. From

I N D O O R   A I R   Q U A L I T Y  
S I M U L A T O R  
Main Menu

Basic Building Design  
HVAC System Description  
Pollutant Characteristics  
Air Cleaners/Sinks  
In-Room Locations  
Start Simulator  
Continue Simulation  
Graphical Output  
Output Results  
Runtime Configuration

Quit to Prior Menu <Esc>

Use the arrow keys to position the cursor.  
Use <Enter> to select the option.

*Figure 1 IAQPC's main menu*

one to six pollutants may be modeled. There are 11 pollutant names to choose from including three sizes of particles, carbon dioxide, and volatile organic compounds (VOC). At this point, however, there are no pollutant-specific calculations, so that any of the pollutant listings can be used to simulate any pollutant as long as the corresponding source and sink terms are correct. Source rates for many common pollutant sources can be changed to reflect the actual rates, if known. For example, if a certain brand of cigarette is to be a source, the particulate production rate can be looked up and entered.

In a manner similar to that used for sources, sink rates can be specified. Four types of passive sinks may be included: horizontal, vertical, furniture, and people. Collection and reemission rates for the chosen pollutants may be input. The

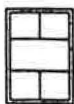
reemission rates allow the sinks to collect and reemit the pollutant. The reemission rate is a fraction of the total collected amount that will be given off in the given time interval.

The user may also choose which types of air cleaners are available and may specify the collection efficiencies for these devices. Up to two room type and two HVAC system cleaners may be selected. Efficiencies for the air cleaners for each pollutant may be specified.

Concentration limits and corresponding averaging periods are also input. These values enable the program to determine a suitable average concentration for each specified pollutant and to compare this with the appropriate limit. In this way, the user can be warned if concentrations will exceed threshold values or air quality standards. The default values

Expanded Floor Plan 3

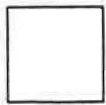
Central Hall  
4 rooms & hall



1 2  
0  
4 3

Hall      Connecting Area (ft<sup>2</sup>)

Outside



HVAC room inlet      .4  
Outside wall(s)      .2  
Next room              0  
Prior room              0  
Hall                      0  
HVAC room return      1

Quit <Esc>

B A S I C   B U I L D I N G  
D E S I G N

Floor Plan Selection 3

Number of Rooms      4

Room Number          0

Volume (ft<sup>3</sup>)            200

Interconnections

Upward Room# Copy    <F3>

Downward Room# Copy <F4>

Building Statistics

Load Building Design

Save Building Design

Quit to Main Menu <Esc>

Use cursor keys to select option.

Use <Enter> to activate option.

Use +/- to change room number.

*Figure 2 Basic design menu*

are those for recognized standards. In addition, the concentration limits are used to normalize the output values before graphing.

Ambient concentrations of pollutants are also specified. The default values are considered to be typical of outdoor air, but some regions will need adjustment. These values may be used as the initial concentrations inside the building.

In addition to specifying source and sink rates, it is necessary to specify their locations. The in-room sources menu allows the choice of which generic sources are present in each room, the hall, and the HVAC system. The in-room sink menu allows the user to select the sinks present. The air cleaners present in any room or the hall are selected, as is the method the program uses to set the initial in-room concentrations (five options are available: zero all concentrations, ambient concentrations, HVAC system concentrations, local equilibrium, and initialize configuration). Again, a summary of the sources and sinks for the building is available as a window inset.

IAQPC allows the user to specify various runtime and menu use options. The runtime configuration options include the time increment to be used by the program. Allowable values are 0.1 to 2.0 hours in increments of 0.1 hour. The print step is the interval at which new values will be printed. The run duration is the length of time in days that the calculations will cover—currently up to 30 days.

The interrupt every (hr) instructs the program to stop calculations at regular intervals. When the program reaches this point, it prints a message to the screen asking the user to press any key to continue. This allows the user to examine the values, then continue or escape, change parameters, and resume calculations. For example, if the user wishes to determine the effect of opening and closing a window every two hours, the interrupt would be set to 2. Then the user would escape, change the outside connection area in the appropriate room, and continue the program.

The menu use options include the choice of highlighting the current choice (bar) or a blinking arrow in front of the choice. The key letter enable allows the user to press the first letter of a choice to select that choice, or the cursor can be moved by cursor keys or a mouse. Graphics display determines whether graphical output will be available. Setting this

option to "off" lets the program run even if the computer does not have graphics capabilities. An on-line calculator is available simply by pressing <F9>. This makes it simple to convert units or calculate areas given dimensions.

The program running options are start simulator, which begins calculations, and continue simulation, which continues the simulation at the point where an interruption occurs. In both cases, the screen will clear, then plot the values as they are calculated. Figure 4 is an example of the graphical output that shows the concentrations of two pollutants over approximately 36 hours.

Output options include a table of the current concentrations, the flow rates as calculated for the building, and a summary of the input data.

## TECHNICAL APPROACH

A fast direct solution method to describe a multizone indoor contaminant distribution was developed. It is assumed that mass is conserved or accounted for in the structure.

If the assumption is made that the neighboring concentrations and source terms do not change during the time step selected, then

$$C_i = C_i(t_0)exp(-L_i t) + P_i(1 - exp(-L_i t))/L_i \quad (1)$$

where

$C_i(t_0)$  = the concentration for room  $i$   
at time  $t = t_0$

$L_i$  = loss rate of pollutants leaving  
room  $i$  per unit time

$P_i$  = production rate of pollutants entering  
room  $i$  per unit time

The discrete solution method approaches the exact solution as the time step decreases. At any given starting time, the concentration for each room is known or set by the initial conditions. After the concentrations of all zones during the time step have been computed, the pollutant concentration for supply air is computed. The concentration in each room that has just been calculated is used as the initial concentration for the next time step. This procedure is repeated until the final time is reached. The order of calculation is not im-

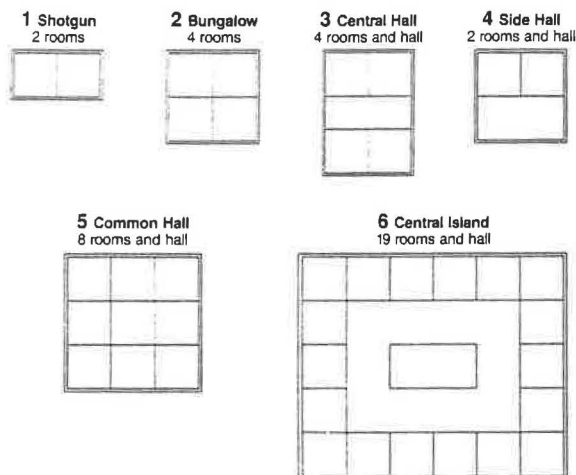


Figure 3 The six available building layouts

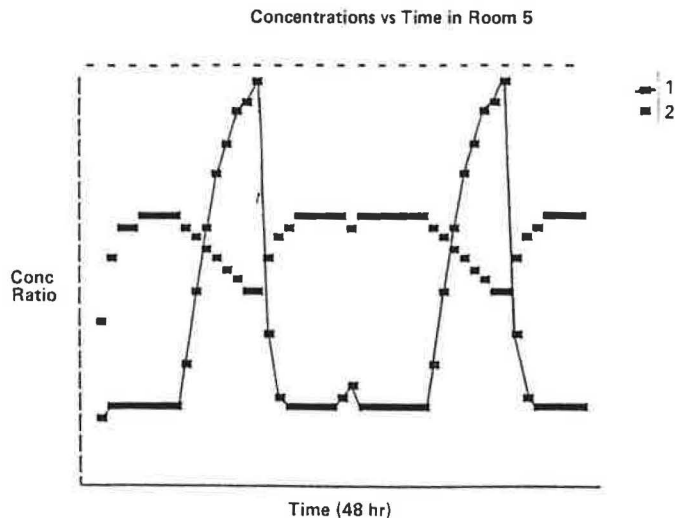


Figure 4 A sample of IAQPC's graphical output

portant. For a complete description of the algorithm, see Yamamoto et al. (1988).

To compare the execution time to run this program with that for the CONTAM model (a state-of-the-art program with extensive algorithms), identical cases were run with both programs. The comparison case, a 12-zone simulation of an office building, represented a building for which experimental data are available (Owen et al. 1986). The algorithm used in IAQPC, another algorithm also developed at this facility, and the CONTAM model were compared. All three gave results that were quite consistent with the experimental results; however, this algorithm ran approximately 10 times as fast as CONTAM (Yamamoto et al. 1988). It also runs much faster than Version 1.

The flow-balancing algorithm uses pressure-driven flows, with a strict pressure balance maintained for the system with "areas" used to represent the flow resistance. The mass flow error in each room is used to provide a relaxation correction to the pressure in the room. Convergence to mass balance in all rooms is the criterion for overall convergence.

## DISCUSSION

IAQPC is a user-friendly program. The incorporation of simple-to-use, easy-to-understand menus into a contaminant calculation program enables any user to benefit from this program. Menu use options make it possible to tailor the menus to an individual. The program can be operated by mouse, with first letter control, with an arrow or a highlighted cursor, and in color or not. These options allow the user to individualize the program for ease in running.

A new user with basic knowledge of concentration levels and building design should have little trouble using the program. The program provides on-screen instructions and a user's manual—complete with tutorial and program flow-chart. A user with no computer experience will need to be cautioned to save data files, turn on the printer, and other basic hints as would be needed for any program use. A user with spreadsheet experience will find this menu design fairly familiar; options are presented, then chosen as in a spreadsheet. A Version 1 user will merely need to become acquainted with the available options. All users should try the tutorial first, then proceed with experimentation. Any user should be able to set up a simple case and obtain results in less than an hour. More complicated cases will take longer to set up simply because of the data entry time. As the program is used, the user will learn more about it and become comfortable with the many options.

Building description is simplified by giving the user a choice of floor plans. The six available floor plans can be used to describe almost any building. This procedure sets up the connections between rooms without the necessity for the user to laboriously specify which room is connected to what. The chosen floor plan need not match the actual layout but should match in function.

Since the connections between rooms are specified by cross-sectional areas, any building may be characterized using only basic floor plans and a survey to determine which doors, etc., are open. It is not necessary to have experimental airflow data in order to determine airflows in the building. However, if detailed  $SF_6$  or other flow rate data are available, the interconnecting areas can be specified, then refined to produce the actual flow rates. In addition, this approach makes it simple to determine the effect of changes in the building, such as the opening of a door or window. Again, the "area" may not correspond exactly to a physical area, but is a state-

ment of the flow resistance. This program may also be used to check plausibility of experimental data. For example, it can verify that measured airflows and concentrations are consistent.

The HVAC data entry options that allow the user to specify total flow and percent makeup air make it possible to determine the effect of these two parameters on the indoor concentrations. These parameters are two of the most important for the system designer and the building HVAC operator. Since energy efficiency is directly related to the flow rate and, even more, to the percentage of outdoor air (which may have to be cooled, heated, or dehumidified), it is important to be able to determine minimum acceptable flows. With IAQPC, these values can be changed quickly and their effects studied. Also, sources can be changed to determine if lower flows would be acceptable if certain sources were eliminated, moved, or vented. In the same way, an experimenter can use these options to aid in experimental design. The results of computer runs will indicate what parameters will be influential and need actual study.

Since this program allows up to six pollutants to be modeled, much time can be saved over the separate runs required per pollutant in previous air quality programs. The generic sources (cigarette, heater, etc.) have default values that are standard for the particular source; this allows the user to specify sources without having to look up source strengths. However, when the user has emissions data for specific sources, these numbers can be input for source strength on final concentrations. For example, if a homeowner wished to decide between brands of heaters based on the resultant pollutant levels, this program would enable the prediction of levels based on the specific heater's byproducts.

In the same way, the possible sinks and air cleaners can be manipulated to determine, for example, the effect of more efficient filters or of removing a charcoal filter. Knowledge of the effect of various air-cleaning devices could benefit a designer by helping to determine the lowest pressure drop for a filter that will yield acceptable air conditions, therefore helping to size the building fans.

Since both the sources and sinks can be specified in any location or combination of locations, IAQPC is very versatile. Sources can be moved to determine, for example, the most reasonable location for the copy machine or how smokers should be placed to have the least impact on an office building as a whole.

The concentration limits, combined with the averaging periods, will make IAQPC a useful tool for building assessment when there is a possibility that air quality standards will be exceeded. This program will help the owner meet safety standards. Changing the concentration limits can be used to increase the comprehensibility of the output graph. If more than one curve occurs in the same region of the graph, the user can change one of the limits in order to shift that portion of the plot. The runtime output and program output options make it possible to obtain the required data in the most readily usable form.

All of the options, combined with the speed of IAQPC, make this program the ideal tool for many HVAC professionals and building occupants, as well as scientists investigating indoor air phenomena. This program and appropriate documentation will be available through normal EPA channels as soon as release approval has been obtained.

**TABLE 1**  
HVAC System Airflows in Test House

Room	Measured Airflows (cfm)
Den	400
Middle Bedroom	165
Corner Bedroom	164
Master Bedroom	165

**TABLE 2**  
Measured Concentrations in Test House (mg/m<sup>3</sup>)

Day/Room	Closet	Corner Bedroom	Master Bedroom	Den
1	107	4.72	3.49	3.84
2	53.6	4.41	3.50	3.30
3	70.9	5.51	4.18	3.80
4	63.0	5.61	4.27	4.02

**TABLE 3**  
Interconnecting Areas (ft<sup>2</sup>) and Volumes (ft<sup>3</sup>)  
Floor Plan 4

Room	Volume	HVAC: In	Ret	Walls: Out	Nxt Rm	Pr Rm	Hall
0	457	0.00	5.00	0.00	0.00	0.00	0.00
1	1375	2.55	0.00	0.13	0.00	0.00	21.00
2	5468	6.70	0.00	0.29	0.00	0.00	34.40
3	1067	0.31	0.00	0.01	0.00	0.00	21.00
4	1124	2.55	0.00	0.13	0.32	0.00	21.00
5	99	0.04	0.00	0.00	0.00	0.32	0.00
Total	9590	12.15	5.00	0.56			

**TABLE 4**  
Airflows (cfm)

Room	ACh/Hr	HV In	HV Ret	Outside	Nxt Rm	Pr Rm	Hall	Total
0	90.3	0	-688	0	0	0	688	-0
1	7.1	162	0	-14	0	0	-147	1
2	4.4	404	0	-32	0	0	-371	1
3	1.2	21	0	-1	0	0	-19	1
4	8.8	161	0	-14	3	0	-150	1
5	2.4	4	0	0	0	-30	-0	1
Total	3.7	752	-688	-61				

**SAMPLE CASE**

This sample case compares the output for IAQPC to experimental data for the EPA test house in Cary, NC. The actual data are briefly discussed. The procedure used to model the case and the input values are listed, then the results are compared. This serves to show the level of accuracy of the program and introduces some of the program options.

**Description of Experiment**

Flow rates were determined in the house when the ventilating system was on. The HVAC system was initially on and was left on for the duration of the test. Moth cakes—p-dichlorobenzene—were placed in one closet. Figure 5 shows the actual layout of the building. The p-dichlorobenzene emission rate was determined to be 1.4 mg/cm<sup>2</sup>·h. The area of the moth cakes was 570 cm<sup>2</sup>. Airflows into the rooms from the HVAC system are given in Table 1. All airflow from the interior to the HVAC system is through the return ducts in the hall. The airflow between the closet and the bedroom was determined to be approximately 2.3 cfm. An infiltration

rate of outdoor air of 0.35 air changes per hour was determined. Concentrations were determined in four locations for four days beginning three days after the cakes were positioned. These are shown in Table 2. For more details, see Sparks et al. (1988).

**Modeling Procedure**

In order to model this case, a floor plan had to be chosen. More than one of the plans could have been used. Since there were no data on flow or sources in many of the rooms, a five-room simulation was chosen. The floor plan shown in Figure 6 was used since there are no interconnections between the master bedroom and the closet. Note that room number 0 is the hall; room number 6 is the HVAC system.

The room volumes were determined directly from the floor plan, then entered into the program. Reasonable guesses were made for all of the interconnecting areas. For example, it was assumed that open doors would connect all the rooms, except the closet, to the hall. This resulted in the use of 21 ft<sup>2</sup> (3 ft by 7 ft) for the interconnection between the four main rooms and the hall. The outlet and return vents

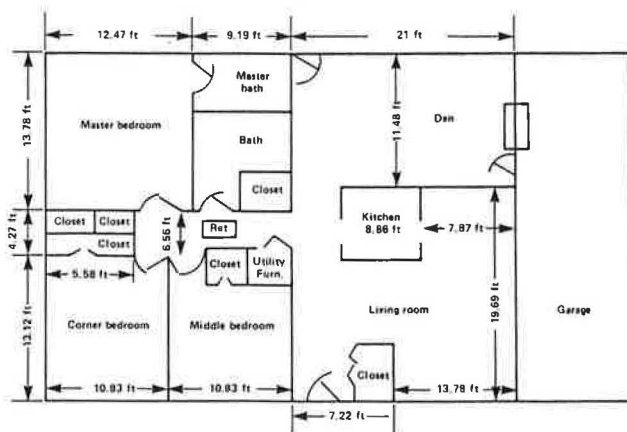


Figure 5 Floor plan of EPA IAQ test house

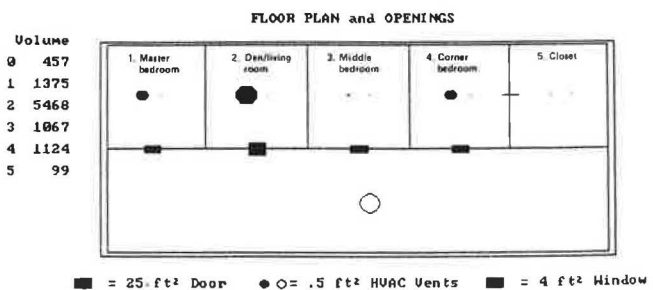


Figure 6 Layout for simulation of EPA test house

TABLE 5

Model Concentrations for Test House (mg/m<sup>3</sup>)

Closet	Corner Bedroom	Master Bedroom	Den
65.8	9.75	8.96	8.96

were assigned much smaller values. The door to the closet was assumed shut, so a small value was given to the area between the room and the closet. In order to force air through the closet, a value was given for an HVAC vent. Also, all four rooms with outside walls were given values to represent cracks or slightly open windows so that air could escape from the building (thus making outdoor air intake possible).

The total volume of the five rooms and the air exchange rate were used to determine the amount of outdoor air entering the building. The flows were added up and entered into the program as the total flow and fraction of outdoor air values. Then the airflows were balanced through the HVAC system design menu. The airflows were then examined and adjustments were made to the interconnecting areas so that the flow rates corresponded closely to the actual values. The final interconnecting areas, room volumes, and flow rates are shown in Tables 3 and 4.

Next, the pollutant choice menu was used to choose dichlorobenzene as the pollutant to be modeled. The generation rate of the generic source (mothcakes) was set as 79.8 mg per 0.1 hour. The appropriate runtime settings were specified: print output to screen, save data to file as generated, print time of 0.5 h, etc.

Then the simulator was run. The on-screen graphical output for the corner bedroom (room 4) is shown in Figure 7. The concentrations reached their final values in fewer than 24 hours so that one set of numbers covers the times for all of the readings. These values are shown in Table 5. In this case, the time to model four days was only 35 seconds.

The closest concentration is well within the range of the experimental values. The other three numbers are fairly close. Obviously, given the detail of the input data, the model does a good job of predicting the actual values.

This sample case shows some of the options and flexibility of IAQPC. It also shows that the calculated concentrations are a good reflection of the measured values.

## CONCLUSIONS

1. IAQPC fills the current need for a quick, user-friendly method of determining potential indoor air problems. This model will allow both building users and designers to determine potential problem areas and IAQ control approaches.
2. Experimental design will be simplified with IAQPC. Variables such as flow rates, makeup air percentage, HVAC schedule, room configuration, sources, and source location that are most likely to influence pollutant concentrations can be determined. It is also possible to use IAQPC to

determine if experimental data are plausible.

3. Experimental data verify that the program does predict actual values.
4. Further experimental data will enable the fine tuning of the program's calculation schemes, in particular, airflow resistance areas and source/sink values.

## PLANNED DEVELOPMENTS

1. Experimental work to characterize indoor sources will be performed after using IAQPC to examine possible outcomes in order to design optimum experiments.
2. Data from experiments will be used to verify or modify the assumptions in the model.
3. Additional sink types and pollutant interactions will be included as these phenomena become better understood. Eventually a model that incorporates costs and health effects will be developed.

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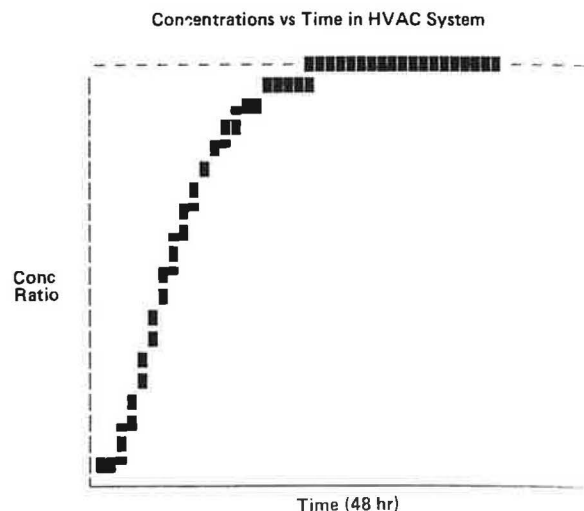


Figure 7 On-screen graphical output for corner bedroom