ESTIMATING THE EVAPORATION RATE AND TIME-VARYING GENERATION RATE OF ACETIC ACID FROM AN ALL-PURPOSE FLOOR CLEANER

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INTRODUCTION

Tier II exposure and risk assessments are dependent upon high quality exposure determinant data that also serve as model inputs. However, since publicly available exposure determinant data are scarce, the risk assessor is left with the option of estimating determinants such as the generation rate, or employing empirical methods to estimate them. When the exposure scenario involves a chemical mixture, estimating the generation rate may not be feasible.

We present an approach for estimating the time-varying generation rate, in this case, for an aqueous acetic acid mixture representative of the base formulation for many consumer and DIY cleaning products that was previously assessed in a screening level assessment.

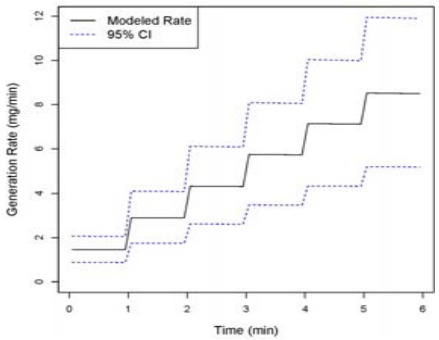
ESTIMATING A TIME –VARYING GENERATION RATE

$$G_1(t) = M_0 k e^{-kt} \quad (1)$$

$$G_2(t) = G_1(t) + M_0\, k e^{-k*(t\_2-t\_1)} \quad (2)$$

$$G_n(t) = M_0 k e^{-kt}\left[\frac{1-e^{-kn}}{1-e^{k}}\right] \quad (3)$$

where
$G_1(t)$ is the generation rate at time t (mg/min)
M_0 is the mass applied at t = 0 (mg)
k is the unknown evaporation rate (min^{-1})
t is the time over which the first spill occurs, 0 < t < 1



Time-varying Generation Rate Estimated From Chamber-Generated Values of k

METHODOLOGY

A two-part study was designed to estimate the evaporation rate, k and the time-varying generation rate $G^n(t)$ under a set of conditions deemed representative of a surface cleaning scenario. The water-based floor cleaning mixture contained acetic acid (4% wt/wt).

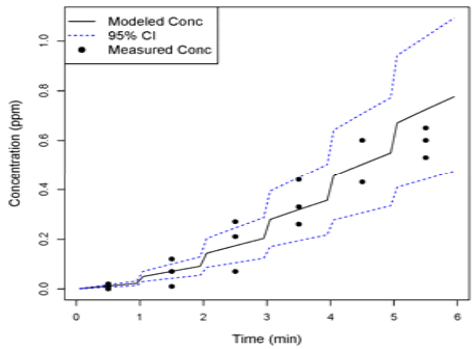
First, tests were conducted in a full size exposure chamber (11.9 m^3) to estimate k under a specific set of conditions, changing only the air exchange rate. Airborne acetic acid concentrations were measured by FTIR. Knowing the air exchange rate, room volume and mass applied at each interval, $G_n(t)$ for acetic acid was estimated using the small spill model.

Second, a field study was conducted to evaluate the time-varying generation rate in a residential environment under similar conditions. Exposures were modeled using the Well Mixed Room model (WMR) and compared with measured exposures in three environment settings: (1) all–purpose room, door closed (2) all-purpose room, door open (3) bathroom

RESULTS

Estimates of k were relatively consistent across air exchange rates. For one minute averaging times, k ranged from 0.0027 to 0.0035 min-1. The 30 second averaging time corresponded to a value of k = 0.0016. The 30 second averaging time corresponded to a value of k = 0.0016. For k estimated from 3 and 6 minute averaging times, k = 0.005.

Modeled TWA concentrations using the WMR model aligned closely with the measured TWA concentrations, albeit underestimating the concentration in room1 (74% of measured TWA) and Room 3 (90% of measured TWA). For Room 2, the predicted TWA exposure exceeded the measured TWA (107%).



Measured and Modeled (WMR model) Acetic Acid Concentrations in Room 2

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CONCLUSIONS

This study demonstrates the feasibility and value of determining reasonably accurate generation rates to develop accurate exposure scenarios. Without this critical model input, the use of reasonable worst case model inputs significantly overestimates the emission rate, especially when estimating emissions from chemical mixtures.

The portability of the evaporation and generation rates were evaluated by comparing measured and modeled acetic acid concentrations for three field scenarios: a residential all-purpose room with the doors closed (room1), the same room with the exterior door open (room2) and a bathroom (room3).

The chamber and field study approach will be particularly useful when refined exposure assessments involving chemical mixtures are needed but generation rates are not publicly available in the peer reviewed literature.

TIME WEIGHTED AVERAGE (TWA) MEASURED AND MODELED ACETIC ACID CONCENTRATIONS

	Time Weighted Average Concentration (ppm)	
	Measured	WMR
Room 1	0.413 (0.334)	0.305 (0.272)
Room 2	0.281 (0.229)	0.301 (0.267)
Room 3	0.864 (0.822)	0.777 (0.681)

Showing mean and (SD) concentrations averaged over six minutes (n=3).
WMR: Well Mixed Room model.

REFERENCES

1. Arnold, S., Ramachandran, G. Kaup, H. Servadio, J. “Estimating the Time-Varying Generation Rate of Acetic Acid from an All-Purpose Floor Cleaner” (submitted).

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