

Integrating a Toxicological Approach for Breakthrough Curves of Organic Vapor Mixtures in the Estimation of Respirator Cartridge Service Life

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ABSTRACT

The estimation of cartridge service life (CSL) for mixtures of contaminants is a complex task. OSHA-CPL-02-00-158 recommends the use of the additivity principle, which assumes that the entire mixture behaves like a pure system of the most volatile contaminant (i.e., sum up the concentration of the components). Here we present a quantitative risk assessment framework to predict potential human health risk when estimating CSL to avoid vapor gas breakthrough inside the mask, premature change schedules, and unnecessary costs. Simulations using the Ideal Adsorbed Solution Theory (IAST) - Langmuir model combined with the modified Wheeler-Jonas equation allowed the calculation of breakthrough curves for vapor mixtures. Acetone was used as an example of a volatile organic contaminant combined in binary mixture with one of the following: m-xylene, o-xylene, styrene, or toluene. Simulations of exposures to acetone (10-700 ppm) and the other contaminant of lower volatility (500 ppm) through a respiratory cartridge with 50 g of carbon at 25°C and a flow rate of 24 L/min were performed. Outlet concentrations were used to determine the Hazard Index (HI) throughout the exposure. The HI is defined as the sum of concentrations for each mixture component normalized by its Occupational Exposure Limit (OEL) Value ($HI > 1$ indicates a health risk). Cartridge service life estimations based on the 10% breakthrough times of acetone and the 10% of HI for the mixture were compared. Simulations of breakthrough curves were in agreement with experimental data previously published. At lower acetone concentrations (< 50 ppm), the simulated CSL using 10% HI of the vapor mixture were up to two times greater than the 10% than the ones calculated following the 10% breakthrough time additive concentration's approach). At higher concentrations of acetone, both approaches gave similar results. The breakthrough time of HI is inversely proportional to the concentration ratio of contaminant 1 (C_1), the more volatile, to contaminant 2 (C_2), the less volatile contaminant, suggesting that using the HI approach can be useful when $C_1/C_2 < 2$.

Keywords: breakthrough curve, vapor mixtures, cartridge service life, hazard index.

INTRODUCTION

The Respiratory Protection Committee (RPC) of the American Industrial Hygiene Association (AIHA) has identified reliable assessment of respirator performance in the laboratory and workplace environment as a research priority (Ettinger, Janssen, & Metzler, 2009). Because the accuracy of cartridge service life prediction models for organic vapors is influenced by environmental conditions (Nelson & Correia, 1976; Ruch, Nelson, Lindeken, Johnsen & Hodgkins, 1972), several investigations have focused on the effect of moisture (Wood 1985), temperature (Nelson, Correia, & Harder, 1976), flow rate/breathing rate (Coyne, Caretti, Scott, Johnson, & Koh, 2006; Linders, Mallens, van Bokhoven, Kapteijn, & Moulijn, 2003; Nelson & Harder, 1972) and concentration (Nelson & Harder, 1976) on cartridge service life.

In our previous work, we have characterized ten activated carbons from commercially available respirator cartridges by using breakthrough experiments in experimental conditions similar to working environments. We showed that predicted adsorption capacities obtained from the characterization of the micropore volume of activated carbon using organic vapors of different vapor pressure fit well with the experimental data (Janvier, Tuduri, Cossement, Drolet, & Lara, 2015). Additionally, we have applied these aforementioned experimental conditions to the design of a miniaturized cartridge, which was able to mitigate the influence of the effect of flow rate and also having a better control on the environmental conditions (temperature, air humidity) (Janvier, Tuduri, Cossement, Drolet, & Lara, 2016).

However, in real working environments, the air is often contaminated with more than one contaminant making the prediction of cartridge service life for vapor mixtures complex. Early works investigated the effects of binary mixtures on respirator cartridge service life and presented qualitative observations (Jonas & Rehmann, 1972; Nelson & Correia, 1976; Swearengen & Weaver, 1988) but these studies lack thorough understanding of multivapor adsorption mechanism. In the 1990s Lara, Yoon and collaborators (Lara, Yoon, & Nelson, 1995; Yoon, Nelson, Lara, Kamel, & Fregeau, 1991; Young Hee Yoon, Nelson, & Lara, 1996) developed a mathematical approach for binary mixtures and multivapors. They showed that breakthrough may occur earlier when in mixtures than it would for the single contaminant. Their descriptive model relied on fitting parameters that have to be obtained from experimental data.

Vahdat, Swearengen, and Johnson (1994) developed a simple method for predicting breakthrough curves for binary mixtures based on the Wheeler-Jonas equation and the IAST (*Ideal Adsorbed Solution Theory*) model combined with the Langmuir equation to obtain adsorption isotherms for each component. This model was successfully applied to binary mixtures of acetone-m-xylene, acetone-styrene, and carbon dioxide-water. Extensive research based on another combination of IAST Dubinin-Radushkevich has been investigated by Wood and Snyder (2007) and resulted in the creation of the program Multivapor™ available on the National Institute for Occupational Safety and Health (NIOSH) website. Also, Vuong and collaborators (2016) have developed a model based on partial differential equations to predict the breakthrough of binary vapor mixtures.

However, the only existing directive for the estimation of cartridge service life for contaminant mixtures is the OSHA compliance directive *CPL 2-0.120, Inspection procedures for the Respiratory Protection Standard*, which recommends the use of the additive concentration effect for multi-component, by which the concentration of all the components are summed up and considered to behave as a pure single contaminant for the most volatile contaminant (OSHA, 1998). This approach is simplistic and does not take into account the quantity and toxicity (e.g. cumulative effect) of the contaminants.

Furthermore, the notion that the concentration required to produce a given effect is constant under all concentration-time conditions does not apply because of the displacement phenomenon, where

the more volatile contaminant is desorbed by the less volatile contaminant, which has greater affinity with the carbon than the less volatile contaminant.

The framework presented here determines the cartridge service life of binary mixtures by integrating a toxicological approach based on the hazard index (HI) principle to predict potential human health risk to ensure proper use of respirator cartridge while avoiding premature change schedules and unnecessary costs. To do so, the Vahdat and the Wheeler-Jonas models were employed to predict breakthrough curves of the following binary systems: acetone- m-xylene, acetone- o-xylene, acetone-toluene and acetone-styrene. The IAST (Ideal Adsorbed Solution Theory) - Langmuir equations were used to predict mixture adsorption capacity from the pure single contaminant adsorption data.

THEORY

Langmuir

The Langmuir equation has a simple form and is used extensively in adsorption systems. The Langmuir equation was selected in this study because the calculation is simple and there are abundant adsorption data in the literature for pure components. Therefore, the adsorption capacity, We for a pure contaminant i using the Langmuir equation is currently used and is expressed in the following form:

$$We = \frac{m_i k_i C}{1 + k_i C} \quad (1)$$

where m and k are Langmuir parameters related to the adsorption capacity and the rate of adsorption for a specific activated carbon-contaminant system, and C is the concentration of the pure contaminant.

The Langmuir parameters are commonly determined by fitting experimental data. However, the adsorption isotherm is different for each system, and a set of parameters needs to be determined.

Ideal Adsorbed Solution Theory (IAST)

The Ideal Adsorbed Solution Theory (IAST) is a well-known model to predict the adsorption of gas mixtures by using adsorption data from pure components (Myers & Prausnitz, 1965). The model is based on the thermodynamic equivalence of the spreading pressure of each adsorbent at equilibrium.

The spreading pressure, Π , corresponds to the difference in surface tension of a clean surface and an adsorbate-adsorbent interface, considering the same temperature. The model assumes that the solution is ideal, which means that no interaction between adsorbent-adsorbate is considered and is expressed as:

$$\frac{\Pi A}{RT} = \int_0^{p_i^0} \frac{W_{\epsilon i}^0}{P} \quad (2)$$

where A is the area of the adsorbent, $W_{\epsilon i}^0$ is the adsorption capacity of the pure component i , P is the total pressure, T is the temperature, and R is the universal gas constant. Vahdat (1994) successfully applied the Langmuir equation to the IAST model with:

$$\frac{\Pi_i A}{RT} = m_i \ln(1 + k_i p_i^0) \quad (3)$$

where p_i^0 is the pure component pressure of component i at the spreading pressure of the mixture. With the postulate that the spreading pressure Π , for each contaminant is equal at the adsorption equilibrium the following equation applies to a binary system:

$$m_1 \ln(1 + k_1 p_1^0) = m_2 \ln(1 + k_2 p_2^0) \quad (4)$$

Additionally, the mole fraction X_1 of component 1 is calculated from:

$$X_1 = \frac{PY_1}{p_1^0} \quad (5)$$

where Y_1 is the mole fraction of component 1 in the gas phase. A similar equation can be written for component 2.

The Modified Wheeler Jonas Model

The modified Wheeler-Jonas model has been extensively used to describe the adsorption of organic vapors in adsorption beds and is expressed as follows (Jonas & Rehrmann 1973; Wheeler & Robell, 1969; Wood & Moyer, 1989):

$$t_B = \frac{We}{C_o Q} \left[W - \frac{\rho_B Q}{K_v} \ln \left(\frac{C_o - C}{C} \right) \right] \quad (6)$$

where t_B is the breakthrough time (min), We is the adsorption capacity (g/g), C_o is the inlet concentration (g/cm³), C (g/cm³) is the outlet concentration, Q is the flow rate (cm³/min), W is the amount of activated carbon (g), ρ_B is the packed bed density (g/cm³), and K_v is the adsorption rate coefficient (min⁻¹), which is dependent on the velocity, u (cm/min).

Wood and Stampfer (1993) proposed an equation based on the fitting of 165 breakthrough curves obtained with 27 hydrocarbons and fluorocarbons with:

$$K_v^{-1} = (1 + 0.027u) \times [(I + S_B \times P_s^{-1})] \times u^{-1} \quad (7)$$

where $S_B = 0.0063 - 0.0055 \ln[(C_o - C)]$, $I = 8.25 \times 10^{-4} \text{ (min} \cdot \text{cm)/s}$ and P_s is the molar polarizability (cm³/mol).

In their study, the adsorption rate constant increased linearly with the linear velocity and no size dependence was observed (Wood & Stampfer, 1993).

The Vahdat et al. model (1994 and 1997) describes a series of equations for each zone that is based on the Wheeler-Jonas equation and the IAST model combined with the Langmuir equation to obtain adsorption isotherms for each component. In this model, Component 1 is more volatile or less adsorbed than component 2. The breakthrough curve concentration profile is divided in four distinct zones and is shown in Figure 1.

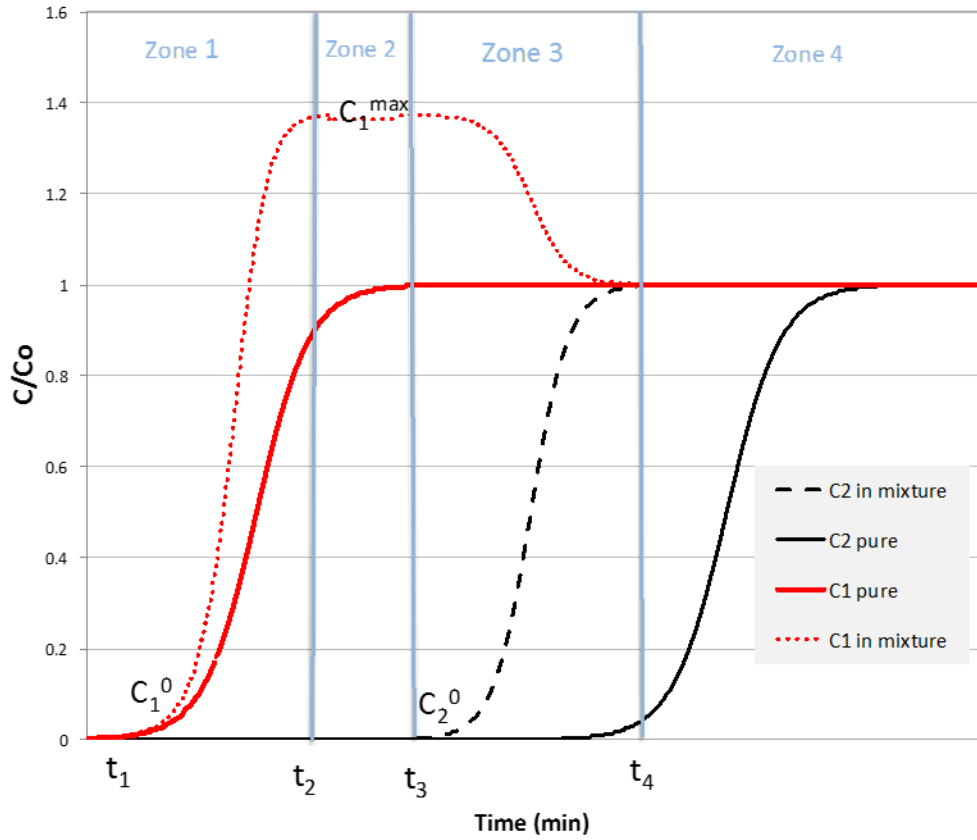


Figure 1. Schematic breakthrough curve of a binary system with inlet concentration of contaminant 1 (C_1^0) and contaminant 2 (C_2^0), and (C_1^{max}) is the maximum concentration of component 1 during the desorption phenomenon.

a) **Zone I**

In zone I, the more volatile component 1, which is weakly adsorbed, breaks through. The breakthrough time of this contaminant relates to adsorption capacity $W_{\epsilon 1}$ and its maximum adsorption capacity, ($W_{\epsilon 1}^{max}$) at the maximum concentration (C_1^{max}) as follows:

$$t_{b1} = \frac{W_{\epsilon 1}^{max}}{\frac{C_1^0 Q}{W - \frac{\rho_B Q}{K_v} \ln\left(\frac{C_1^{max} - C_1}{C_1}\right)} + \frac{C_2^0 \rho_B (W_{\epsilon 1}^{max} - W_{\epsilon 1})}{W(W_{\epsilon 2} \rho_B + \epsilon C_2^0)}} \quad \text{for } t_{b1} < t_2 \quad (8)$$

where ϵ is the bed porosity, C_1 is the outlet concentration of contaminant 1, C_2^0 is the inlet concentration of contaminant 2.

b) **Zone II**

In Zone II, Contaminant 1 reaches its maximum concentration (C_1^{max}), which is higher than its initial inlet concentration, C_1^0 :

$$C_1 = C_1^{max} \quad \text{for } t_3 > t > t_2 \quad (9)$$

The maximum concentration can be found from the mass balance equation as follows:

$$C_1^{max} = \frac{2[QC_1^0 t_4 - W(W_{e1}) - \varepsilon V C_1^0 - QC_1^0(t_4 - t_3)/2]}{Q[t_3 + t_4 - t_2 - t_1]} \quad (10 - a)$$

where V is the volume of the bed. Initially, C_1^{max} may be approximated by calculating the value with :

$$C_1^{max} = C_1^0 \left(\frac{W_{e1}^0 - W_{e1}}{W_{e2}} \right) C_2^0 \quad (10 - b)$$

c) **Zone III:**

In zone III, Contaminant 2, which is more strongly adsorbed, breaks through and reaches its maximum concentration and is described with Eq. 6 by using the adsorption capacity of contaminant 2 in the mixture (W_{e2}) instead of W_e . Contaminant 1's concentration decreases from its maximum concentration (C_1^{max}) and is expressed as follows:

$$C_1 = C_1^{max} - (C_1^{max} - C_1^0) \frac{C_2}{C_2^0} \quad \text{for } t > t_3 \quad (11)$$

d) **Zone IV**

In zone IV, the carbon bed is saturated with both contaminant 1 and contaminant 2 and breakthrough concentrations are equal to the inlet concentrations C_1^0 and C_2^0 , respectively.

Breakthrough curves for each effluent correspond to concentrations that will eventually be inside the worker's mask, especially in the case of a volatile contaminant where contribution to overall risk is considered fairly high (McKone, 1987). To further evaluate the toxicity effect of breakthrough contaminant mixtures and evaluate the potential health risks to workers, it is important to apply risk assessment principles.

Hazard Index

The risk assessment based on the combined action of each component in a chemical mixture may be characterized by using the Hazard index (HI) approach, which was originally proposed by the US Environmental Protection Agency mixture guidelines (US EPA, 1986). This approach is proposed for mixtures containing components having the same toxic effect, in the same organ via the same mode of action. This approach assumes that the components of the mixture are additive in concentration (or dose) of the mixture components and is expressed by the sum of hazard quotients calculated of each component. The HI can be calculated as follows:

$$HI = \sum_{i=1}^n \frac{D_i}{RfD_i} \quad (12)$$

where the exposure doses (or concentrations) of each component of the mixture (D_i) are normalized by the guideline exposure values, i.e., dose or concentration considered safe (e.g. Occupational Exposure Limit value (OEL), reference dose (RfD), etc.). When the hazard index exceeds unity, there may be concern for potential health effects. If HI is less than 1, then it will pose no risk to calculate the

breakthrough time of a mixture. The hazard index may incorporate an uncertainty factor (UF) or safety factor of 10, for mixtures of chemicals where little information is known about the potential of interactions amongst components, or if relatively high concentrations of the mixture compounds are present (Drinking Water and Health, Volume 9, 1989). In such cases, it is calculated as:

$$HI = (UF) \sum_{i=1}^n \frac{D_i}{RfD_i} \quad (13)$$

METHODS

Data Selection

To apply the HI principle, the selection criteria of the binary system were selected on the basis of three factors: (i) the first contaminant is volatile and less harmful compared to contaminant 2; (ii) components of the binary system have to induce the same toxic effect, and (iii) available single component adsorption data are available to solve the quadratic IAST-Langmuir equation. Table I lists the physical and chemical properties of the contaminants along with their major toxic effects. This study specifically excluded binary mixtures of contaminants where the most volatile component is at the same time the most toxic contaminant.

Table I. Contaminants Physicochemical Properties and Associated Toxicity (CNESST, 2015)

Solvent	Density (g/cm ³)	Boiling point (°C)	Vapor Pressure (mm Hg)	Odor Threshold (ppm)	Major effect	toxic OEL (ppm)
Acetone	0.784	56.29	185	50	Neurotoxicity	500
Toluene	0.866	110.6	22	6.7	Neurotoxicity, Reproductive effect	50
o-Xylene	0.88	144.4	4.97	5.4	Neurotoxicity, Reproductive effect	100
m-Xylene	0.864	139.1	5.9	0.6	Neurotoxicity	100
Styrene	0.906	145	5	0.14	Possible carcinogen, Neurotoxicity	50

The adsorption isotherms of pure contaminants and their binary gas mixtures for the two activated carbons listed in Table II were fitted with the Langmuir equation. Then, the ideal adsorbed solution theory (IAST) in conjunction with the Langmuir single-component isotherm were used to calculate the adsorption of the mixtures on the two activated carbons at a flow rate of 24 L/min, temperature of 25°C, and carbon weight of 50 g for simulations of exposures to acetone (10-700 ppm) and the other contaminant of lower volatility (500 ppm). Parameters listed in Table II of Carbon A were used for the simulations and those of Carbon B were used to validate the IAST- Langmuir model with the experimental data.

Table II. Adsorbent Data Used in the Simulation of Binary Breakthrough Curves

Adsorbent	Flow rate (L/min)	Density (g/cm ³)	Temperature (°C)	Surface (m ² /g)	Area	Amount (g)	Ref.
Carbon A	24	0.43	25	1280		50	(Vahdat, 1997)
Carbon B	24	0.45	25	1170		50	(Y H Yoon et al., 1991)

Then, the predicted data of mixture and component gas adsorption and contaminant equilibrium concentration were simulated and analyzed for the following binary mixture systems: acetone/toluene, acetone/m-xylene, acetone/o-xylene, and acetone/styrene. Finally, using the calculated breakthrough concentration as a function of time, a hazard index was calculated using the outlet concentrations of the mixture components to predict the theoretical service life for the safe use of a given respirator cartridge.

Calculations of Breakthrough Curves for Binary Vapor Mixtures

The Microsoft Excel program was used for the calculations using the quadratic equation to solve for the unknown parameters. The pure component pressure of contaminant 1 at the spreading pressure of the mixture, P_1^o was obtained by solving equations 4 and 5 with:

$$\frac{1 + k_1 P_1^o}{1 + k_2 P_2^o} = \exp\left(\frac{m_2}{m_1}\right) \quad (14)$$

$$X_1 + X_2 = 1 \quad (15)$$

$$\frac{PY_1}{P_1^o} + \frac{PY_2}{P_2^o} = 1 \quad (16)$$

$$x_1 = \frac{PY_1}{P_1^o} \quad (17)$$

To derive implicit quadratic equations, let

$$c = \exp(m_2/m_1) \quad (19)$$

Substituting Eq.19 into Eq. 14 gives:

$$1 + k_1 P_1^o = c(1 + k_2 P_2^o) \quad (20)$$

$$k_1 P_1^o - c k_2 P_2^o + (1 - c) = 0 \quad (21)$$

Rearranging Eq. 16 gives:

$$(PY_1 P_2^o) / [(P_1^o P_2^o) + (PY_2 P_1^o) / (P_1^o P_2^o)] = (P_1^o P_2^o) / (P_1^o P_2^o) \quad (21)$$

which can be simplified to :

$$(PY_2 P_1^o) / (P_1^o - PY_1) = P_2^o \quad (22)$$

Now substituting Eq. 22 into Eq.21 gives the following quadratic equation:

$$k_1 P_1^{o2} + (-k_1 PY_1 - c k_2 PY_2 + 1 - c) P_1^o - (1 - c) PY_1 = 0 \quad (23)$$

Having the following implicit quadratic solution:

$$P_1^o = \frac{-(-k_1 PY_1 - c k_2 PY_2 + 1 - c) \pm \sqrt{(-k_1 PY_1 - c k_2 PY_2 + 1 - c)^2 - 4k_1(1 - c)PY_1}}{2k_1} \quad (24)$$

Because it is a quadratic equation, two solutions are returned. However, only one solution is physically consistent. The major flow chart of the calculations is shown in Figure 2. Basically, Langmuir parameters of the pure components are used in combination with the IAST model to determine the

adsorption capacities of the individual components in the mixture using the parameters of the adsorption systems (flow rate, pressure, temperature, carbon weight, density, concentration) listed in Table II for the binary mixture. Then, component 1 and component 2 of the mixture were calculated for each zone of Figure 1 using the Vahdat model.

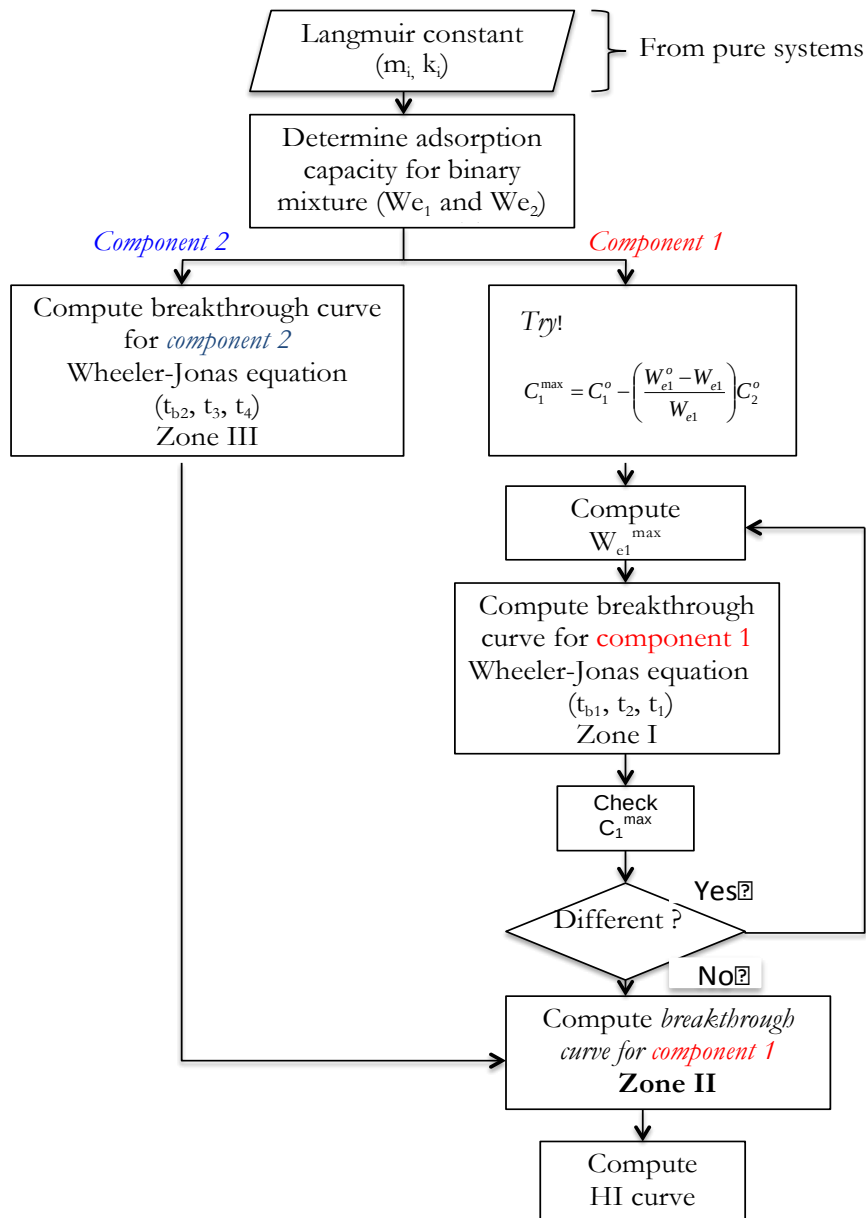


Figure 2. Flow chart for calculation of adsorption capacity and breakthrough curve of binary vapors mixtures where $C_1^{\max}$ can initially be estimated and checked with equations 6.10-a and 6.10-b (represented by “Different” in the flowchart).

RESULTS AND DISCUSSION

Validation of Prediction Model

Using single contaminant adsorption data, IAST, and parameters of binary vapor mixtures, breakthrough curves of the binary systems of acetone/m-xylene using the Vahdat model were validated against previously published data (Lara et al., 1995; Vahdat et al., 1994) and the comparison is shown in Table III. All three simulations revealed reproducibility of the experimental data and closely matched the Vahdat Model.

Table III. Comparison of Predicted Maximum Concentration Ratios of Acetone with Experimental Data and the Vahdat Model (1994)

ne	Concentration (ppm)		C_{max}^1/C_1^o		
	Aceto	m-Xylene	Experime ntal[20]	Vahdat Model (1994)	This Study
	749	260	1.21	1.23	1.21
	474	490	1.55	1.55	1.54
	248	730	2.37	2.33	2.31

C_{max}^1 is the maximum concentration of contaminant 1 and C_1^o is the inlet concentration of contaminant 1

An example of the above resulting adsorption breakthrough curves in the binary system of acetone/m-xylene are shown in Figure 3. The additive principle curve, which considers that the mixtures behaves as a pure contaminant by summing up the concentration of each component to acetone, was also computed. Because acetone is weakly adsorbed compared to m-xylene, the breakthrough of the former occurs early and is desorbed by the strongly adsorbed m-xylene according to the competing adsorption effect. Therefore, acetone is displaced by m-xylene and enters the gas stream, causing outlet concentration of acetone to increase beyond its inlet concentration.

Effect of Concentration Ratio on the Hazard Index (HI)

The HI curves for the breakthrough concentration fractions presented in **Table III**, were computed and are plotted in Figure 4. Two distinctive plateaus are observed for all HI plots: the first one occurs on the onset of the breakthrough of contaminant 2 (m-xylene); the second one at the maximum concentration of acetone. Depending on the concentration ratio of acetone to m-xylene, the shape of the HI curve varied and its positions shifted (see Figure 4).

When the concentration of acetone was about three times less than m-xylene ($C_1/C_2 = 0.34$), the HI curve increased steeply and its characteristic curve shifted to the right. When the concentration of acetone was almost equal to that of m-xylene ($C_1/C_2 = 0.97$), spreading of HI curve occurred and the curve shifted to the left of HI plot of $C_1/C_2 = 0.34$. Then, when the acetone concentration was 2.8 times that of m-xylene, the HI curve decreased and exhibited the most spreading along the x-axis.

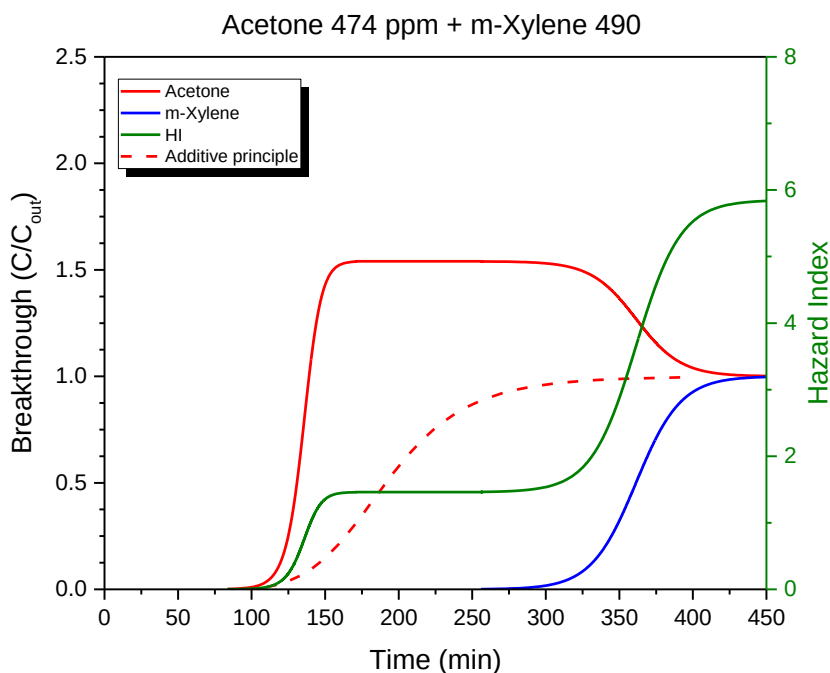


Figure 3. Hazard index and breakthrough curve for acetone (474 ppm) and m-xylene (490 ppm) on respirator cartridge in the binary system. The additive principal curve is calculated by adding the sum of the concentration of each component to acetone.

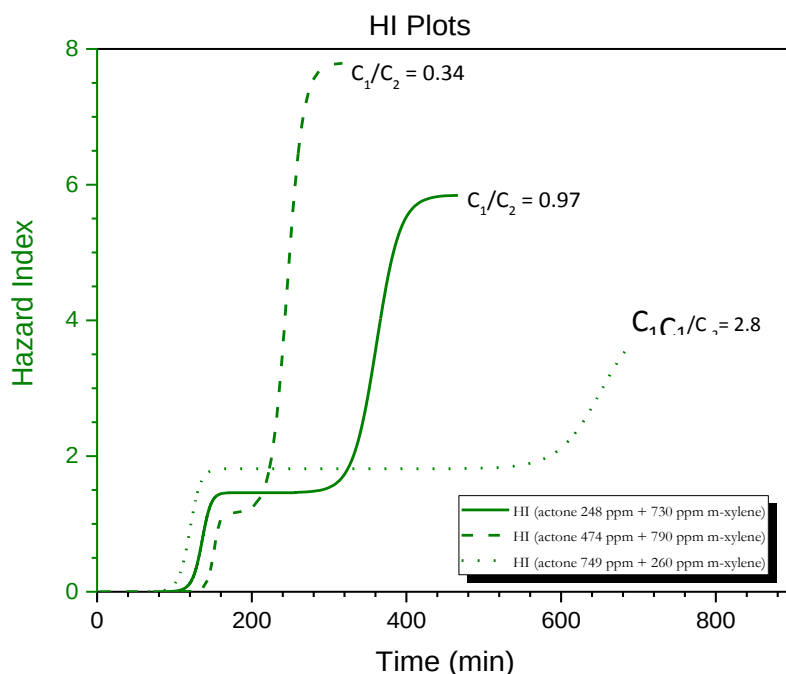


Figure 4. Effect of the concentration ratio of acetone (C_1) to m-xylene (C_2) on the Hazard index curve.

In this scenario, when $HI > 1$, breakthrough time values pose an unreasonable health risk and occur before the breakthrough of the second contaminant, m-xylene. As stated in the U.S. EPA (1986) guidelines, the hazard index should be interpreted as an approximation of the non-carcinogenic risk posed by exposure to the mixture and not considered as an absolute risk value.

Simulations

Results of the of breakthrough curves for the binary vapor mixtures of acetone/o-xylene at various concentration scenarios for acetone while the concentration of o-xylene remained fixed at 500 ppm are shown in Figure 5. A protection factor of 10, which replaces the uncertainty factor, was included into HI. At very low concentrations of acetone (< 25 ppm), a marked difference of about 100 minutes is observed between the 10% breakthrough times ($t_b 10\%$) and 10% HI breakthrough times for the binary system of acetone/o-xylene. Above the concentration of 50 ppm of acetone, the 10% HI breakthrough times are not significantly different to the calculated 10% breakthrough times. However, when the protection factor is not considered, a difference of up to 170 min below 400 ppm is observed. When the concentration of acetone is equivalent or greater to the concentration of o-xylene, all breakthrough time indicators ($t_b 10\%$, $t_b 10\% HI$, $t_b HI$) are more or less the same.

The results of the HI breakthrough times for the binary vapor mixtures of acetone/toluene are shown in Figure 6. When the concentration of acetone is 10 ppm, a difference of more than 100 min between $t_b 10\%$ and $t_b 10\% HI$ is observed. If the uncertainty factor of 10 for HI is removed, a difference up to 170 minutes is seen between $t_b 10\%$ and $t_b HI$ when the concentration of acetone is below 225 ppm in the binary system of acetone/toluene.

The results of the HI breakthrough times for the binary vapor mixtures of acetone/styrene are shown in Figure 7. For various inlet concentrations of acetone, the HI breakthrough times for the adsorption mixture showed no significant difference between the $t_b 10\%$ and $t_b 10\% HI$. However, when the concentration of toluene is 305 ppm and the concentration of acetone is 503 ppm, the difference between $t_b 10\%$ and $t_b HI$ is up to 240 minutes.

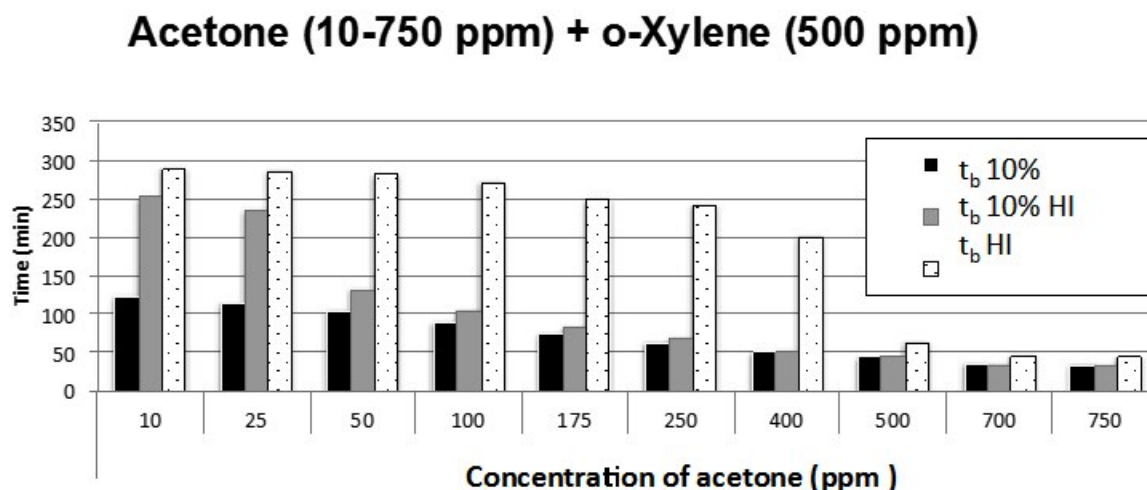


Figure 5. Comparison of cartridge service life using 10% breakthrough time ($t_b 10\%$), hazard index (HI), and $t_b 10\% HI$ when $HI = 1$ for the binary system of acetone/o-xylene.

Acetone (10-700 ppm) + Toluene (450 ppm)

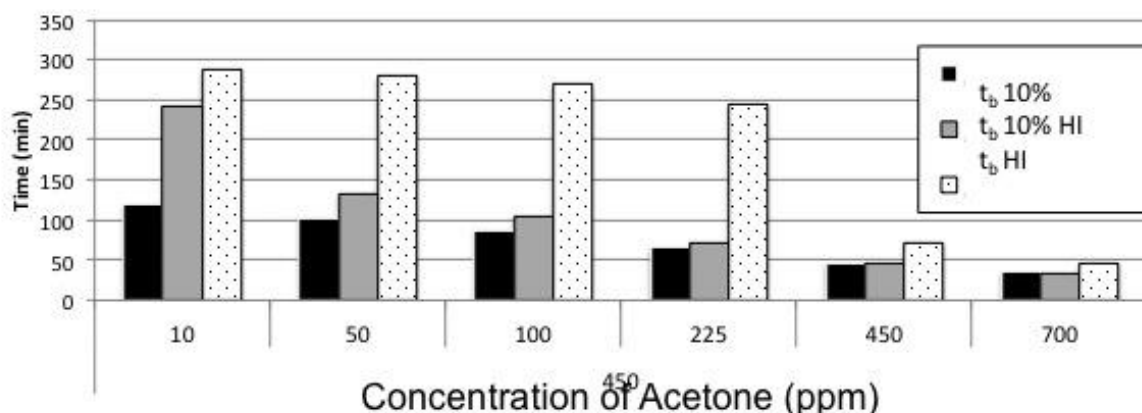


Figure 6. Comparison of cartridge service life using 10% breakthrough time (t_b 10%), hazard index (HI), and t_b 10 % HI when HI = equals to 1 for the binary system of acetone/toluene.

Acetone (256-510 ppm) + Styrene (305-998 ppm)

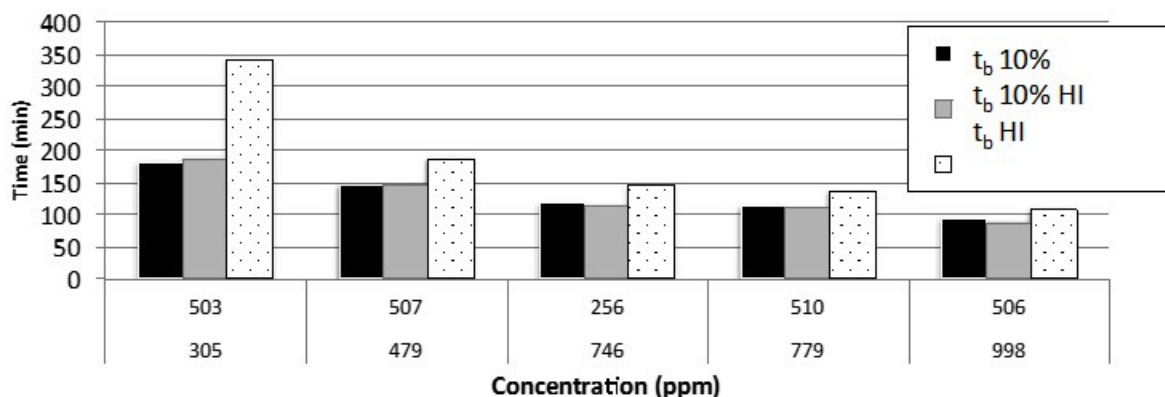


Figure 7. Comparison of cartridge service life using 10% breakthrough time (t_b 10%), hazard index (HI), and t_b 10 % HI when HI = equals to 1 for the binary system of acetone/styrene.

Effect of the Concentration Ratio on HI

The effect of the concentration ratio of contaminant 1 (C_1) to contaminant 2 (C_2) on the breakthrough time when $HI=1$ ($t_b HI=1$) was studied in Figure 8. The relationship appears to be inversely proportional; as C_1/C_2 increases, $t_b HI=1$ decreases. The asymptote is reached around $C_1/C_2 = 2$ for vapor mixtures of acetone + m-xylene and acetone + styrene, whereas for binary systems of acetone + o-xylene and acetone + toluene it occurs earlier $C_1/C_2 = 1.5$ and $C_1/C_2 = 1$, respectively. This result implies that

using the breakthrough time when $HI = 1$ to calculate the cartridge service life for binary systems would be more useful at low concentration fractions of contaminant 1 to contaminant 2.

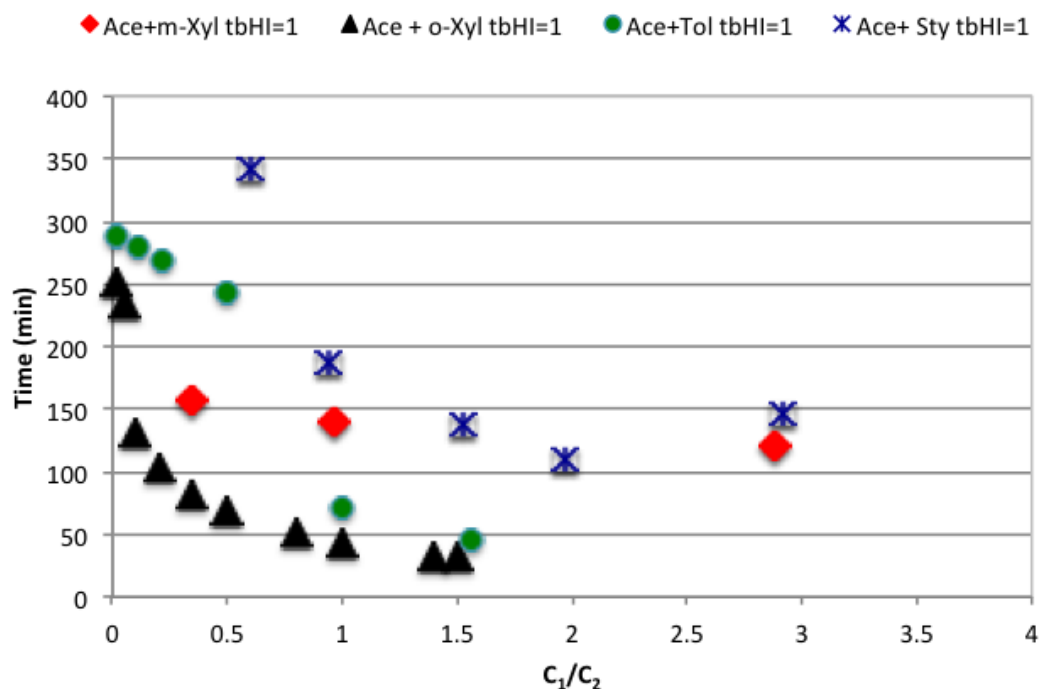


Figure 8. Effect of C_1/C_2 on t_b $HI = 1$ for binary systems.

CONCLUSIONS

Breakthrough curves of mixture contaminants were simulated using the Vahdat model and agreed well with the experimental data for the binary system of acetone and m-xylene. The results obtained highlight the importance of integrating a toxicological approach to predict mixture breakthrough curves for binary vapor mixtures particularly at low concentration fraction for contaminant 1 ($C_1/C_2 < 2$). The simulated cartridge service life using the breakthrough times of 10% HI were up to two times greater than the 10% breakthrough times of acetone in the mixture. At higher concentrations of acetone, both approaches gave similar results. The HI approach is a useful tool to characterize the risk related to exposures to mixtures of contaminants. Its use in combination with breakthrough time prediction models can assure a safe use of respirators and optimize estimation of cartridge service life. The HI approach should be considered in future development of predictive software tools.

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