Comparison of two IAQ calculation methods

W. Brad M. Stanley*, Christopher O. Muller

Purafil, Inc.; Atlanta, GA, USA

ABSTRACT
Calculating the contamination concentrations in a space or the required ventilation for a space has been a difficult and confusing part in the application of the IAQ Procedure of *ANSI/ASHRAE Standard 62, Ventilation for Acceptable Indoor Air Quality*. Appendix D of ASHRAE Standard 62 currently presents one method for performing these calculations, but it is limited to the steady-state analysis of a single zone. More recently, the Indoor Air Quality Design Tool (IAQDT) was developed by the National Institute of Standards and Technology to facilitate these calculations and to include transient effects. This paper reports on the application of both methods to a single zone, showing the results of the each method to be very similar, with exceptions occurring when transient effects are important.

INDEX TERMS
Design; Modelling; Indoor air quality; ASHRAE Standard 62; Indoor air quality procedure

INTRODUCTION
ASHRAE's standard titled 'Ventilation for Acceptable Indoor Air Quality', *ANSI/ASHRAE Standard 62-2001* (hereafter Std 62)' provides formulas in Appendix D for calculating space contaminant concentrations of a zone for application with the standard's Indoor Air Quality (IAQ) Procedure. These equations are based on a single-zone mass balance under steady state conditions. They have been used for many years to calculate contaminant concentrations in a zone and compare them to guideline levels.

The US National Institute of Standards and Technology (NIST) has developed the Indoor Air Quality Design Tool (IAQDT) to aid in contaminant-based design of ventilation systems, such as the IAQ Procedure of Std 62 (Walton, 2003). The IAQDT calculates transient concentrations of contaminants based on the HVAC system configuration and operation. It differs from the Std 62 Appendix D in that it does not assume steady state conditions to exist.

A comparison of a sample office space using these two approaches is performed. Some items to consider are the resulting contaminant concentrations in the zone, reasons for the differences and appropriateness of each model for office building scenarios.

ASHRAE Standard 62 Mathematical Model (ASHRAE, 2001)
The formulas provided in Std 62 Appendix D take into account (among other things) the amount of outdoor air, contaminant generation rate(s), outdoor contaminant concentrations, filter locations and efficiencies, ventilation effectiveness, supply air circulation rate and the fraction recirculated. The schematic of a representative system is shown in Figure 1.

* Corresponding author. E-mail: brad_stanley@purafil.com

The variables in this model are defined as follows:

V_o = volumetric flow of outdoor air, from ambient into air handling system (AHS);
V_r = volumetric flow of return air, from the zone to the AHS and ambient air;
V_s = volumetric flow of supply air, from the AHS;
R = recirculation flow factor;
F_r = flow reduction factor, used with variable air volume (VAV) systems;
C_o = contaminant concentration in the outdoor air;
C_s = contaminant concentration in the occupied zone;
E_f = filter efficiency for contaminant;
E_v = ventilation effectiveness;
N = contaminant generation rate in the zone;
A, B = filter locations in the recirculation air and the supply (mixed) air, respectively.

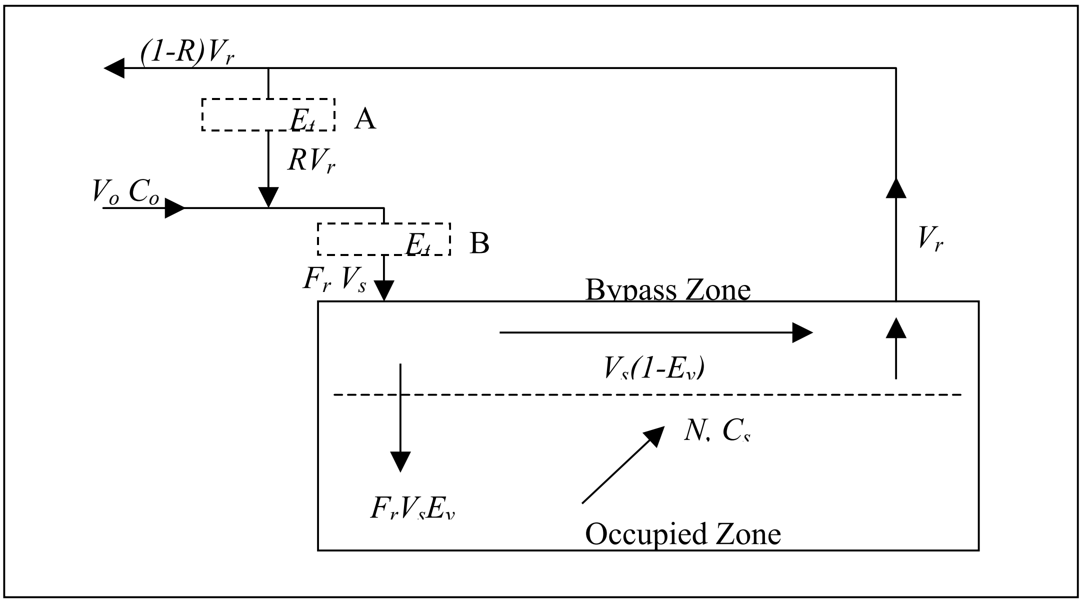

Figure 1 ASHRAE Standard 62 Appendix D single-zone system.

This model is intended to model one zone at a time. In the simplest form, the user would use constant generation rates and filter efficiencies, and the mechanical system properties to determine the total concentration in the space or the amount of outside air or recirculation air needed. For the purposes here, the concentration of the contaminant in the space will be calculated and compared to a guideline level. An example of those formulas is shown in Table 1 for the setup modelled in this work.

Table 1 Std 62 Appendix D—space contaminant concentration formulas

Class	Filter location	HVAC flow type	Outdoor airflow type	Space contaminant concentration
V	B	Constant	Constant	$C_s = \dfrac{N + E_v V_o (1 - E_f) C_o}{E_v (V_o + R V_r E_f)}$

NIST IAQDT (Walton, 2003)
The mathematical model behind the IAQDT is based on mass balances of a single-zone system. This system (or zone) over which the balances are written is shown in Figure 2. It takes into account the amount of outside air, recirculation, total supply air and infiltration to

the space as well as the amount of exhaust, return air and exfiltration from the space. Air cleaning technologies applied in the HVAC system or in the space can be modelled if efficiencies and flows are determined.

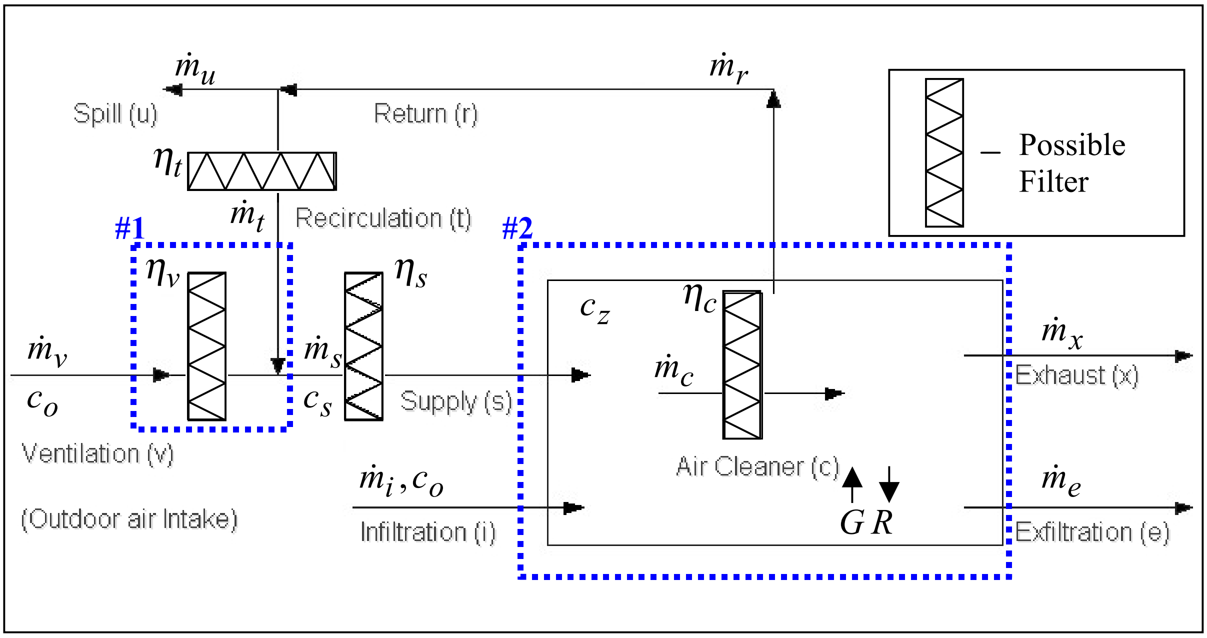

Figure 2 Single-zone system.

The variables in this model are defined as follows:

c_o = contaminant concentration in the outdoor air, kg/kg;
c_s = contaminant concentration in the mixed supply air, kg/kg;
c_z = contaminant concentration in the zone and return air; kg/kg;
η_v = filter efficiency for the ventilation air stream;
η_t = filter efficiency for the recirculation air stream;
η_s = filter efficiency for the supply air stream;
η_c = filter efficiency for the air cleaner;
G = contaminant generation rate in the zone;
R = contaminant removal (sink) coefficient in the zone.

The concentration of each contaminant in the zone can be calculated by simultaneously solving Eqns (1) and (2). These are based on a mass balance for the contaminant concentration on the supply flow over system #1 and a mass balance for the rate of change of contaminant concentrations in the zone over system #2. These equations are solved throughout a day from midnight (00:00) to midnight (24:00) until steady state is reached, i.e. the contaminant concentration at the end of the day equals the contaminant concentration at the beginning of the day. These calculated concentrations throughout the day are saved and compared to limit concentrations for further reporting

$$\dot{m}_s c_s = \dot{m}_v \left(1-\eta_v\right) c_o + \dot{m}_t \left(1-\eta_t\right) c_z \tag{1}$$

$$\left(\frac{\rho_z V_z}{\Delta t} + \dot{m}_c \eta_c + \dot{m}_r + \dot{m}_x + \dot{m}_e + \sum R\right) c_{z,t} - \dot{m}_s \left(1-\eta_s\right) c_{s,t} = \frac{\rho_z V_z}{\Delta t} c_{z,t-\Delta t} + \dot{m}_i c_o + \sum G \tag{2}$$

METHODS

The comparison of these two models involved the sample zone parameters listed in Table 2. These parameters were entered into the Std 62 formulas as well as the IAQDT software, which also utilized schedules for the generation rates and ventilation periods. The Std 62 formulas were used with constant, always on generation and ventilation rates to find the steady state properties. The contaminant concentrations and generation rates used are shown in Table 3.

Table 2 Example zone parameters

Parameter	Description/value	Schedule
System properties		
Filter location	Supply Airstream	n.a.
HVAC flow type	Constant	n.a.
Outdoor airflow type	Constant	n.a.
System values		
Area (m^2 [ft^2])	929 [10 000]	n.a.
Volume (m^3 [ft^3], 2.7 m [9 ft] ceilings)	2549 [90 000]	n.a.
Occupancy (7 people/92.9 m^2 ([1000 ft^2])	70	6 a.m. to 6 p.m.
Supply airflow (m^3/h [cfm])	16 990 [10 000]	Always on
Ventilation Airflow (m^3/hr [cfm])	595 [350]	6 a.m. to 6 p.m.

n.a., not applicable.

Table 3 Contaminant concentrations and generation rates (Wang, 1975; Sheldon *et al.*, 1988; Brightman *et al.*, 1995)[a]

Contaminant	Generation rate	Schedule
Bioeffluent generation rates (mg/day/person)		
Acetone	50.7	6 a.m. to 6 p.m.
Ammonia	32.2	6 a.m. to 6 p.m.
Hydrogen sulphide	2.73	6 a.m. to 6 p.m.
Methyl Alcohol	74.4	6 a.m. to 6 p.m.
Phenol	9.5	6 a.m. to 6 p.m.
Building generation rates (mg/min/m^2 [mg/min/ft^2])		
TVOC	0.01357 [0.001261]	Always on
Formaldehyde	0.001657 [0.0001539]	Always on

[a]Bioeffluent rates taken from Wang. Building generation rates were developed from data in the other sources referenced.

The outdoor air contaminant concentrations were taken from the EPA AIRS database and other studies and are listed with the results in the next section. A filter efficiency of 25% (E_f = 0.25) was used for all contaminants except ammonia and carbon monoxide, against which the filter had no effectiveness (E_f = 0).

RESULTS

Results from each method are shown in Table 4. The difference between them was less than 1% as compared to the guideline values, with the exception of ammonia and carbon monoxide.

The cause of this greater than 1% difference is shown in Figure 3. This shows concentration versus time data for both ammonia and sulphur dioxide as derived by the IAQDT. Since the ammonia is not being removed by the filtration and has an internal source, it is able to build up to some extent. The sulphur dioxide does not have an internal source and is removed by the filtration system, so that the concentration levels off fairly rapidly. Therefore, the ammonia concentration increases as it is approaching the Std 62 concentration when the internal source (the occupants) is turned off at 6 p.m. Then the concentration begins to go back down towards the unoccupied minimum. Thus, the concentration determined by the Std 62 formulas for ammonia was higher than the IAQDT concentration because the Std 62 formulas calculate steady state conditions based on what can be assumed the worst case, constant occupancy and minimum airflows.

Table 4 Comparison of results from IAQDT and Std 62 formulas

Contaminant	Maximum concentration(mg/m^3)		Guideline[a] (mg/m^3)	% difference (based on limit)
	IAQDT	Std 62		
Acetone	0.03311	0.03309	7.00	0.00%
Ammonia	0.15213	0.16142	0.50	1.86%
Carbon monoxide	3.29115	3.43681	10.31	1.41%
Formaldehyde	0.02031	0.02031	0.12	0.00%
Hydrogen sulphide	0.00174	0.00174	0.04	0.00%
Methyl alcohol	0.04623	0.04623	1.50	0.00%
Nitrogen dioxide	0.00400	0.00393	0.10	0.07%
Ozone	0.02162	0.02127	0.24	0.15%
Phenol	0.00594	0.00594	0.10	0.00%
Sulphur dioxide	0.00076	0.00075	0.08	0.02%
TVOC	0.16772	0.16769	1.00	0.00%

[a]ASHRAE (1981, 2001); EPA (1990) and Tucker (1988).

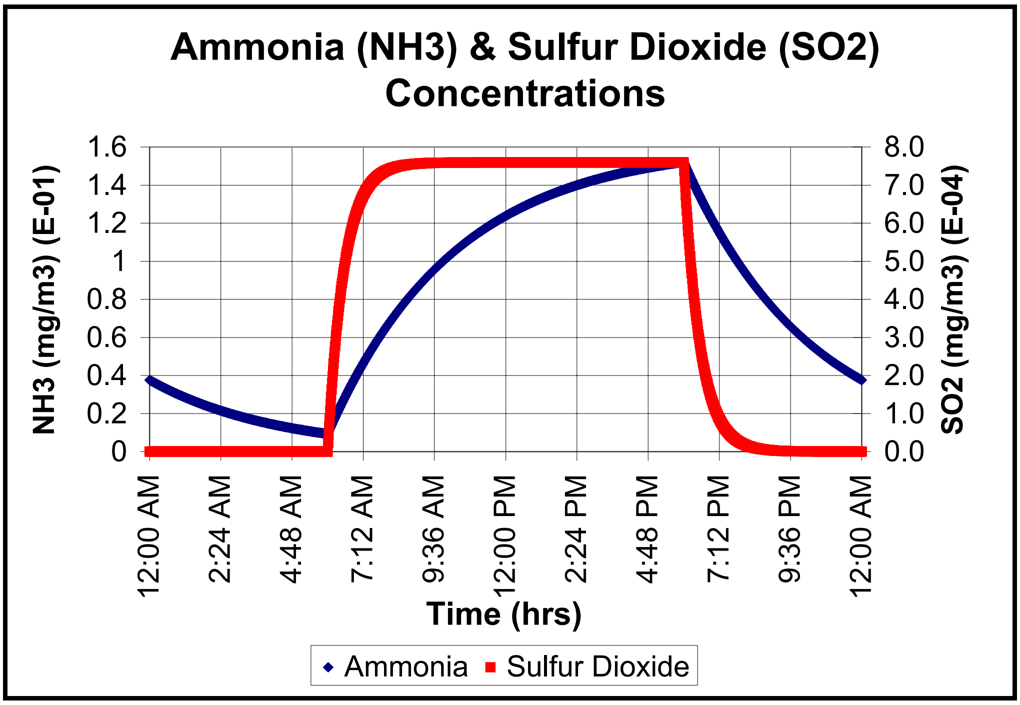

Figure 3 Contaminant concentrations versus time for ammonia and sulphur dioxide.

Carbon monoxide is a contaminant only from the outside air, but it is not being filtered and so goes through a similar pattern as ammonia. All the other compounds were filtered and reached a steady state rather quickly as compared to these two. Therefore, other differences between the results are mainly due to the number of decimal places in the spreadsheet and the IAQDT.

CONCLUSIONS

The two models discussed are based on mass balances of an HVAC system and give similar results for a given set of conditions. Main differences between the two methods can be attributed to the IAQDT software calculating transient concentrations as opposed to the long term, steady state concentrations calculated by Std 62 equations.

These two models can be applied as follows. If the worst possible scenario is desired, in terms of highest indoor concentrations, the Std 62 formulas as well as the IAQDT can be used with constant, always on generation rates and minimum airflows to derive steady state contaminant concentrations. If transient effects of HVAC operation on contaminant concentrations are desired, the IAQDT serves as a good tool to view how the contaminant concentrations change with time. Based on this study, both methods can be applicable to office spaces for contaminant based design.

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