

# **A screening model for predicting concentrations of volatile organic chemicals in shower stall air**

PAUL F. SANDERS

*Division of Science, Research and Technology, New Jersey Department of Environmental Protection, P.O. Box 409, Trenton, NJ 08625*

Telephone: (609)292-9998

FAX: (609)292-7340

e-mail: [paul.sanders@dep.state.nj.us](mailto:paul.sanders@dep.state.nj.us)

## **Abstract**

A simple equilibrium model was developed to predict maximum possible concentrations of volatile organic chemicals that may occur in shower stall air from the use of contaminated water during a showering event. The only site-specific parameter that must be known to use the model is the contaminant concentration in the influent water. Data was compiled from four previous studies for which vapor concentrations of contaminants in experimental shower stalls were measured. Peak concentrations reported in these experiments were compared to model-predicted concentrations. Experimental peak concentrations were typically within an order magnitude of concentrations predicted from the model (used under standard conditions), with the predicted value almost always being the higher of the two concentrations. When the model-predicted values were adjusted for experimentally reported values for water temperature, air exchange rates, and water flow rates, agreement between experimental and predicted values improved; predicted values usually were in the range of 1 to 3 times the experimental peak concentrations. The behavior of the model suggests that it would be useful as a screening tool for estimating maximum concentrations of volatile organic chemicals in shower stall air, arising from the use of contaminated water during a showering event. Example calculations of shower water criteria to protect against unacceptable inhalation exposures indicated that at times these criteria were lower than drinking water Maximum Contaminant Levels or other criteria based on ingestion of the water.

## **Introduction**

During the past decade, increasing attention has been given to the potential for significant inhalation exposures to volatile organic chemicals (VOCs) during showering (Moya et al., 1999; Keating et al., 1997; Giardino and Andelman, 1996; Weisel and Jo, 1996; Tancrede et al., 1992). Requests for assessments of this exposure pathway have recently become more frequent at the author's agency as awareness of its potential importance has increased. While residents of dwellings with VOC-contaminated water may be instructed to drink bottled water until a water treatment system is installed, it has also been necessary to make rapid decisions as to whether or not contaminated water may be used in the meantime for other purposes, such as for showering. This decision usually must be made when only one piece of information is known: the concentration of the VOC in the influent shower water.

Models that evaluate the potential inhalation of VOCs during showering have been evolving as the kinetics of contaminant volatilization from shower systems has become better

understood. First, the kinetics of chemical transfer between the shower water and the surrounding airspace has been studied. This transfer process is best described by the well established two-film model (Lewis and Whitman, 1924), which has recently been applied to shower systems (Moya et al., 1999; Little, 1992). Moya et al. describes a multi-step procedure for calculating concentrations of contaminants in shower stall air as function of time using this method (Moya et al., 1999). A second area of research has focused on the kinetics of air exchange between the shower stall and the rest of the bathroom and/or other rooms in the occupied structure (Little, 1992; McKone, 1987; Wilkes et al., 1996). While both of these approaches are recommended for more advanced analysis, they are too detailed for routine use as a screening tool. For screening purposes, a rapid, simple assessment of maximum contaminant concentrations that may be encountered in shower stall air is desired. Another drawback to kinetic-based models is that, while theoretically rigorous, they require data that is not available without a site-specific investigation. Such investigations are generally not conducted unless absolutely necessary, because of the disruption caused to residents and the high level of concern that it typically generates.

In this study, a simple equilibrium model has been developed to calculate a conservative estimate of the maximum concentration of a VOC that might be observed in shower stall air as a function of its concentration in the influent water. Other than the concentration of the VOC in water, the model requires only a temperature-adjusted Henry's law constant. Optionally, an estimate of the total volume of air exchanged from the shower stall and the total volume of water used may be incorporated. In order to evaluate the usefulness of the model, its predictions are compared to concentrations of VOCs measured in four recent experimental studies using model shower chambers.

## Methods

### *Screening Model*

The model is derived from the expression for the dimensionless form of the Henry's law constant, expressed in terms of moles of contaminant in each compartment:

$$H = \frac{n_{air} / V_{air}}{(n_{total} - n_{air}) / V_{water}} \quad (1)$$

where  $n_{air}$  refers to the numbers of moles in the air compartment at equilibrium,  $n_{total}$  is the total number of moles of contaminant in the shower system,  $V_{air}$  is the volume of the shower stall, with the option of including the total volume of air exchanged from the stall during the shower event, and  $V_{water}$  is the total volume of water used during a showering event. The moles of contaminants in the shower air,  $n_{air}$ , may be expressed as  $(C_{air} V_{air})/M$ , where  $C_{air}$  is the concentration of the contaminant in the air compartment at equilibrium (mass/volume) and  $M$  is its molecular weight. The total moles,  $n_{total}$ , is set as  $(C_{water} V_{water})/M$ , where  $C_{water}$  is the contaminant concentration in the influent shower water (mass/volume). This factor simply calculates the total moles of contaminant based on the volume of water used, and ignores contaminant exiting the system via the shower drain or air exchange. Substituting these expressions into Equation 1 and solving for the predicted equilibrium contaminant concentration in air from a known concentration in influent shower water yields

$$C_{air} = C_{water} \frac{HV_{water}}{HV_{air} + V_{water}} \quad (2)$$

where  $H$  is the dimensionless Henry's law constant at the temperature of the shower water.

### *Calculation of equilibrium air concentrations*

Using Equation 2 and reported influent contaminant concentrations from experimental studies, equilibrium air concentrations were calculated for chloroform, trichloroethene, ethylbenzene, toluene, cyclohexane, ethyl acetate, and acetone. Concentrations were calculated in two ways: 1) using standard values for all input parameters except for the influent VOC concentration in water, and 2) additionally adjusting  $V_{air}$ ,  $V_{water}$  and  $H$  for the total air exchanged, total water consumed, and the actual water temperatures reported by the investigators. The standard values for the model parameters were as follows: shower stall volume, 1.5 m<sup>3</sup>, no air exchange; shower water volume, 0.1 m<sup>3</sup> (10 minute shower duration with a 10 L/minute shower flow rate); shower water temperature for calculating the Henry's law constant, 40°C. The 10 minute shower duration corresponds to the 80<sup>th</sup> percentile value reported by Burmaster (1998). Relative to the reported studies, the shower stall volume was typical, the water temperature was equal to or above most temperatures, and the flow rate was a typical maximum value. Henry's law constants were calculated using temperature-dependant relationships for this parameter reported in recent research (Robbins et al., 1993; Gosset, 1987; Ashworth et al., 1988; Schoene and Steinhanses, 1985; Enviromega, 1993). The U. S. Geological Survey has conveniently summarized experimentally determined temperature-dependant relationships for the Henry's law constant for many VOCs (Rathbun, 1998). Alternatively, a theoretical approach is available to calculate Henry's law constants at a desired temperature using the Clapeyron equation and a chemical's critical temperature, boiling point, and enthalpy of vaporization (USEPA, 2000a).

### *Experimental Shower Systems*

Data was extracted from four recent studies employing experimental shower systems for which contaminant concentrations in the shower stall air were directly measured (Moya et al., 1999; Keating et al., 1997; Giardino and Andelman, 1996; Jo et al., 1990). Peak contaminant concentrations were used for comparison to the screening model (except for results from Jo et al. (1990), who reported time-averaged air concentrations). The experimental conditions for these studies varied widely with regard to shower stall air exchange rates (0-379 L/min), shower water temperatures (19-46°C) and contaminant concentrations in the influent shower water (Table 1). Values for  $V_{air}$  and  $V_{water}$  were calculated from reported shower stall volumes, air exchange rates, water flow rates, and shower duration times.

## **Results and Discussion**

Experimentally measured contaminant concentrations in shower air were compared to predicted concentrations for eighty-nine reported experiments from four investigators, a subset of which

are listed here (Table 1). For the experiments of Moya et al., Keating et al., and Giardino and Andleman, the range of experimental conditions employed are illustrated. The experiments of Jo et al. were all run under similar experimental conditions; results from the first five experiments are shown. Differences between the calculated and measured concentrations are reported as the ratio of the two values for convenience. A statistical summary of the ratio values was also prepared (Table 2). The experimental concentrations of Jo et al. were time-averaged, rather than peak values. The statistical summary was therefore calculated both with and without those experiments.

The most striking observation that can be made is the relatively close agreement between concentrations predicted with the screening model and the experimentally determined peak concentrations. When screening model calculations were adjusted for experimentally reported values for  $V_{air}$ ,  $V_{water}$  and water temperature, the average ratio of predicted concentrations to measured peak concentrations was less than three (Table 2). This ratio was reduced to less than two when the time-averaged data of Jo et al. was removed from the data set. When the ratios were determined using standard shower conditions, the mean ratio was approximately seven either with or without the data set of Jo et al. (Table 2).

Predicted concentrations were generally higher than measured results; the reason for this lies in the formulation of the screening model as a simple equilibrium system. The model does not account for the kinetics of contaminant volatilization or its loss from the shower system via air exchange and water exiting the shower drain. The entire mass of contaminant entering the system during the shower run is simply partitioned between the air and water phase under equilibrium conditions. Thus, a conservative (high) prediction of contaminant concentrations would be expected. Such a conservative prediction is desirable in a screening model, as long as the prediction is not unreasonably high. It has been suggested that a screening model should give an order-of-magnitude estimate of actual contaminant concentrations (Donigian, 1983). This condition was always met when the calculation was adjusted for experimental  $V_{air}$ ,  $V_{water}$  and water temperature values. Even when run under standard conditions, this order of magnitude agreement was achieved more than 80% of the time, and the highest ratios were still not excessively high (between 20 and 30 for some of the cyclohexane experiments).

Another desirable feature of a screening model is that it should not under predict experimental concentrations. When run under standard conditions, the model under predicted experimentally measured concentrations only 4 times out of 89 experiments, and in those four cases the under prediction was less than a factor of two. Use of the model with experimentally adjusted values for  $V_{air}$ ,  $V_{water}$  and temperature yielded predictions for 6 of 89 experiments that were between 58 and 80% of the measured values. An additional 12 predictions were only marginally low (between 80% and 100% of the measured values). While the under prediction was again less than a factor of two in all cases, it would be somewhat more prudent to calculate concentrations using standard conditions. This is also recommended for another reason: values for  $V_{air}$ ,  $V_{water}$  and water temperature are not known for actual cases without site-specific investigation. The somewhat greater over prediction of peak shower concentration that results is not excessive (a factor of seven, on average).

Attempts to quantitatively correlate the calculated ratios to the Henry's law constant or other parameters yielded poor results, due to the inherent differences in the experimental conditions between the studies and the variable mass recoveries reported. However, two general trends were observed. First, the ratios for the experiments of Jo et al. were often higher than for

Table 1. Comparison of Calculated to Experimental Contaminant Concentrations in Shower Air: Representative Results<sup>a</sup>

Contaminant	Investigator	Expt. No.	Time of shower (min)	Experimental data					Air concentrations from model (mg/m <sup>3</sup> )		Ratio of calculated to experimental concentrations			
				V <sub>water</sub> (m <sup>3</sup> )	V <sub>air</sub> (m <sup>3</sup> )	Influent water temperature (°C)	Influent water concentration (mg/L)	Peak concentration in shower air (mg/m <sup>3</sup> )	Adjusted conditions <sup>b</sup>	Standard conditions <sup>c</sup>	Adjusted conditions <sup>b</sup>	Standard conditions <sup>c</sup>		
Chloroform	Keating et al. (1997)	1	10	0.034	3.7	35	57	630	506	3090	0.8	4.9		
		2	10	0.034	3.7	45	58.7	780	529	3183	0.7	4.1		
		5	10	0.034	3.7	40	55.6	430	498	3014	1.2	7.0		
	Giardino and Andelman (1996)	11	11.1	0.056	2.2	42	0.582	16	13	32	0.8	2.0		
		12	11.1	0.056	4.0	27	0.555	7.7	7	30	0.9	3.9		
		13	11.1	0.111	1.8	28	0.677	24.9	31	37	1.2	1.5		
	Jo et al. (1990)	1	10	0.087	1.7	40	0.0129	0.0692 <sup>d</sup>	0.6	0.7	8.3	10.1		
		2	10	0.087	1.7	40	0.013	0.0581 <sup>d</sup>	0.6	0.7	9.9	12.1		
		3	10	0.087	1.7	40	0.02	0.1242 <sup>d</sup>	0.9	1.1	7.1	8.7		
		4	10	0.087	1.7	40	0.021	0.897 <sup>d</sup>	0.9	1.1	1.0	1.3		
		5	10	0.087	1.7	40	0.0228	0.899 <sup>d</sup>	1.0	1.2	1.1	1.4		
	Trichloroethene	Giardino and Andelman (1996)	2	21.7	0.111	7.4	22	0.959	14.3	14	58	1.0	4.1	
			3	18.6	0.184	2.0	21	0.493	42.8	36	30	0.8	0.7	
5			18.6	0.093	3.0	46	0.922	41.9	27	56	0.7	1.3		
6			18.6	0.093	6.5	44	0.589	13.7	8	36	0.6	2.6		
7			18.6	0.186	2.0	33	0.519	54.9	41	31	0.7	0.6		
8			18.6	0.184	5.7	32	0.875	33	27	53	0.8	1.6		
Cyclohexane			Moya et al. (1999)	1	8	0.073	4.6	21	1.8	6.9	28	119	4.1	17.3
				3	8	0.049	4.5	21	3.1	7.9	33	205	4.2	26.0
	5	8		0.073	4.7	35	2.6	9.3	40	172	4.3	18.5		
	7	8		0.049	4.6	36	1.9	6.3	20	126	3.2	20.0		
Ethylbenzene	Moya et al. (1999)	1	8	0.073	4.6	21	6.1	29	91	368	3.1	12.7		
		3	8	0.049	4.5	21	7.5	26	77	453	3.0	17.4		
		5	8	0.073	4.7	35	8	35	120	483	3.4	13.8		
		7	8	0.049	4.6	36	5.2	30	54	314	1.8	10.5		
Toluene	Moya et al. (1999)	1	8	0.073	4.6	21	4.5	41	66	261	1.6	6.4		
		3	8	0.049	4.5	21	7	34	72	406	2.1	11.9		
		5	8	0.073	4.7	35	6.4	56	95	371	1.7	6.6		
		7	8	0.049	4.6	36	5.6	47	58	325	1.2	6.9		
Ethyl acetate	Moya et al. (1999)	1	8	0.073	4.6	21	26.2	68	87	219	1.3	3.2		
		3	8	0.049	4.5	21	25.8	57	78	215	1.4	3.8		
		5	8	0.073	4.7	35	24.4	130	125	204	1.0	1.6		
		7	8	0.049	4.6	36	23.6	81	108	197	1.3	2.4		
Acetone	Moya et al. (1999)	1	8	0.073	4.6	21	38.1	36	36	105	1.0	2.9		
		3	8	0.049	4.5	21	42	35	38	116	1.1	3.3		
		5	8	0.073	4.7	35	41.6	77	80	115	1.0	1.5		
		7	8	0.049	4.6	36	41.1	71	79	113	1.1	1.6		

<sup>a</sup> Experimental contaminant concentrations in air are peak values measured unless otherwise noted. Total number of experiments = 89.

<sup>b</sup> V<sub>water</sub>, V<sub>air</sub>, and Henry's law constant adjusted for experimental conditions

<sup>c</sup> Standard conditions as described in text

<sup>d</sup> Experimental concentrations are average values over duration of shower runs

**Table 2. Ratio of Calculated to Experimental Contaminant Concentrations in Shower Air: Statistical Summary**

	Model calculations adjusted for experimental conditions <sup>a</sup>		Model calculations under standard conditions <sup>b</sup>	
	All experimental data (n=89)	All data except Jo et al. (n=70)	All experimental data (n=89)	All data except Jo et al. (n=70)
Average ratio	2.7	1.7	7.2	7.0
Std. dev. of ratio	2.4	1.1	5.8	6.4
Ratio range	0.6-9.9	0.6-5.6	0.6-26	0.6-26

<sup>a</sup> Experimental values for water temperature,  $V_{air}$  and  $V_{water}$

<sup>b</sup> Standard values for water temperature,  $V_{air}$  and  $V_{water}$  as given in text

other studies, which may be attributable to the time-averaged, rather than peak, concentrations reported in this study. Second, consideration of only the results of Moya et al. allows for comparison of five different chemicals under consistent experimental conditions, since the experiments were run using a mixture of the chemicals studied. Moya et al. suggested that a rapid approach to equilibrium might occur with compounds with low values of Henry's law constants, because the amount of mass transfer required is small. This suggests that the simple equilibrium-based screening model used in this study may be most accurate for contaminants with lower values for the Henry's law constant. This hypothesis is supported by the results of this study, in that the two chemicals with the lowest values for the dimensionless Henry's law constant at 40°C (acetone, 0.003, and ethyl acetate, 0.009) had ratios of predicted-to-measured concentrations (using site-specific conditions) of approximately one (Table 1). Ethyl benzene and toluene have higher Henry's law constants (0.64 and 0.444 at 40°C, respectively), and yielded average ratios of 2.6 and 1.6. Cyclohexane, with the highest Henry's law constant (11.7 at 40°C), yielded an average ratio of 3.6. Moya reported lower mass recoveries for the chemicals with higher Henry's law constants. This could lead to ratios as high as 1.5 for cyclohexane and ethyl benzene based on the recoveries reported. However, since ratios larger than this were observed for these two chemicals, it appears that they were not able partition to equilibrium conditions in the shower experiments because of amount of mass transfer required was high, particularly for cyclohexane.

A simple rearrangement of Equation 2 may be used to predict acceptable influent water concentrations from an allowed air concentration in the shower stall. The latter concentration would be a function of the inhalation toxicity endpoint selected by the user and the inhalation exposure time assumed. For noncarcinogens, the acceptable water concentration is

$$C_{water} = RfC \frac{1440}{10} \frac{HV_{air} + V_{water}}{HV_{water}} \quad (3)$$

where  $RfC$  is the inhalation reference concentration, and the ratio of 1440/10 is an adjustment made for the dose that would normally be received over 24 hours (1440 minutes) being concentrated into a 10 minute shower exposure time period. For carcinogens, the equivalent equation is

$$C_{water} = \frac{10^{-6}}{URF} \frac{1440}{10} \frac{HV_{air} + V_{water}}{HV_{water}} \quad (4)$$

where  $10^{-6}$  is the acceptable risk level and  $URF$  is the inhalation unit risk factor. It has been estimated that dermal exposure may be roughly equivalent to inhalation exposure during a showering event (Jo et al., 1990). Incorporating this assumption into the calculation of an acceptable water concentration would require dividing the result from Equations (3) and (4) by a factor of two.

Example shower water criteria for selected VOCs to protect against unacceptable inhalation exposures are listed in Tables 3 and 4. Table 3 lists six noncarcinogens of potential concern, and Table 4 lists five carcinogens. Inhalation reference concentrations ( $RfCs$ ) and unit risk factors ( $URFs$ ) were taken from the USEPA IRIS or HEAST databases (USEPA, 2002; USEPA, 1997). Also shown in these tables are current New Jersey groundwater health criteria, based on ingestion of groundwater (NJDEP, 1993) and Maximum Contaminant Levels (MCLs) for several of the chemicals in drinking water (NJDEP, 1994; USEPA, 2000b). Henry's law constants at 40°C for these calculations were determined using a software package available from the Environmental Protection Agency (USEPA, 2000a).

**Table 3. Acceptable VOC Concentrations in Shower Stall Water to Protect Against Unacceptable Inhalation Exposures: Noncarcinogens**

Chemical	Reference Concentration (RfC) in Air ( $\mu\text{g}/\text{m}^3$ ) <sup>a</sup>	Shower Water Criteria ( $\mu\text{g}/\text{L}$ )		NJDEP Groundwater Health Criteria <sup>b</sup> ( $\mu\text{g}/\text{L}$ )
		No dermal absorption	With dermal absorption	
Acetone	350	19,400	9,700	700
1,1-Dichloroethane	50	130	65	50 <sup>c</sup>
1,2-Dichloroethene (cis)	35	93	46	70 <sup>c</sup>
1,2-Dichloroethene (trans)	60	140	70	100 <sup>c</sup>
MTBE	300	1700	850	70 <sup>c</sup>
Tertiary buty alcohol (TBA)	61	7,800	3,900	100

<sup>a</sup>USEPA(2002); USEPA(1997)

<sup>b</sup>NJDEP(1993)

<sup>c</sup>equals Maximum Contaminant Level (USEPA(2000b); NJDEP(1994))

If dermal adsorption is ignored, the shower water criteria shown for the example noncarcinogens are all higher than the New Jersey groundwater criteria and/or MCLs (Table 3). When adjustment is made for dermal adsorption, the criteria for *cis*- and *trans*-1,2-dichloroethene fall slightly lower than the criteria based on adsorption, but overall the shower inhalation pathway for these chemicals is not a significant concern relative to the ingestion pathway.

**Table 4. Acceptable VOC Concentrations in Shower Stall Water to Protect Against Unacceptable Inhalation Exposures: Carcinogens**

Chemical	Unit Risk Factor (URF) in Air ( $\mu\text{g}/\text{m}^3$ ) <sup>-1a</sup>	Shower Water Criteria ( $\mu\text{g}/\text{L}$ )		NJDEP Groundwater Health Criteria <sup>b</sup> ( $\mu\text{g}/\text{L}$ )	Maximum Contaminant Level (MCL) <sup>c</sup> ( $\mu\text{g}/\text{L}$ )
		No dermal absorption	With dermal absorption		
Benzene	$8.3 \times 10^{-6}$	0.30	0.15	0.2	1
Carbon tetrachloride	$1.5 \times 10^{-5}$	0.15	0.08	0.4	2
Chloroform	$2.3 \times 10^{-5}$	0.12	0.06	70	
Trichloroethene	$1.7 \times 10^{-6}$	1.38	0.69	1	1
1,1-Dichloroethene	$5.0 \times 10^{-5}$	0.04	0.02	1	2

<sup>a</sup>USEPA(2002); USEPA(1997)

<sup>b</sup>NJDEP(1993)

<sup>c</sup>USEPA(2000b); NJDEP(1994)

For the example carcinogens, shower water criteria were usually lower than the corresponding MCL values and the groundwater health criteria, particularly if the criteria were adjusted for dermal exposure during showering (Table 4). Of particular note is chloroform, which does not have an MCL but does have a groundwater criterion of 70  $\mu\text{g}/\text{L}$  based on ingestion. The shower water criteria for chloroform of 0.12  $\mu\text{g}/\text{L}$  (0.06  $\mu\text{g}/\text{L}$  with adjustment for dermal exposure) is substantially lower than the groundwater criteria and suggests that the showering exposure pathway may be worthy of further consideration for some chemicals when VOCs are regulated in potable water.

The results of this study suggest that the simple model described may serve as a useful and reasonably conservative screening tool for deciding whether or not potential inhalation exposures resulting from VOC-contaminated shower water are significant relative to other exposure pathways such as ingestion. For site-specific cases, the model may suggest whether the inhalation exposure pathway warrants further investigation. For follow-up site-specific investigation, either on-site measurements, or alternatively, more sophisticated models, such as the two-film model approach, described by Little and Moya et al., are recommended.

### Acknowledgments

This research was supported through the New Jersey A-280 Drinking Water Research Fund. The author thanks Cynthia Howard-Reed for providing additional information pertaining to the experiments of Moya et al. The author also thanks Thomas Ledoux, Gloria Post and Alan Stern for assistance with risk assessment issues pertaining to the study.

### Supplementary Information

Model-calculated and experimentally measured peak contaminant concentrations in shower stall air for all experiments used in this study are shown in the Appendix.

## References

- Ashworth R.A., Howe G.B., Mullins M.E., and Rogers T.N. Air-water partitioning coefficients of organics in dilute aqueous solutions. *J Hazard. Mater.* 1988: 18: 25-36.
- Burmester D.E. A lognormal distribution for time spent showering. *Risk Anal.* 1998: 18: 33-35.
- Donigian A.S. Model predictions vs. field observations: The model validation/testing process. In: Swan R.L., and Eschenroeder A., eds. *Fate of Chemicals in the Environment*. ACS Symposium Series No. 225. American Chemical Society: Washington, DC, 1983; 151-171.
- Enviromega. Collection system organic release algorithm: User's Manual. Environmega, Inc.: Flamborough, Ontario, Canada, 1993; 13.
- Giardino N.J., and Andelman J.B. Characterization of the emissions of trichloroethylene, chloroform, and 1,2 dibromo-3-chloropropane in a full-size, experimental shower. *J Exposure Anal. Environ. Epidemiol.* 1996: 6: 413-423.
- Gossett J.M. Measurement of Henry's law constants for C<sub>1</sub> and C<sub>2</sub> chlorinated hydrocarbons. *Environ. Sci. Technol.* 1987: 21: 202-208.
- Jo W.K., Weisel C.P., and Liroy P.J. Routes of chloroform exposure and body burden from showering with chlorinated tap water. *Risk Anal.* 1990: 10: 575-580.
- Keating G.A., McKone T.E., and Gillett J.W. Measured and estimated air concentrations of chloroform in showers: effects of water temperature and aerosols. *Atmos. Environ.* 1997: 31: 123-130.
- Lewis W.K., and Whitman W.G. *Ind.Eng. Chem.* 1924:16: 1215-1220.
- Little J.C. Applying the two-resistance theory to contaminant volatilization in showers. *Environ. Sci. Technol.* 1992: 26: 1341-1349.
- Moya J., Howard-Reed C., and Corsi R.L. Volatilization of chemicals from tap water to indoor air from contaminated water used for showering. *Environ. Sci. Technol.* 1999: 33: 2321-2327.
- McKone T.E. Human exposure to volatile organic compounds in household tap water: the indoor inhalation pathway. *Environ. Sci. Technol.* 1987: 12: 1194-1201.
- NJDEP. New Jersey Drinking Water Quality Institute. Maximum Contaminant Level Recommendations for Hazardous Contaminants in Drinking Water. Submitted to the New Jersey Department of Environmental Protection: Trenton, NJ. 1994.
- NJDEP. New Jersey Ground Water Quality Standards. N.J.A.C. 7:9-6. New Jersey Dept. of Environmental Protection: Trenton, NJ. 1993.

Rathbun R.E. *Transport, Behavior, and Fate of Volatile Organic Compounds in Streams*. U.S. Geological Survey Professional Paper 1589. U.S. Government Printing Office: Washington, DC, 1998.

Robbins G.A., Wang S., and Stuart J.D. Using the static headspace method to determine Henry's law constants. *Anal. Chem.* 1993: 65: 3113-3118.

Schoene K., and Steinhanes J. Determination of Henry's law constant by automated head spacegas chromatography: Determination of dissolved gases. *Fresenius Z. Anal. Chem.* 1985: 321: 538-543.

Tancrede M., Yanagisawa Y., and Wilson R. Volatilization of volatile organic compounds from showersI. Analytical method and quantitative assessment. *Atmos. Environ.* 1992: 26A: 1103-1111.

USEPA. (U.S. Environmental Protection Agency) Integrated Risk Information System (IRIS) (<http://toxnet.nlm.nih.gov>). Updated February 13, 2002. Office of Research and Development, National Center for Environmental Assessment: Washington, DC, 2002.

USEPA. User's guide for the Johnson and Ettinger (1991) model for subsurface vapor intrusion into buildings (revised). U.S. Environmental Protection Agency, Office of Emergency and Remedial Response: Washington, DC, 2000a.

USEPA. National Primary Drinking Water Regulations. 40 CFR141.1. U.S. Environmental Protection Agency, Office of Water: Washington, DC, 2000b.

USEPA. Health Effects Assessment Summary Tables. FY 1997 Update. EPA-540/R-97-036. Office of Research and Development and Office of Solid Waste and Emergency Response: Washington, DC, 1997.

Weisel, C.P.; Jo, W.K. Ingestion, inhalation, and dermal exposures to chloroform and trichloroethene from tap water. *Environ. Health Perspec.* 1996: 104, 48-51.

Wilkes C.R., Small M.J., Davidson C.I., and Andelman J.B. Modeling the effects of water usage and cobehavior on inhalation exposures to contaminants volatilized from household water. *J Exposure AnaL Environ. Epidemiol.* 1996: 6: 393-412.

## APPENDIX

Supporting Information for "A screening model for predicting concentrations of volatile organic chemicals in shower stall air", by Paul F. Sanders

Calculated versus Measured Experimental Contaminant Concentrations in Shower Air: All Experiments<sup>a</sup>

Contaminant	Investigator	Expt No. conditions <sup>c</sup>	Experimental Data						Air concentrations from model (mg/m <sup>3</sup> )		Ratio of calculated to experimental	
			Time of Shower (min)	$V_{waters}$ (m <sup>3</sup> )	$V_{airs}$ (m <sup>3</sup> )	Influent water temperature (°C)	Influent water concentration (mg/L)	Peak concentration in shower air (mg/m <sup>3</sup> )	Adjusted conditions <sup>b</sup>	Standard conditions <sup>c</sup>	Adjusted conditions <sup>b</sup>	Standard
			concentrations									
Chloroform	Keating et al. (1)	1	10	0.034	3.7	35	57	630	506	3090	0.8	4.9
		2	10	0.034	3.7	45	58.7	780	529	3183	0.7	4.1
		3	10	0.034	3.7	35	60	520	533	3253	1.0	6.3
		4	10	0.034	3.7	45	50.9	530	459	2760	0.9	5.2
		5	10	0.034	3.7	40	55.6	430	498	3014	1.2	7.0
		6	10	0.034	3.7	40	56.6	310	507	3069	1.6	9.9
	Giardino and Andelman (2)	10	11.1	0.056	2.3	26	0.634	11.1	13	34	1.2	3.1
		11	11.1	0.056	2.2	42	0.582	16	13	32	0.8	2.0
		12	11.1	0.056	4.0	27	0.555	7.7	7	30	0.9	3.9
		13	11.1	0.111	1.8	28	0.677	24.9	31	37	1.2	1.5
		14	11.1	0.056	2.3	29	1.11	19.6	23	60	1.2	3.1
	Jo et al. (3)	1	10	0.087	1.7	40	0.0129	0.0692 <sup>d</sup>	0.6	0.7	8.3	10.1
		2	10	0.087	1.7	40	0.013	0.0581 <sup>d</sup>	0.6	0.7	9.9	12.1
		3	10	0.087	1.7	40	0.02	0.1242 <sup>d</sup>	0.9	1.1	7.1	8.7
		4	10	0.087	1.7	40	0.021	0.897 <sup>d</sup>	0.9	1.1	1.0	1.3
		5	10	0.087	1.7	40	0.0228	0.899 <sup>d</sup>	1.0	1.2	1.1	1.4
		6	10	0.087	1.7	40	0.0237	0.1172 <sup>d</sup>	1.0	1.3	9.0	11.0
		7	10	0.087	1.7	40	0.0242	0.2 <sup>d</sup>	1.1	1.3	5.4	6.6
		8	10	0.087	1.7	40	0.0248	0.1748 <sup>d</sup>	1.1	1.3	6.3	7.7
9		10	0.087	1.7	40	0.0265	0.1681 <sup>d</sup>	1.2	1.4	7.0	8.5	
10		10	0.087	1.7	40	0.0278	0.1952 <sup>d</sup>	1.2	1.5	6.3	7.7	
11		10	0.087	1.7	40	0.0308	0.2002 <sup>d</sup>	1.4	1.7	6.8	8.3	
12		10	0.087	1.7	40	0.0316	0.2259 <sup>d</sup>	1.4	1.7	6.2	7.6	
13		10	0.087	1.7	40	0.04	0.3269 <sup>d</sup>	1.8	2.2	5.4	6.6	
14	10	0.087	1.7	40	0.022	0.1259 <sup>d</sup>	1.0	1.2	7.7	9.5		
15	10	0.087	1.7	40	0.0232	0.1192 <sup>d</sup>	1.0	1.3	8.6	10.6		
16	10	0.087	1.7	40	0.0254	0.1341 <sup>d</sup>	1.1	1.4	8.4	10.3		
17	10	0.087	1.7	40	0.0289	0.1963 <sup>d</sup>	1.3	1.6	6.5	8.0		
18	10	0.087	1.7	40	0.0291	0.2278 <sup>d</sup>	1.3	1.6	5.7	6.9		
19	10	0.087	1.7	40	0.0356	0.3134 <sup>d</sup>	1.6	1.9	5.0	6.2		
Trichloroethene	Giardino and Andelman (2)	1	23.1	0.116	3.5	27	0.486	19.6	15	29	0.8	1.5
		2	21.7	0.111	7.4	22	0.959	14.3	14	58	1.0	4.1
		3	18.6	0.184	2.0	21	0.493	42.8	36	30	0.8	0.7
		4	18.6	0.186	6.0	19	0.422	14.7	12	25	0.8	1.7
		5	18.6	0.093	3.0	46	0.922	41.9	27	56	0.7	1.3
		6	18.6	0.093	6.5	44	0.589	13.7	8	36	0.6	2.6
		7	18.6	0.186	2.0	33	0.519	54.9	41	31	0.7	0.6
		8	18.6	0.184	5.7	32	0.875	33	27	53	0.8	1.6
		9	18.6	0.184	2.1	25	0.792	58.3	57	48	1.0	0.8

Contaminant	Investigator	Expt No. conditions <sup>c</sup>	Experimental Data						Air concentrations from model (mg/m <sup>3</sup> )		Ratio of calculated to experimental	
			Time of Shower (min)	$V_{waters}$ (m <sup>3</sup> )	$V_{airs}$ (m <sup>3</sup> )	Influent water	Influent water	Peak concentration	Adjusted conditions <sup>b</sup>	Standard conditions <sup>c</sup>	Adjusted conditions <sup>b</sup>	Standard
						temperature (°C)	concentration (mg/L)	in shower air (mg/m <sup>3</sup> )				
Cyclohexane	Moya et al. (4)	1	8	0.073	4.6	21	1.8	6.9	28	119	4.1	17.3
		2	8	0.073	4.4	22	3.3	9.7	54	219	5.6	22.6
		3	8	0.049	4.5	21	3.1	7.9	33	205	4.2	26.0
		4	8	0.049	4.5	22	2	6.3	22	133	3.4	21.0
		5	8	0.073	4.7	35	2.6	9.3	40	172	4.3	18.5
		6	8	0.073	4.5	34	1.6	5.4	26	106	4.8	19.6
		6 rep	8	0.073	4.7	34	0.71	6.5	11	47	1.7	7.2
		7	8	0.049	4.6	36	1.9	6.3	20	126	3.2	20.0
Ethylbenzene	Moya et al. (4)	8	8	0.049	4.6	35	1.8	6	19	119	3.2	19.9
		8 rep	8	0.049	4.6	34	0.84	5.7	9	56	1.6	9.8
		1	8	0.073	4.6	21	6.1	29	91	368	3.1	12.7
		2	8	0.073	4.4	22	7.3	32	114	441	3.6	13.8
		3	8	0.049	4.5	21	7.5	26	77	453	3.0	17.4
		4	8	0.049	4.5	22	5.5	18	57	332	3.2	18.4
		5	8	0.073	4.7	35	8	35	120	483	3.4	13.8
		6	8	0.073	4.5	34	4.6	34	72	278	2.1	8.2
Toluene	Moya et al. (4)	6 rep	8	0.073	4.7	34	3.9	34	59	235	1.7	6.9
		7	8	0.049	4.6	36	5.2	30	54	314	1.8	10.5
		8	8	0.049	4.6	35	5.6	29	58	338	2.0	11.7
		8 rep	8	0.049	4.6	34	4.5	27	47	272	1.7	10.1
		1	8	0.073	4.6	21	4.5	41	66	261	1.6	6.4
		2	8	0.073	4.4	22	7	57	108	406	1.9	7.1
		3	8	0.049	4.5	21	7	34	72	406	2.1	11.9
		4	8	0.049	4.5	22	6.1	36	63	354	1.7	9.8
Ethyl acetate	Moya et al. (4)	5	8	0.073	4.7	35	6.4	56	95	371	1.7	6.6
		6	8	0.073	4.5	34	5.3	55	82	307	1.5	5.6
		6 rep	8	0.073	4.7	34	5.1	62	77	296	1.2	4.8
		7	8	0.049	4.6	36	5.6	47	58	325	1.2	6.9
		8	8	0.049	4.6	35	6	48	61	348	1.3	7.2
		8 rep	8	0.049	4.6	34	5.4	47	56	313	1.2	6.7
		1	8	0.073	4.6	21	26.2	68	87	219	1.3	3.2
		2	8	0.073	4.4	22	21.9	81	76	183	0.9	2.3
Acetone	Moya et al. (4)	3	8	0.049	4.5	21	25.8	57	78	215	1.4	3.8
		4	8	0.049	4.5	22	30.9	83	96	258	1.2	3.1
		5	8	0.073	4.7	35	24.4	130	125	204	1.0	1.6
		6	8	0.073	4.5	34	23.6	120	119	197	1.0	1.6
		6 rep	8	0.073	4.7	34	24.7	140	124	206	0.9	1.5
		7	8	0.049	4.6	36	23.6	81	108	197	1.3	2.4
		8	8	0.049	4.6	35	23.7	120	105	198	0.9	1.6
		8 rep	8	0.049	4.6	34	24	130	104	200	0.8	1.5

Contaminant	concentrations Investigator Expt No. conditions <sup>c</sup>		Experimental Data						Air concentrations from model (mg/m <sup>3</sup> )		Ratio of calculated to experimental	
			Time of Shower (min)	V <sub>waters</sub> (m <sup>3</sup> )	V <sub>airs</sub> (m <sup>3</sup> )	Influent water temperature (°C)	Influent water concentration (mg/L)	Peak concentration in shower air (mg/m <sup>3</sup> )	Adjusted conditions <sup>b</sup>	Standard conditions <sup>c</sup>	Adjusted conditions <sup>b</sup>	Standard
Acetone	Moya et al. (4)	6 6 rep 7 8 8 rep	8 8 8 8 8	0.073 0.073 0.049 0.049 0.049	4.5 4.7 4.6 4.6 4.6	34 34 36 35 34	40.4 39.9 41.1 41.8 40.1	76 81 71 78 120	75 74 79 76 70	111 110 113 115 111	1.0 0.9 1.1 1.0 0.6	1.5 1.4 1.6 1.5 0.9

<sup>a</sup>Experimental contaminant concentrations in air are peak values measured unless otherwise noted. Total number of experiments = 89.

<sup>b</sup>V<sub>water</sub>, V<sub>air</sub> and Henry's law constant adjusted for experimental conditions

<sup>c</sup>Standard conditions as described in text

<sup>d</sup>Experimental concentrations are average values over duration of shower runs

### References

1. Keating, G.A.; McKone, T.E.; Gillett, J.W. Measured and estimated air concentrations of chloroform in showers: effects of water temperature and aerosols. *Atmos. Environ.* (1997) 31:123-130.
2. Giardino, N.J.; Andelman, J.B. Characterization of the emissions of trichloroethylene, chloroform, and 1,2-dibromo-3-chloropropane in a full-size, experimental shower. *J. Exposure Anal. Environ. Epidemiol.* (1996) 6: 413-423.
3. Jo, W.K.; Weisel, C.P.; Liou, P.J. Routes of chloroform exposure and body burden from showering with chlorinated tap water. *Risk Anal.* (1990) 10: 575-580.
4. Moya, J.; Howard-Reed, C.; Corsi, R.L. Volatilization of chemicals from tap water to indoor air from contaminated water used for showering. *Environ. Sci. Technol.* (1999) 33: 2321-2327.