ABSTRACT

STEPHEN MICHAEL BAKALYAR. Testing of a Model to Estimate Vapor Concentration of Various Organic Chemicals. (Under the direction of Dr. PARKER C. REIST)

A model developed by Dr. Parker C. Reist to predict the build-up and decay rates of vapor concentrations following a chemical spill and clean-up was tested. The chemicals tested were: acetone, butyl acetate, ethyl acetate, hexane, methylene chloride, methyl ethyl ketone, and toluene. The evaporation rates of these chemicals were determined both by prediction, using a model developed by I. Kawamura and D. Mackay, and empirically and these rates were used in the Reist model. Chamber experiments were done to measure actual build-up and decay of vapor concentrations for simulated spills and simulated clean-up. The chamber experimental results were compared to the model's predicted results. The Reist model, used with the Kawamura-Mackay predicted evaporation rate, can be useful in estimating equilibrium concentration and the time required to reach the equilibrium concentration.

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INTRODUCTION

A major concern of the industrial hygienist is the protection of the worker against exposure to vapors from solvents and other organic chemicals. Vapor evolution from chemical spills, open surface tanks, or from any open container may contribute significantly to that exposure. Quantifying the potential exposure is the best means of determining the risk to the worker.

Air sampling is an effective way of determining airborne concentrations of chemical vapors but results are not immediate and time may be critical, as in the case of a spill in the workplace. Direct reading instruments offer immediate results but these instruments are usually specific for the chemical detected and the likelihood of the average workplace having such instruments for each chemical used is very low. Detector tubes offer immediate results, are available for a wide range of chemicals, and are easy to use. However, the accuracy of these tubes may be as poor as +/- 50% [4]. Also, in spill situations, it may not be advisable to enter the spill area, especially if the chemical is hazardous. The ideal method would allow prediction of the concentration of the airborne vapor without having to expose anyone unnecessarily.

Currently, there are methods for determining ventilation rates to control vapor concentrations below the Threshold

Limit Value (TLV) [1] and for determining the evaporation rates of various chemicals [2,3,9,11]. There is, however, nothing in the literature that presents a model for the prediction of the build-up of vapors and the equilibrium concentration that can be expected following a chemical spill, and the decay of the concentration following clean-up or removal of the chemical. Such a model was recently developed [7]. The purpose of this research was to test this model.

BACKGROUND

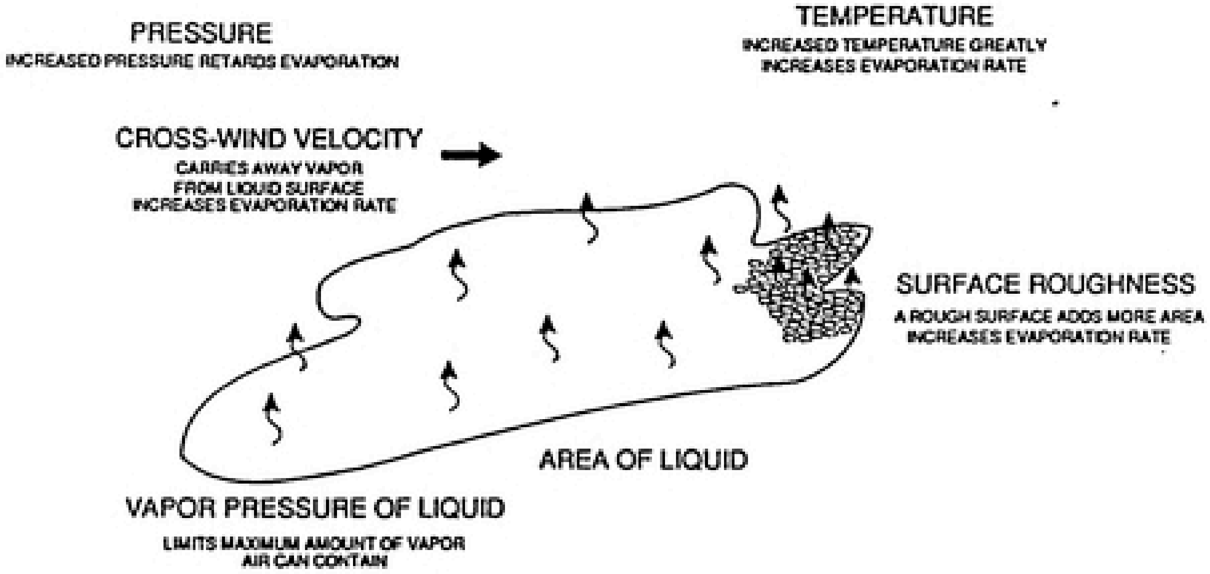
Determining the evaporation rate of a chemical is a crucial element in the process of ascertaining the build-up rate and maximum concentration in a workplace. The rate of evaporation of a chemical is dependent upon many factors. Some of the key factors are: the vapor pressure of the chemical; the partial pressure of the vapor over the surface of the chemical; the air temperature and chemical temperature; in the case of a spill, the temperature of the surface on which the chemical is spilled; velocity of air across the surface of the chemical; the volume of the chemical available to evaporate; and the surface area of the chemical. Since many of these factors are dependent upon one another, prediction of the concentration of vapor above a chemical can be very difficult. Mixtures present even more complex problems, such as the difficulty in determining the vapor pressure. For this reason, only pure chemicals were used in this study. Figure 1 [7] illustrates some of the factors affecting the evaporation of a chemical.

Mellan [6] made some general observations concerning the rate at which chemicals evaporate:

(1) Evaporation rates are not inversely proportional to the boiling points, but liquids within a single homologous series of compounds do evaporate more rapidly if their boiling points are lower.

FIGURE 1

FACTORS AFFECTING EVAPORATION RATE OF LIQUID



(2) Liquids from separate homologous series with equal boiling points have entirely different evaporation rates.

(3) Hydroxyl groups greatly retard the evaporation rate, so that compounds such as alcohols and water evaporate much slower than one would otherwise expect.

(4) If two compounds have identical boiling points, in general the one with higher molecular weight will tend to evaporate more rapidly.

(5) Vaporization results in a temperature drop in the liquid, unless heat is supplied from the surroundings.

According to Gray [2], theoretical approaches to the problem of predicting evaporation rates start by considering heat transfer, develop an elaborate theory of pure heat transfer, and then point out that mass transfer can be treated similarly with a substitution of coefficients. He states that investigation into both heat and mass transfer determined that the two do not interfere with one another even though they occur simultaneously when liquids evaporate. As a result, either heat or mass transfer can be considered and the other ignored.

A ventilation manual [1] commonly used today by industrial hygienists uses a mass balance approach to determine airborne vapor concentrations. This approach is based on the control of air contaminants by dilution ventilation. The method recommended for determining the evaporation rate is through examination of records of a plant's chemical consumption, with the assumption that the evolution of the chemical is uniform. Kawamura and Mackay [3] found that evaporation rates are usually not uniform. They state that neglecting factors such as evaporative cooling, direct heat transfer between the chemical and air, and between the chemical and the ground, can cause the evaporation rate to be overestimated by as much as a factor of four, especially for volatile chemicals.

The problems in designing a model to predict atmospheric vapor concentrations over an evaporating liquid are many. A variety of factors influence evaporation rate, and the way these factors interact with one another make the task that much more difficult. As yet undetermined factors may also exist that further complicate the issue. The models in this study incorporate the most current knowledge concerning the evaporation rate phenomenon. The effectiveness of the models is determined by comparing the results of actual experiments to those calculated using the models.

THE MODEL

The following model was developed to predict the effect of evaporation on air concentration levels in spaces having different volume and flow characteristics [7]. This model (hereafter called the Reist model) is based on mass balance and predicts an exponential build-up of contaminant until an equilibrium concentration is reached. It also includes a decay element to predict how quickly the contaminant is removed from the air once the chemical source is removed. The equilibrium concentration predicted is dependent only on the rate of evaporation of the chemical and the volume of air exhausted from the room.

Definition of terms:

Figure 2 depicts the following terms used in the development of the model:

Q - Make-up air flow into and out of the room
C_i - Incoming concentration of contaminant in make-up air
C_s - Concentration of contaminant in room at start of decay
X - Volume of room
C - Concentration of contaminant in room
Q_r - Recirculating airflow (this flow does not remove contaminant although it may contribute to increased room concentrations by increasing velocity across the evaporating surface)

Q_r - Flow of air through air cleaner, if any

n - Efficiency of air cleaner

m - Rate of generation of contaminant

K - Factor which accounts for room air not being well mixed

The development:

As a first step a mass balance is considered:

mass in - mass out = mass change

$$QC_I+m+(1-n)Q_rC-Q_rC-QC = X/K\ dC/dt \qquad (1)$$

which simplifies to

$$QC_I+m-(nQ_r+Q)C = X/K\ dC/dt \qquad (2)$$

Let $R = QC_I+m$, and $S = (nQ_r+Q)C$ so that $dS = (nQ_r+Q)dC$.

Then

$$R - S = (X/K)(1/(nQ_r+Q))(dS/dt) \qquad (3)$$

Now let

$$T = (X/K)(1/(nQ_r+Q))$$

and $W = R - S$ so that $dW = -dS$. Then

$$W = -TdW/dt \qquad (4)$$

$$-dT/T = dW/W \qquad (5)$$

Integrating and exponentiating gives

$$W = \exp(-1/T)\exp h \qquad (6)$$

where h is a constant.

The build-up, decay, and steady state equations:

For initial conditions of $t = 0$ and $C = 0$, the constant *h* in equation (6) can be evaluated to give the build-up equation:

$$C = (1/(nQ_r+Q))(QC_i+m)(1-\exp^{-t/\tau}) \tag{7}$$

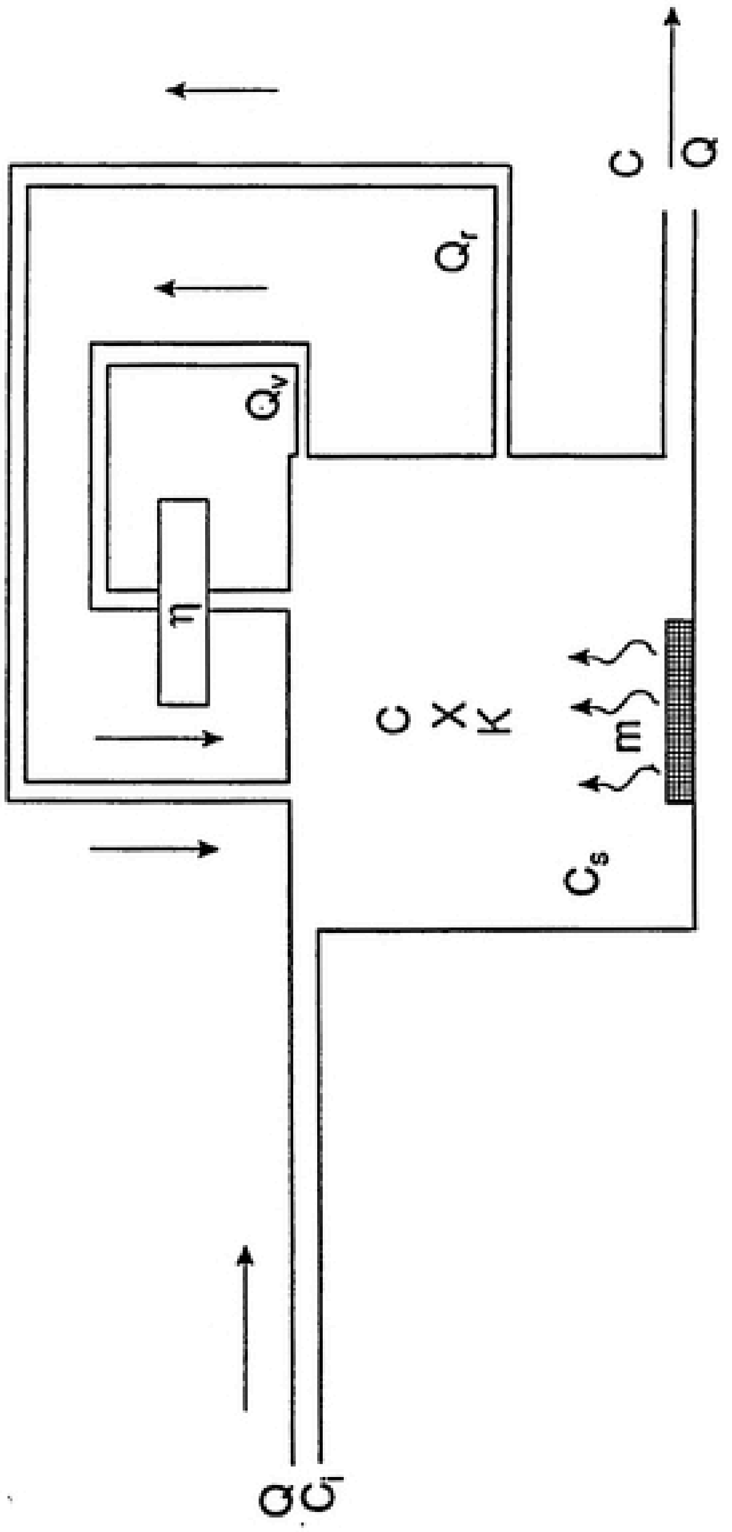
For decay of concentration from a room, the initial conditions are $C = C_s$ at $t = 0$. Then the constant *h* in equation (6) can be evaluated to give:

$$C = ((QC_i+m)/(nQ_r+Q))(1-\exp^{-t/\tau})+C_s\exp^{-t/\tau}) \tag{8}$$

For equilibrium conditions:

$$C_s = m/Q \tag{9}$$

Figure 2. Depiction of terms used in the Reist model.



PREVIOUS WORK

Past attempts have focused primarily on developing models or methods of estimating evaporation rates that could in turn be used to estimate concentrations. In the literature there is no model which estimates concentrations directly. The theme presented in the following methods and models centers on the estimation of evaporation rates.

Stiver and Mackay [9] give methods for quantifying the rate of environmental evaporation of liquid mixtures such as crude oils and petroleum products under a variety of environmental conditions. Three methods are presented: tray evaporation, gas stripping, and distillation. A form of the tray evaporation method was used in this research and is discussed in the next section. This method was chosen because of its simplicity and because the liquid surface and air interface are similar to that of a real chemical spill.

Gray [2] developed a system of equations for predicting the evaporation rates of solvents. He contends that his equations could be used by the industrial hygienist, with diffusion equations developed elsewhere, to predict the atmospheric concentrations of vapors from spilled toxic liquids. He presented three formulas to predict the evaporation rates of simple liquids in ducts and two to predict the evaporation rates in open air. His models, however, are not easily used, requiring a variety of parameters (some of which are not readily acquired), and too much effort for ease of use in an emergency situation.

Kawamura and Mackay [3] developed two models to estimate the evaporation rate of volatile and non-volatile liquids resulting from ground spills. The models, termed the "direct evaporation" method and the "surface temperature" method, were designed to be used outdoors and are based on a quasi steady state heat balance around the chemical pool.

The surface temperature method (hereafter called the Kawamura-Mackay model) was used in this research as a means of predicting the evaporation rate of each chemical under conditions similar to those determined empirically. This model was chosen due to its relative simplicity of use over the other models noted above. A comparison of the Kawamura-Mackay model and the Gray model was done. Table 1 gives the results of this comparison. An average difference of 22% was found and deemed acceptable, providing sufficient justification for use of the simpler model. The predicted evaporation rates found using the Kawamura-Mackay were used in the Reist model and compared to the vapor concentrations measured over a simulated spill.

TABLE 1: Comparison of Gray's Results and Kawamura-Mackay Predictions for Evaporation Rates for Xylene at Various Velocities

Velocity (fpm)	Gray's Results (g/min-cm^2)	Kawamura-Mackay Prediction (g/min-cm^2)	% Diff
23.43	0.0002988	0.000220	26.34
52.56	0.000612	0.000389	36.30
98.44	0.000718	0.000606	15.50
196.85	0.000836	0.000987	18.09
252	0.001046	0.001182	13.08
Average Difference			21.86

The Kawamura-Mackay model bases the driving force for evaporation on the vapor pressure of the chemical evaluated at the surface of the chemical pool. According to Kawamura and Mackay, the surface temperature of the chemical pool must be known and is a function of radiative heat transfer by solar insolation, evaporative cooling, and direct heat transfer between the chemical pool and the air, and between the pool and the ground. Furthermore, the effects of the evaporative cooling and direct heat transfer terms are most significant for volatile chemicals. This is due to the depression of the surface and pool temperatures relative to the ambient temperature as a result of the evaporative cooling of the chemical.

For the purposes of this research, solar influences in the Kawamura-Mackay model were neglected since all empirical data were collected indoors.

The basic Kawamura-Mackay model:

$$E = k\ M\ P(Ts)/RT \qquad (10)$$

where: k = mass transfer coefficient (m/h)

M = molecular weight

$P(Ts)$ = vapor pressure of the chemical evaluated at the surface of the pool (Pa)

R = gas constant (8.314 Pa m^3/mol K)

T = absolute temperature (K)

E = evaporation rate ($g/m^2\ h$)

The mass transfer coefficient (k) is a function of the dimensionless Schmidt number (Sc) which is 2.11, the velocity (U) in m/h across the surface of the liquid, and the downwind pool length or diameter (X) in m and is given as:

$$k = 0.029U^{0.78}\ X^{-0.11}\ Sc^{-0.67} \qquad (11)$$

The vapor pressure at the surface of the pool ($P(Ts)$) is given as: $P(Ts) = 133 \exp\{2.3\{a-[b/(Ts-273+c)]\}\}$ (12) where a, b, and c are constants for each chemical [5] and Ts (surface temperature) is determined using Newton's method.

Kawamura and Mackay report a difference between the predicted and experimental evaporation rates of from 1 to 32% with an average of 12% using this method. They state that this is an acceptable error for models used under environmental emergency conditions.

TESTING THE REIST MODEL

Overview:

The purpose of this research was to determine how well the Reist model predicts concentration build-up, the equilibrium concentration, and the concentration decay rate for given conditions following a chemical spill in a workplace and the clean-up of the spill. The conditions that must be known (Table 2) are related to the particular physical properties of chemical and physical characteristics of the room in which the spill occurs.

The first experiment, the evaporation rate test, was done to determine the uniformity of the evaporation rate of each chemical under ambient conditions with little or no air movement across the surface of the liquid chemical. The second experiment, the velocity test, was done to determine the evaporation rate of each chemical as a function of the increase in air velocity across the surface of the liquid chemical. The results of this second experiment were used in the Reist model to predict concentration build-up and decay. The third experiment, the chamber test, was a simulated chemical spill. A pan of the chemical was placed in a chamber and the build-up of vapor concentration measured using a MIRAN. Once the concentration reached equilibrium the pan was removed from the chamber to measure the concentration decay rate. Two runs were done in the chamber for each

TABLE 2: Conditions Required for Reist Model

1. Room volume – ft^3
2. Air flow through room – cfm
3. Air temperature in room – degrees C
4. Air velocity over surface of liquid – fpm
5. Evaporation (generation) rate of liquid – g/min-cm^2
6. Molecular weight of liquid – g/mol
7. Spill area – cm^2

chemical. The chamber exhaust ventilation system was turned on and the door was closed during each run. In Run 1 the pan was simply placed in the chamber on a cart. In Run 2 the pan was placed on a cart with a small fan positioned to blow air across the liquid surface to increase the surface velocity.

The characteristics of the chamber - chamber dimensions, air velocity across the top of the liquid in the pan, and air flow through the room - were determined empirically, and used in the Reist model. The results of the Reist model prediction, using these empirical data, were compared to the chamber test results to determine the effectiveness of the Reist model in predicting concentration build-up and decay. Then, the Reist model predictions, using the Kawamura-Mackay model evaporation rate predictions, were compared to the measured concentrations.

The experiments and equipment used are outlined in detail in Appendix A. The following chemicals were tested: acetone, butyl acetate, ethyl acetate, n-hexane, methylene chloride, methyl ethyl ketone (MEK), and toluene. Acetone, ethyl acetate, hexane, MEK, and toluene were chosen because of their common use in industry. Butyl acetate and methylene chloride were chosen as examples of chemicals with extreme vapor pressures. The procedures used in testing these chemicals are briefly described below.

Evaporation Rate Test:

A petri dish bottom, 9cm (8.7cm for MEK) in diameter, was filled almost to the top with chemical and placed on the balance pan of a Mettler balance. The balance was inside a chemical fume hood with the sash in the full open position and the exhaust fan on. The velocity of air passing through the balance was measured with a thermoanemometer velocity meter and was found to be negligible (less than 10 fpm). The chemical and dish were weighed initially and periodically and the results recorded along with the air temperature in the balance.

Velocity Tests:

Evaporation rate tests were done at several velocities: 65 feet per minute (fpm), 110 fpm, 220 fpm, 300 fpm, and 425 fpm. A petri dish, 9 cm in diameter (8.7 cm for acetone and MEK), filled with chemical was placed in the balance, weighed, and the weight recorded. A flexible exhaust hood, with a blastgate located just behind the hood portion, was positioned at the left door of the balance to allow air to be drawn through the balance and across the surface of the chemical in the petri dish (Figure 3). The blastgate was used to regulate the air flow through the balance. Cardboard squares were taped to both the left and right door areas to reduce surface area and allow for higher velocity ranges through the balance. The probe of a thermoanemometer velocity

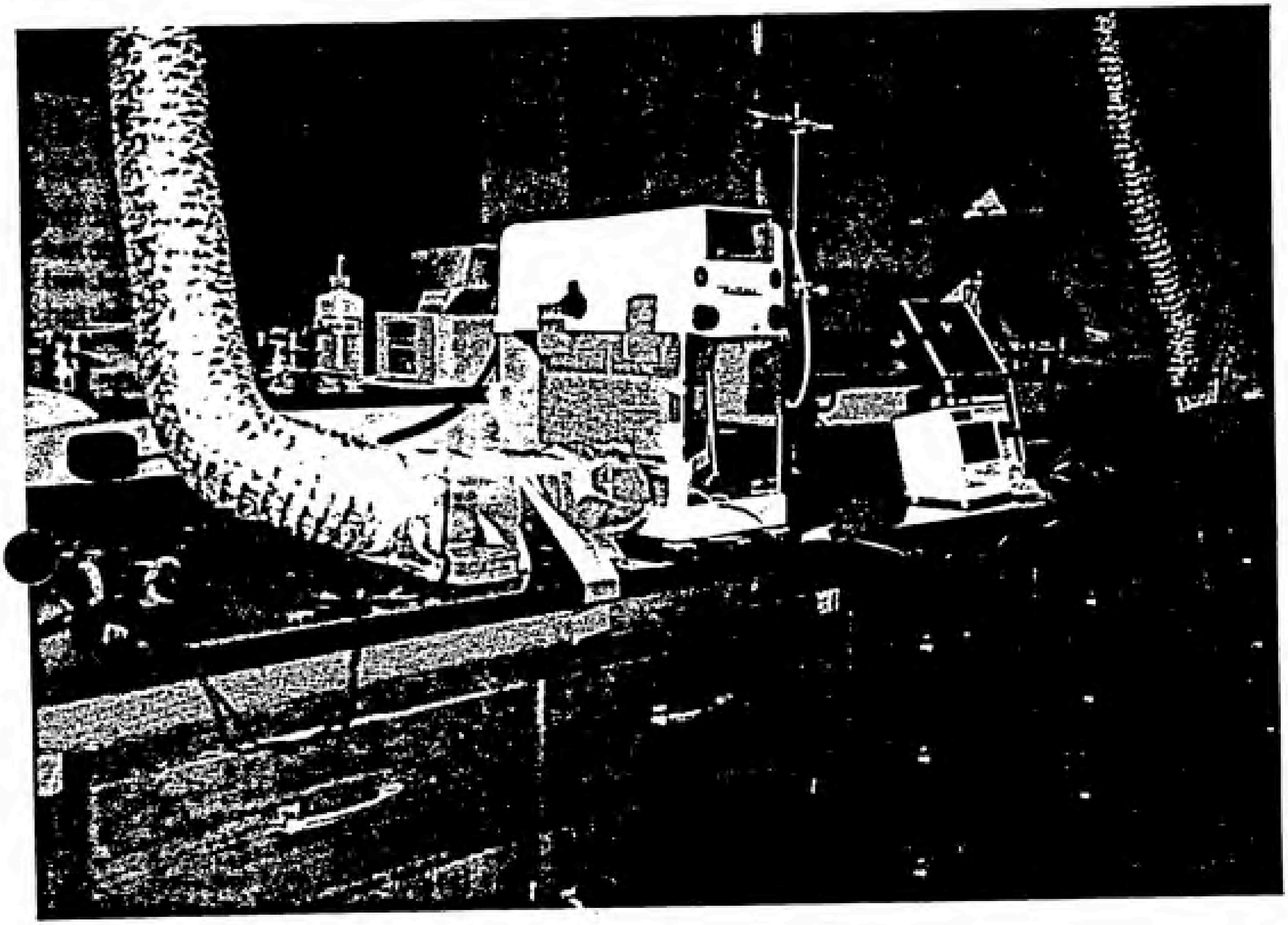


Figure 3. Velocity test equipment set-up.

meter was taped to the right side of the balance to measure the velocity of air across the top of the petri dish. Measurements were taken at 0, 2, 4, and 6 minute intervals for each velocity.

Temperature was measured for each chemical at 110 fpm surface velocity to determine the effect of surface velocity on liquid temperature. The setup described above was used. A type-J thermocouple was placed in the liquid to measure the temperature and the results recorded using the data logger.

Miniature Infrared Analyzer (MIRAN) Calibration:

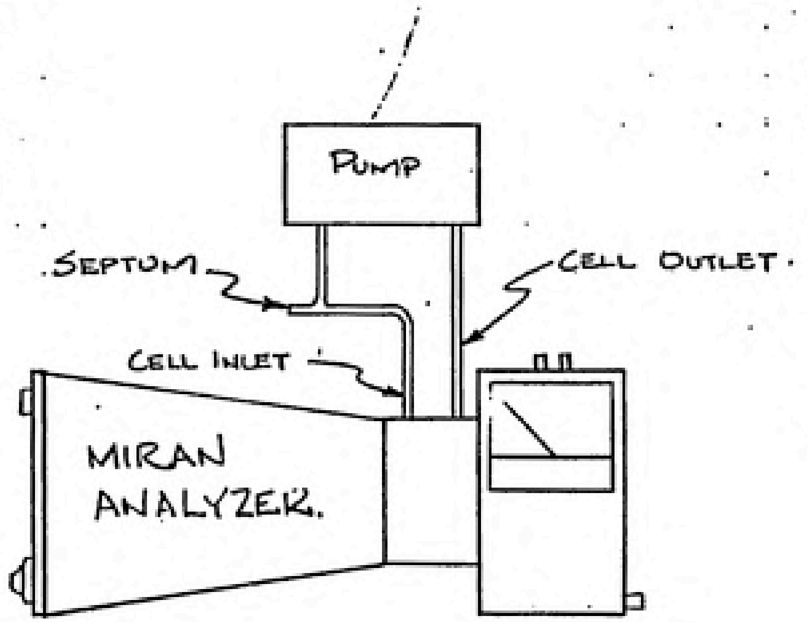
All chemical concentrations were measured using a MIRAN which was calibrated in the following manner. First, the analytical wavelength and pathlength were determined (see Appendix A). Then, a known concentration of vapor was prepared in a calibration flask [9]. Aliquots of the chemical vapor were then injected into the closed loop configured MIRAN (Figure 4), and the absorbance was noted after each injection.

Chamber Tests:

The chamber tests were done in an 830 cubic foot room with exhaust ventilation vents located near the floor, on each side of the wall opposite the door. The flow through the room was determined by measuring the average face velocity at each vent, multiplying the face velocity by the area of each vent

Figure. 4

SCHEMATIC DIAGRAM OF CLOSED LOOP CALIBRATION SYSTEM.



to get the flow through each vent, and then adding the results to get the total flow through the room. The survey was done with the door closed and the exhaust ventilation system on. Measurements were taken using a thermoanemometer velocity meter.

A cart was positioned in the center of the chamber. A probe and tubing assembly, connected to the MIRAN (Figures 5, 6, and 7), was taped to the cart at a height of 52 inches (") from the floor. A teflon coated pan, 8" X 12" X 2", was positioned on the base of the cart (9" off the floor). A small fan connected to a variable transformer was also placed on the base of the cart and positioned to blow air across the top of the pan (Figure 7).

The air velocity across the liquid surface in the pan was estimated in the following way. Due to the turbulence in the chamber caused by the high flow rate, it was very difficult to measure the surface velocity using a thermoanemometer. Instead, the surface velocity for each run was found by determining the evaporation rate inside the chamber. This was done by measuring the liquid volume evaporated for each chemical and by using the results to find the velocity on the evaporation rate vs velocity curves (Figures 8-14). The average of these results was a 400 fpm surface velocity for

Figure 5. MIRAN with probe and tubing assembly.

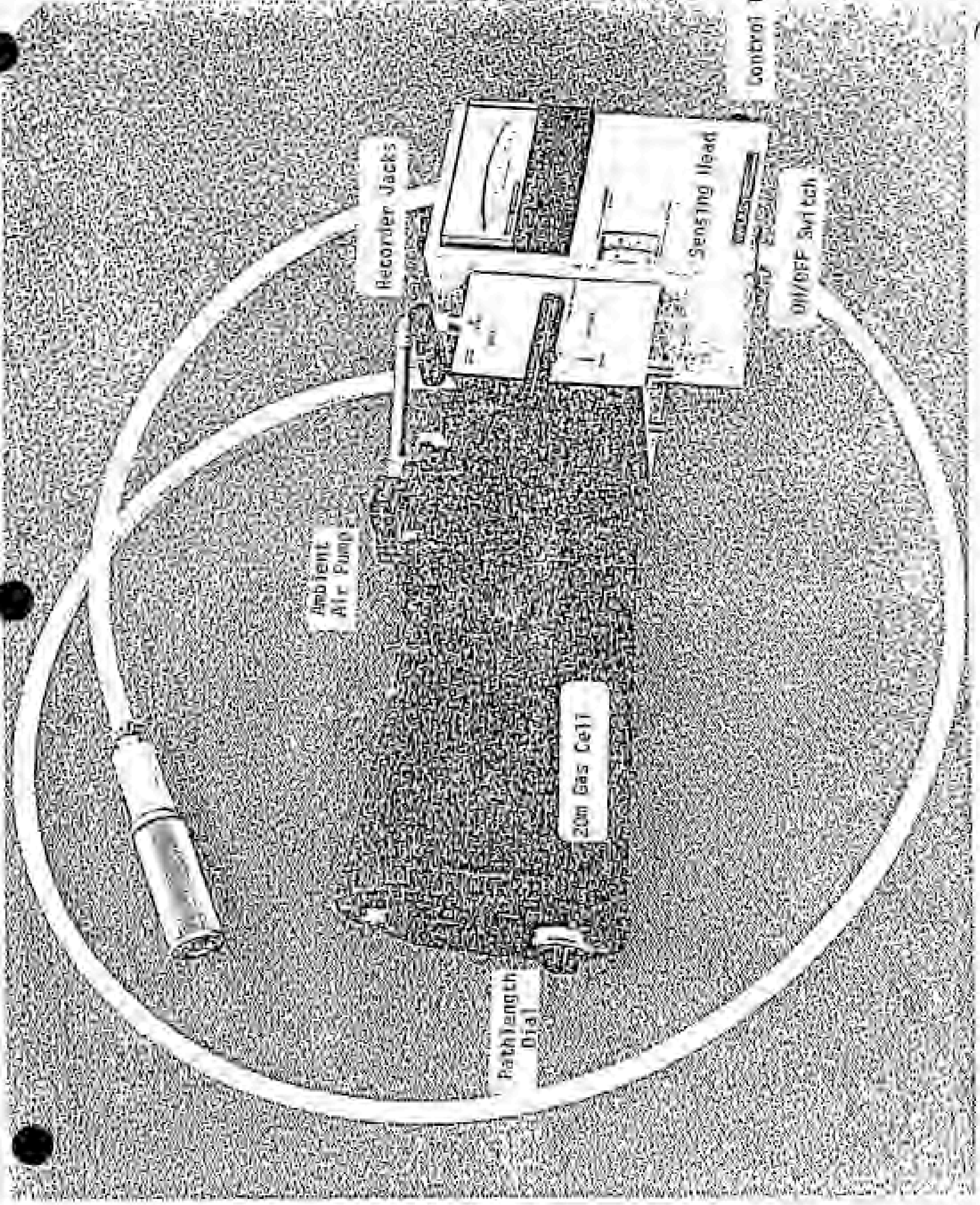


Fig 5

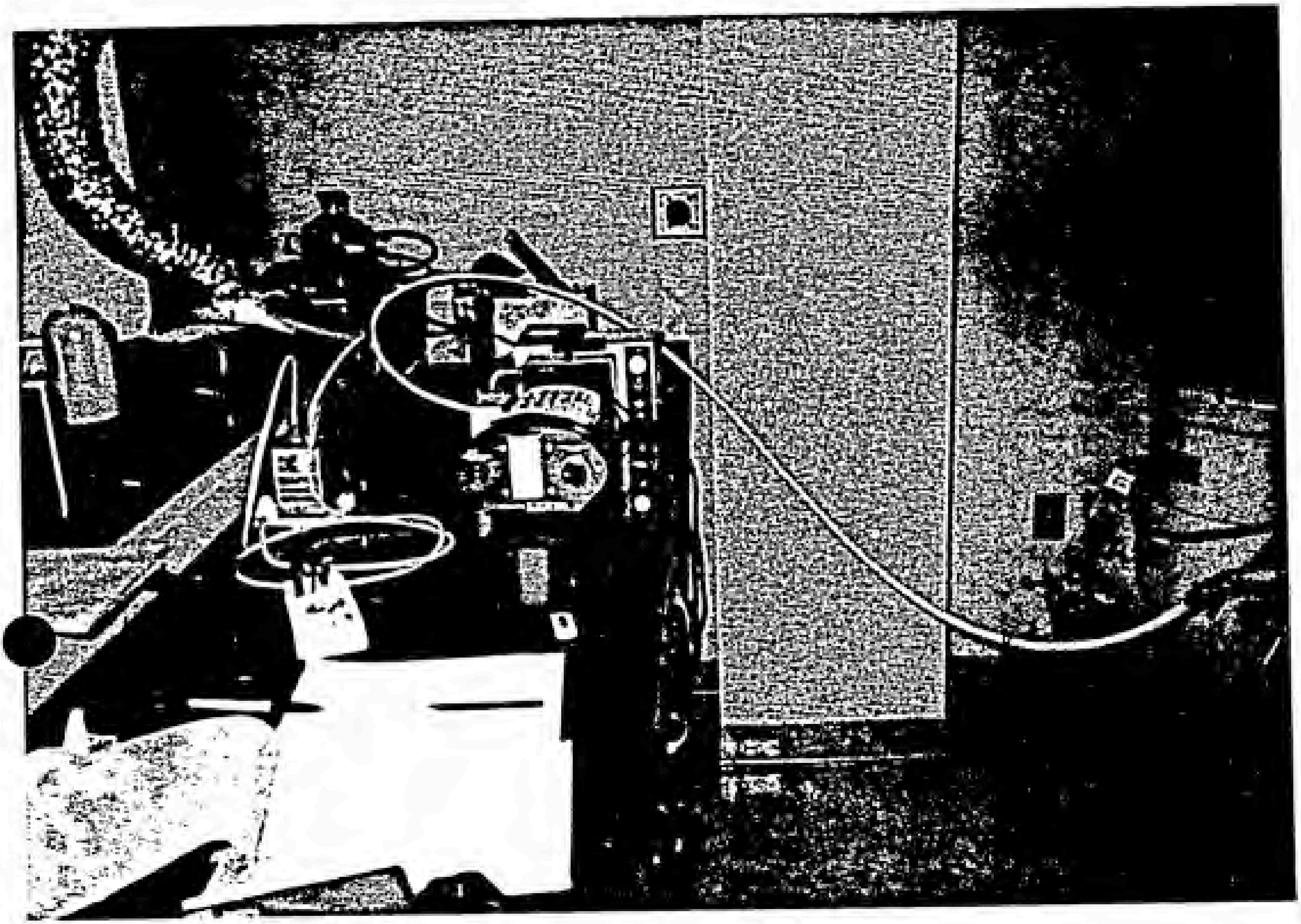


Figure 6. MIRAN chamber test set-up.

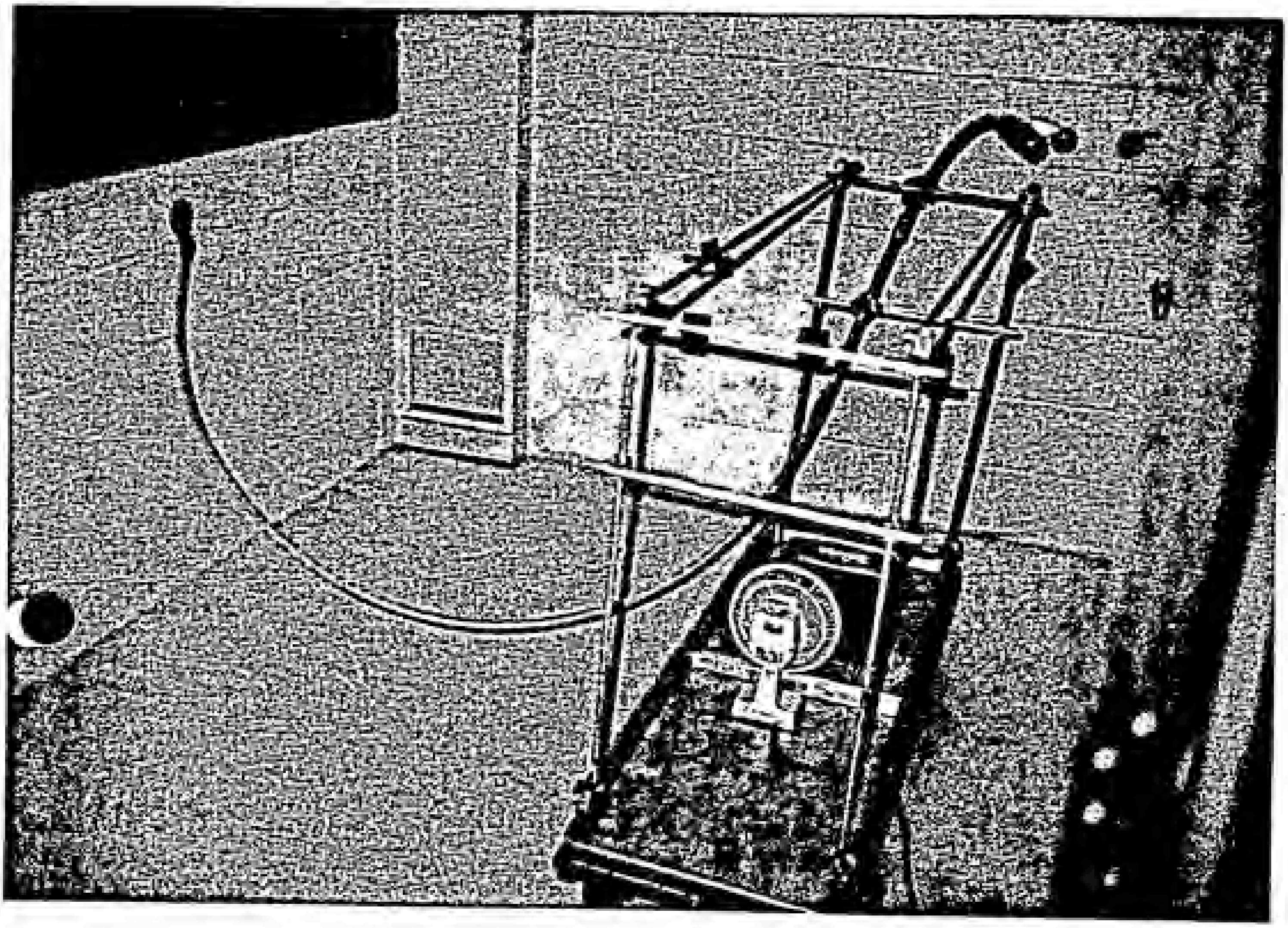


Figure 7. Chamber test equipment set-up.

Run 1 (without the fan) and a 600 fpm surface velocity for Run 2 (with the fan).

Each run involved two phases: concentration build-up and concentration decay. Concentration build-up was measured by pouring about one liter of chemical into the pan, closing the door, and recording the change in absorbance measured in the MIRAN on the data logger. Once the absorbance stopped increasing, the pan was removed from the chamber and the decay measured. The air temperature was simultaneously recorded by the data logger via a Type-J thermocouple.

RESULTS

Evaporation Rate Test Results:

Data for each evaporation rate test are recorded in Tables 1A-7A. (All tables and figures with the designation "A" are located in the Appendix). Figures 1A-7A show the weight of liquid remaining as a function of time. A regression analysis was also done on the data and the resultant regression curve plotted.

The air pressure was not measured but was assumed to be 1 atmosphere. The air temperature in the room averaged 22.5 degrees Centigrade (C) and did not vary more than +/- 1 degree C. The liquid temperature of the chemicals was not measured for this test. The evaporation rate for each chemical tested is uniform over time (R^2 > .99). Table 3 summarizes these evaporation test results.

Velocity Test Results:

The data for each velocity test are recorded in Tables 8A-14A. The regression curves in Figures 8-14 show evaporation rate as a function of velocity data. The room temperature and pressure conditions and assumptions are the same as the evaporation rate test. The changes in liquid temperature during a velocity test of 110 fpm are recorded in Table 15A. The temperature of the liquid for each chemical decreased with time as shown in Figure 15. Similar results

TABLE 3: Summary of Evaporation Rate Tests

Chemical Name	Air Temperature (C)	Evaporation Rate (g/min-cm^2)	R^2	Vapor Pressure @ Temp (psia)
Acetone	23	0.00561	0.996	4.09
Butyl Acetate	23.4	0.00078	0.997	0.201
Ethyl Acetate	22.3	0.00403	0.997	1.6
Hexane	22.2	0.00483	0.994	2.56
Methylene Chloride	23.3	0.00921	0.995	7.76
MEK	22	0.00425	0.997	1.51
Toluene	21.8	0.00254	0.998	0.465

were noted for each chemical during each velocity test and for each chamber run. The overall effect of increasing the velocity across the surface of the liquid caused the evaporation rate to increase. Table 4 summarizes the evaporation rate data for each velocity test.

MIRAN Calibration:

Tables 16A-22A list the calibration conditions for each chemical. Figures 8A-14A show the calibration curves for each chemical tested. A spreadsheet was constructed using LOTUS 1-2-3 to facilitate calculating the flask and MIRAN concentrations and to predict extraction and injection volumes required to attain the desired MIRAN concentrations. Table 23A is an example of this spreadsheet with the formulas listed. Tables 24A-30A give, for each chemical: the MIRAN settings used, physical properties of the chemical, room temperature, vapor pressure at that room temperature (see Table 31A for vapor pressure information) [5], lower explosion limit (for safety purposes) [10], amount of the liquid injected into the calibration flask, resultant concentration in the flask, aliquots extracted from the flask and injected into the MIRAN, resultant concentrations in the MIRAN, and chamber data.

TABLE 4: Summary of Velocity Test Evaporation Rates

Chemical Name	Air Temperature (C)	Air Velocity (fpm)	Evaporation Rate (g/min-cm^2)	R^2	Vapor Pressure @ Temp (psia)
Acetone	22	65	0.00642	0.969	3.92
		110	0.00759		
		220	0.00814		
		300	0.0096		
		425	0.0115		
Butyl Acetate	23	65	0.00086	0.979	0.0197
		110	0.00119		
		220	0.00162		
		300	0.0019		
		425	0.00226		
Ethyl Acetate	23	65	0.00513	0.929	1.66
		110	0.00585		
		220	0.00666		
		300	0.00787		
		425	0.008		
Hexane	22.8	65	0.0069	0.994	2.57
		110	0.00808		
		220	0.0115		
		300	0.0147		
		425	0.0196		
Methylene Chloride	23.3	65	0.00866	0.985	7.76
		110	0.00878		
		220	0.0103		
		300	0.0114		
		425	0.0135		
MEK	22	65	0.00357	0.869	1.53
		110	0.00509		
		220	0.00651		
		300	0.00706		
		425	0.00753		
Toluene	23	65	0.00331	0.97	0.49
		110	0.00365		
		220	0.00451		
		300	0.0046		
		425	0.0054		

Chamber Test Results:

The results of the chamber ventilation survey are recorded in Table 32A. The volume of the chamber was found to be 830 ft^3 and the air flow through the chamber was 713 cubic feet per minute (cfm). These data and the following data were used in the Reist model to construct the predicted concentration curves: room air temperature, molecular weight of the chemical, air velocity over the liquid surface, surface area of the liquid in the pan (619 cm^2), and a mixing factor ($k = 1$). The air velocities over the liquid surface were estimated, for each run, as described earlier, by extracting them from the evaporation rate curves based on the measured evaporation rate of the chemical in the chamber. A sample calculation for a single build-up concentration point for acetone using the Reist model is found in the Appendix.

The data collected during the chamber tests are recorded in Tables 33A-39A. These data were used to construct the observed concentration curves. These curves were plotted against the predicted build-up and decay curves using measured evaporation rates (Figures 16-29). The predicted and measured curves require a similar time to reach the equilibrium concentrations. The times required for the concentration to decay are also similar. For equilibrium concentrations, the model over-predicts three of the chemicals and under-predicts three of the chemicals for each run. In the remaining case, one run is over-predicted and the other is very close to the measured concentrations.

The Kawamura-Mackay Model Results:

The Kawamura-Mackay model was used to predict the evaporation rates for each of the chemicals under the conditions described in the previous section. These predicted evaporation rates, listed in Table 40A and summarized in Table 5, were then used in the Reist model to construct a second set of predicted concentration curves for each run. These curves were plotted against the measured concentration curves and are depicted in Figures 30-43.

The predicted equilibrium concentrations, in all cases but one, are lower than the measured equilibrium concentrations. Table 6 lists the equilibrium concentrations for the measured concentrations, predicted concentrations using measured evaporation rates, and predicted concentrations using the Kawamura-Mackay evaporation rates. The difference between the predicted and the experimental equilibrium concentrations are also listed.

In general, the predicted equilibrium concentrations, using both the measured evaporation rates and the Kawamura-Mackay predicted rates, agreed well with the experimental equilibrium concentrations. At equilibrium, the difference

TABLE 5: Summary of Kawamura-Mackay Predicted Evaporation Rates

Chemical Name	Air Temperature (C)	Air Velocity (fpm)	Evaporation Rate (g/min-cm^2)	R^2	Vapor Pressure @ Temp (psia)
Acetone	22	65	0.00241	0.995	3.92
		110	0.00323		
		220	0.00487		
		300	0.00593		
		425	0.00746		
Butyl Acetate	23	65	0.000562	0.996	0.0197
		110	0.000804		
		220	0.0013		
		300	0.00163		
		425	0.0021		
Ethyl Acetate	23	65	0.00216	0.995	1.66
		110	0.00296		
		220	0.00452		
		300	0.00555		
		425	0.00701		
Hexane	22.8	65	0.00292	0.995	2.57
		110	0.00393		
		220	0.00601		
		300	0.00732		
		425	0.00923		
Methylene Chloride	23.3	65	0.0051	0.996	7.76
		110	0.00672		
		220	0.01		
		300	0.0121		
		425	0.0152		
MEK	22	65	0.00168	0.995	1.53
		110	0.00229		
		220	0.00353		
		300	0.00434		
		425	0.00549		
Toluene	23	65	0.000961	0.995	0.49
		110	0.00135		
		220	0.00215		
		300	0.00266		
		425	0.00339		

TABLE 6: Comparison of Equilibrium Concentration Results (in ppm)

Chemical Name	Run#	Chamber Test Measurements	Reist Prediction Using Measured Evaporation Rates and % Diff Compared to Chamber Test Measurements		Reist Prediction Using Karamura-Mackay Evaporation Rates and % Diff Compared to Chamber Test Measurements	
				%Diff		% Diff
Acetone	1	103	139	-35	88	15
	2	135	172	-27	121	10
Butyl Acetate	1	15	17	-13	17	-13
	2	17	22	-29	24	-41
Ethyl Acetate	1	78	68	13	56	28
	2	96	81	16	78	19
Hexane	1	126	157	-25	76	40
	2	132	217	-64	105	20
Methylene Chloride	1	152	111	27	129	15
	2	262	134	49	179	32
MEK	1	75	79	-5	53	29
	2	101	99	2	73	28
Toluene	1	56	41	27	24	57
	2	61	49	20	34	44
Average Difference				25		28

between the experimental concentrations and those predicted using measured evaporation rates ranged from 2 to 64%, with an average of 25%. The difference between the experimental concentrations and those predicted using the Kawamura-Mackay predicted evaporation rates ranged from 10 to 57%, with an average of 28%.

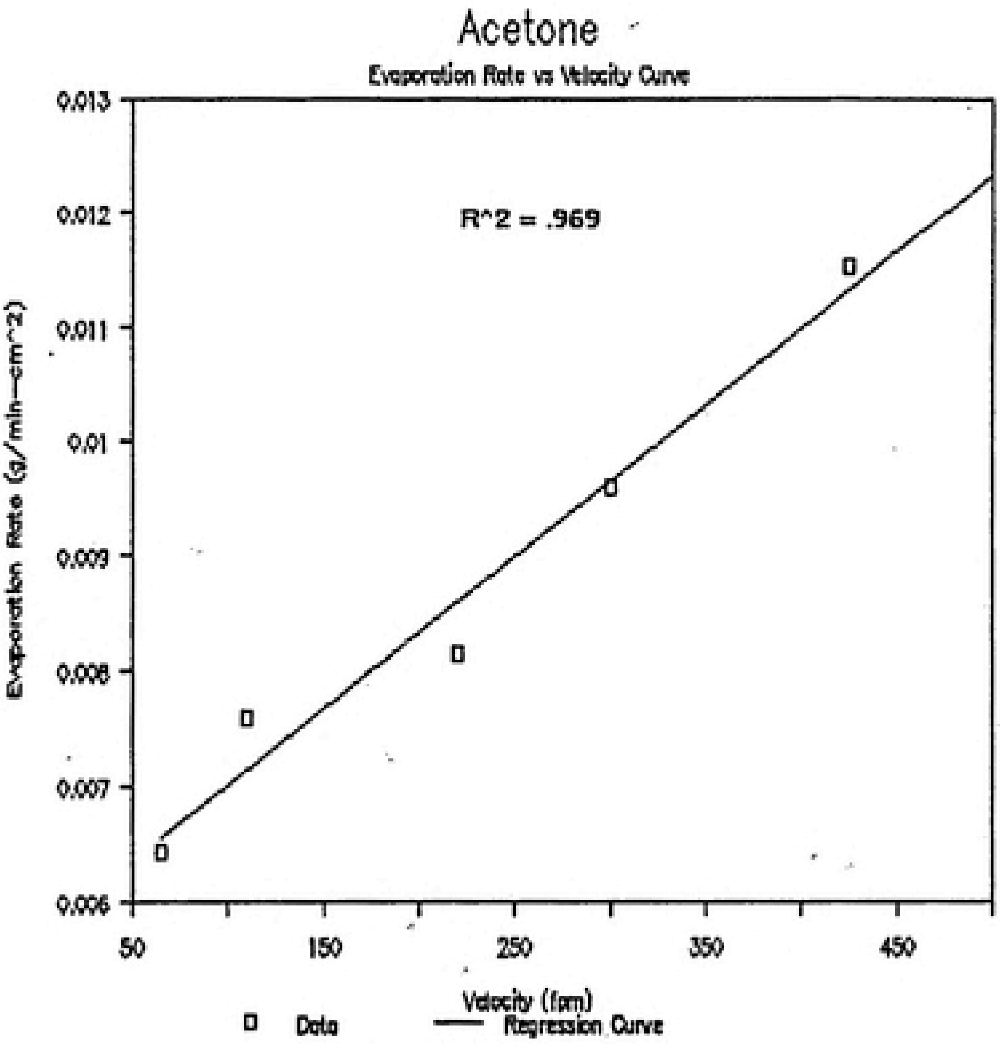


Figure 8. Velocity test evaporation rate curve.

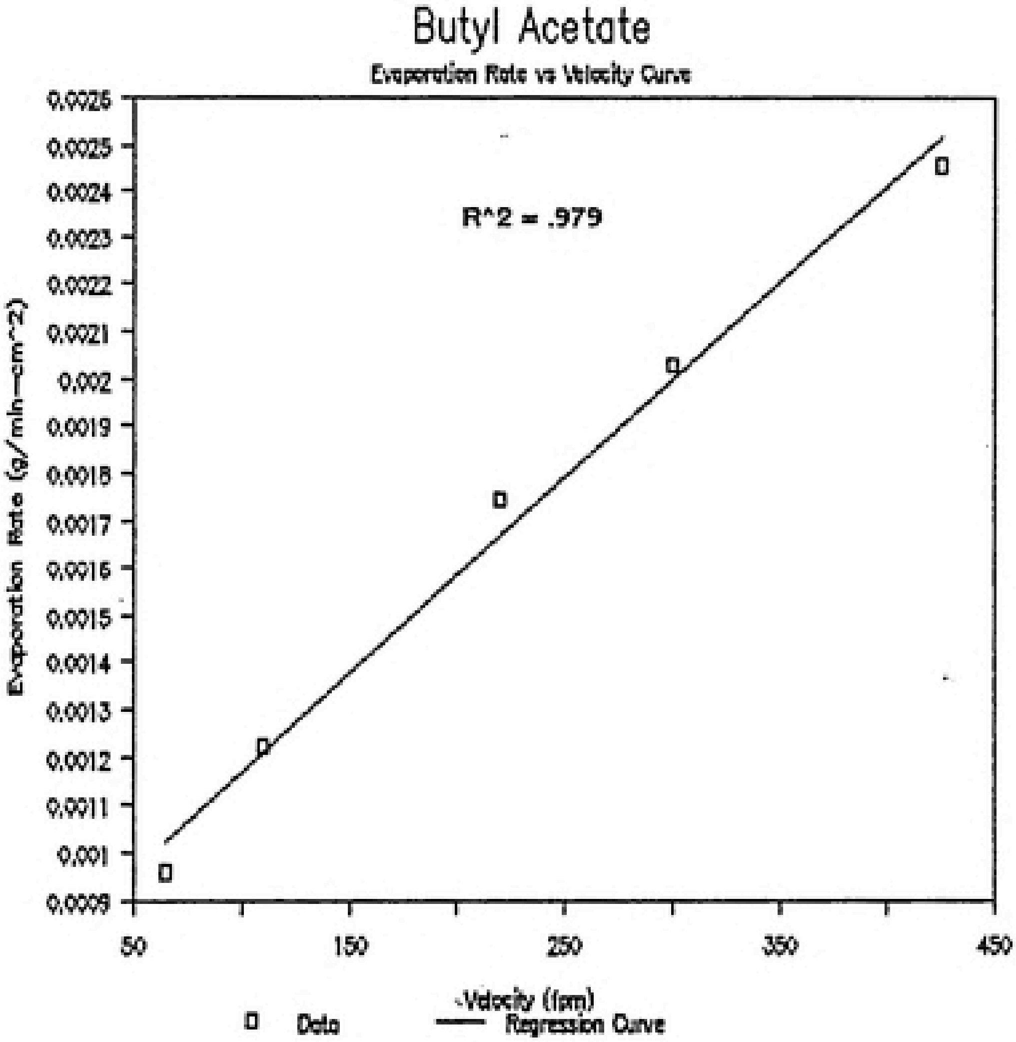


Figure 9. Velocity test evaporation rate curve.

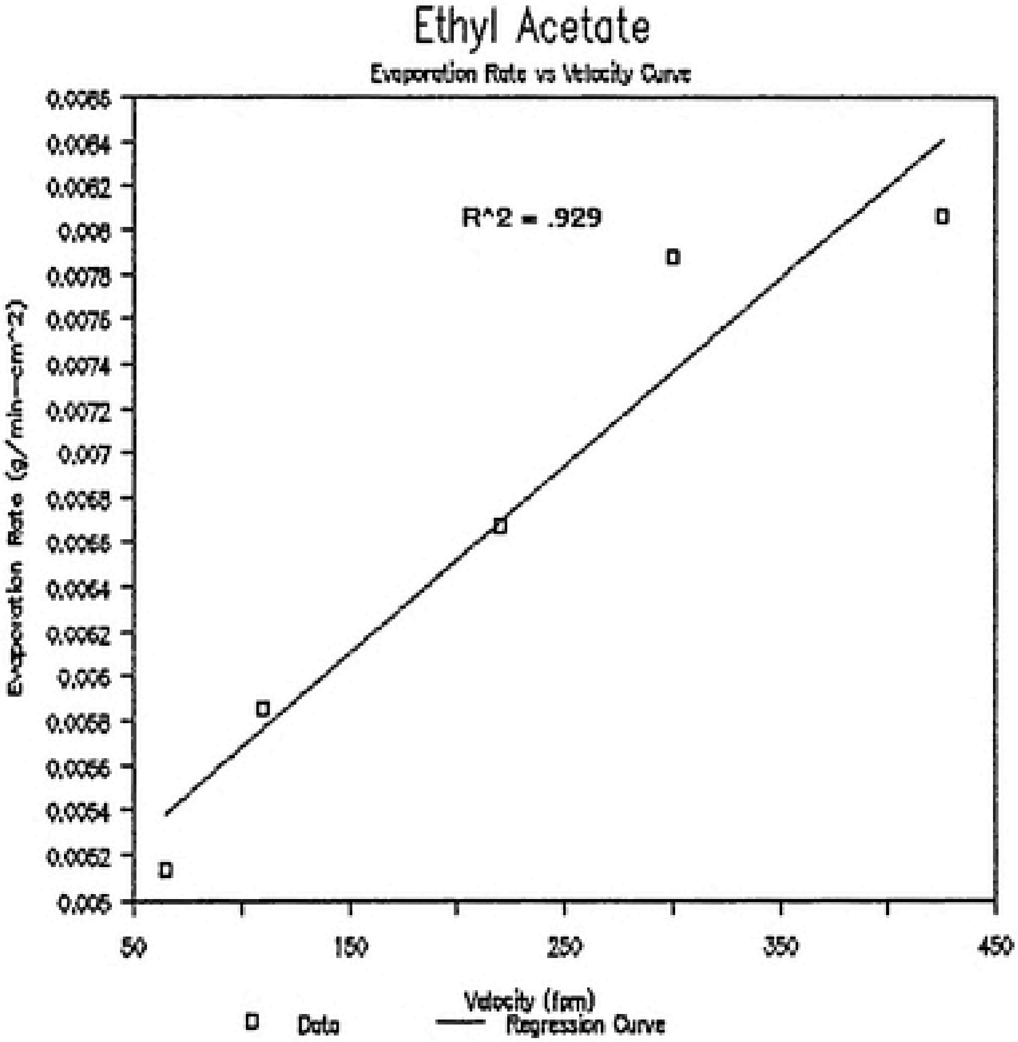


Figure 10. Velocity test evaporation rate curve.

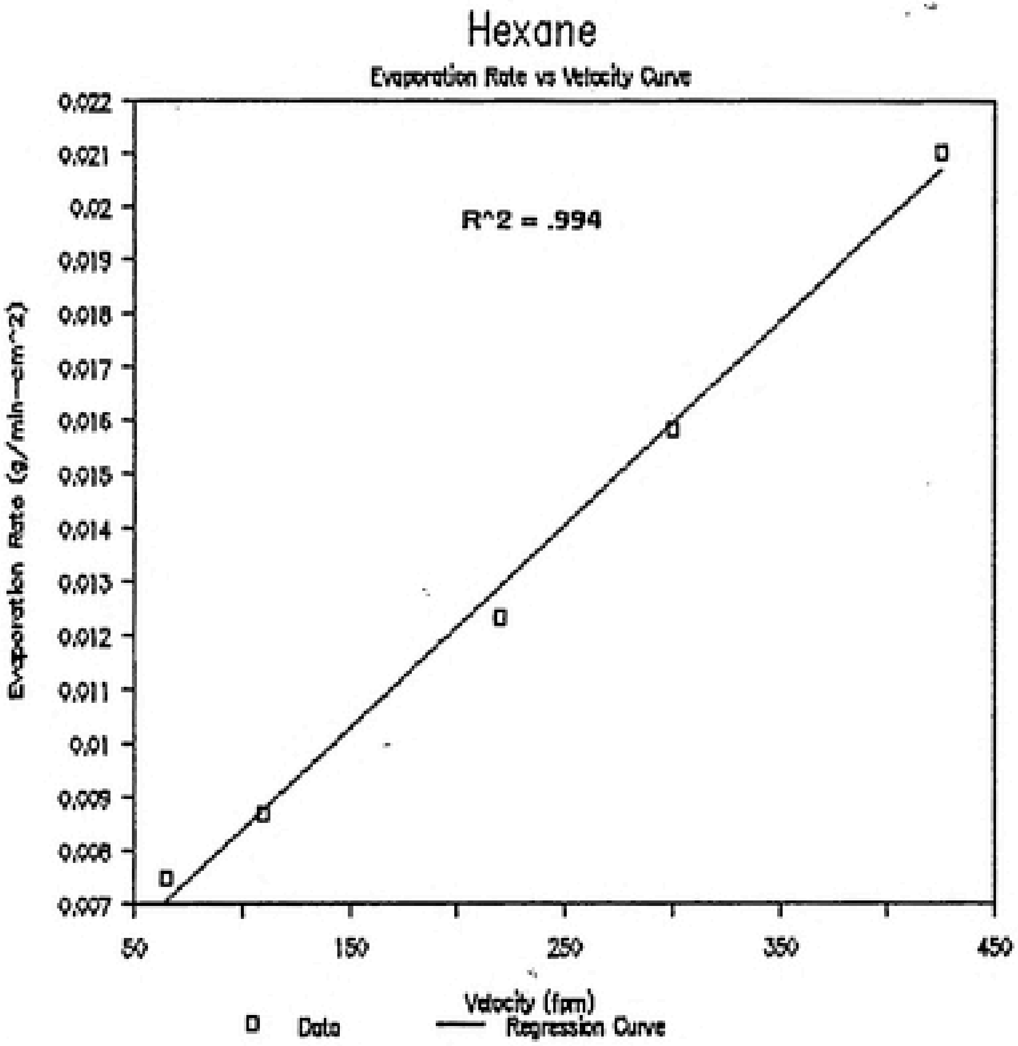


Figure 11. Velocity test evaporation rate curve.

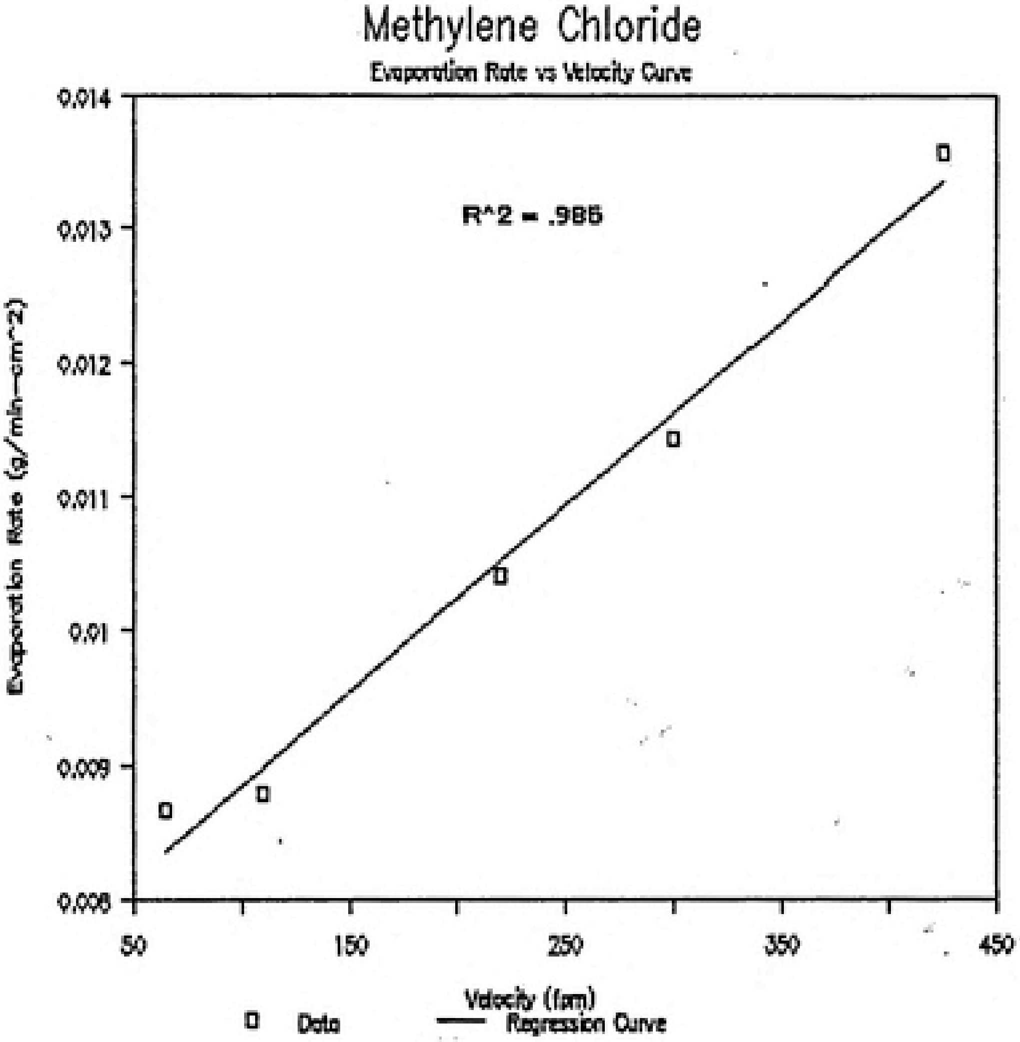


Figure 12. Velocity test evaporation rate curve.

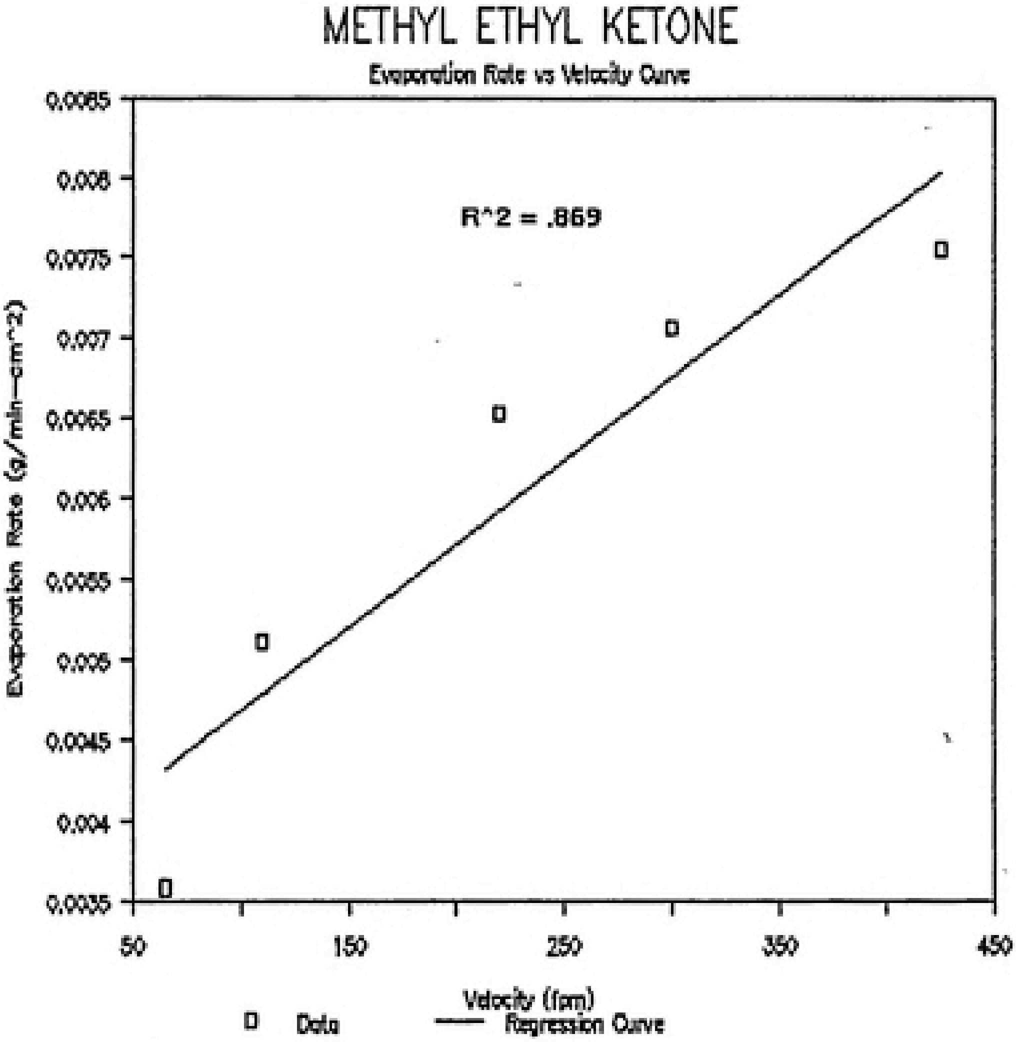


Figure 13. Velocity test evaporation rate curve.

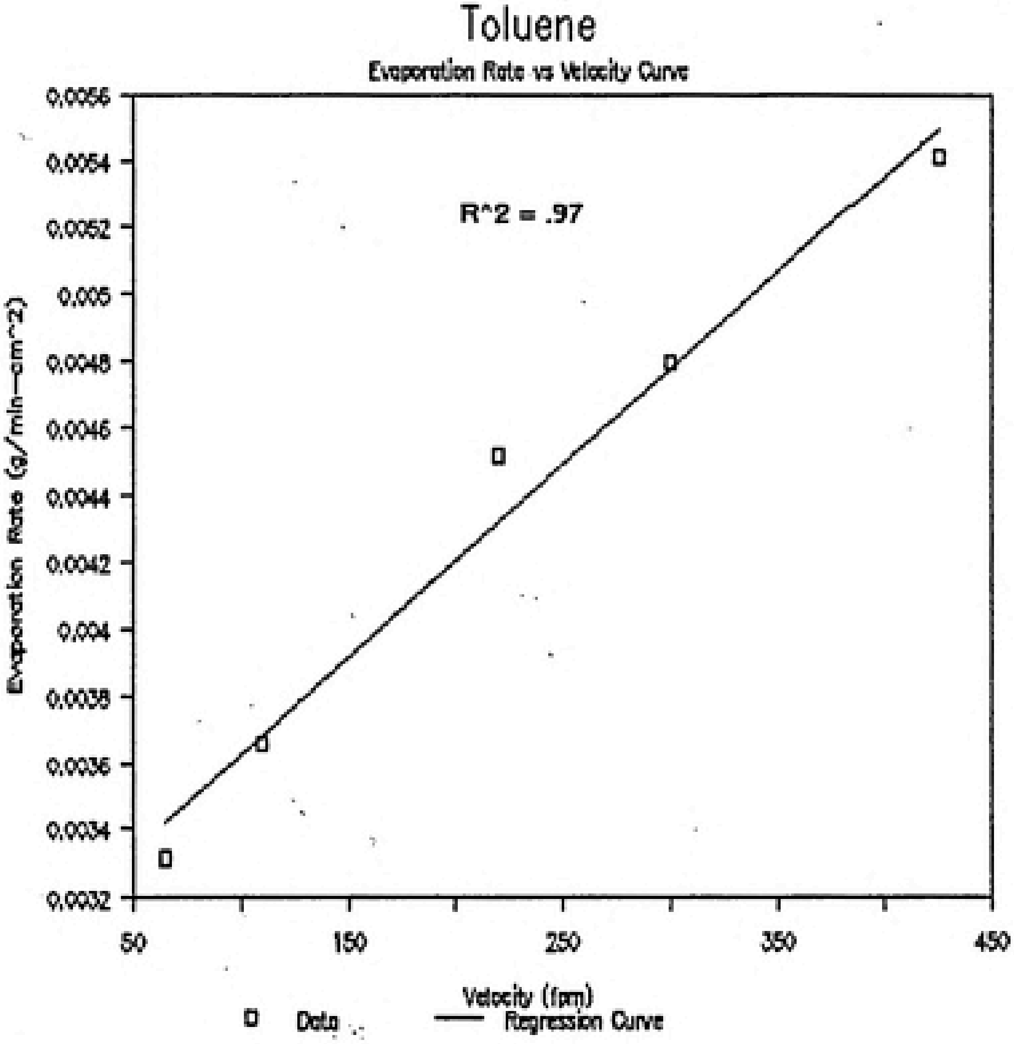


Figure 14.—Velocity test evaporation rate curve.

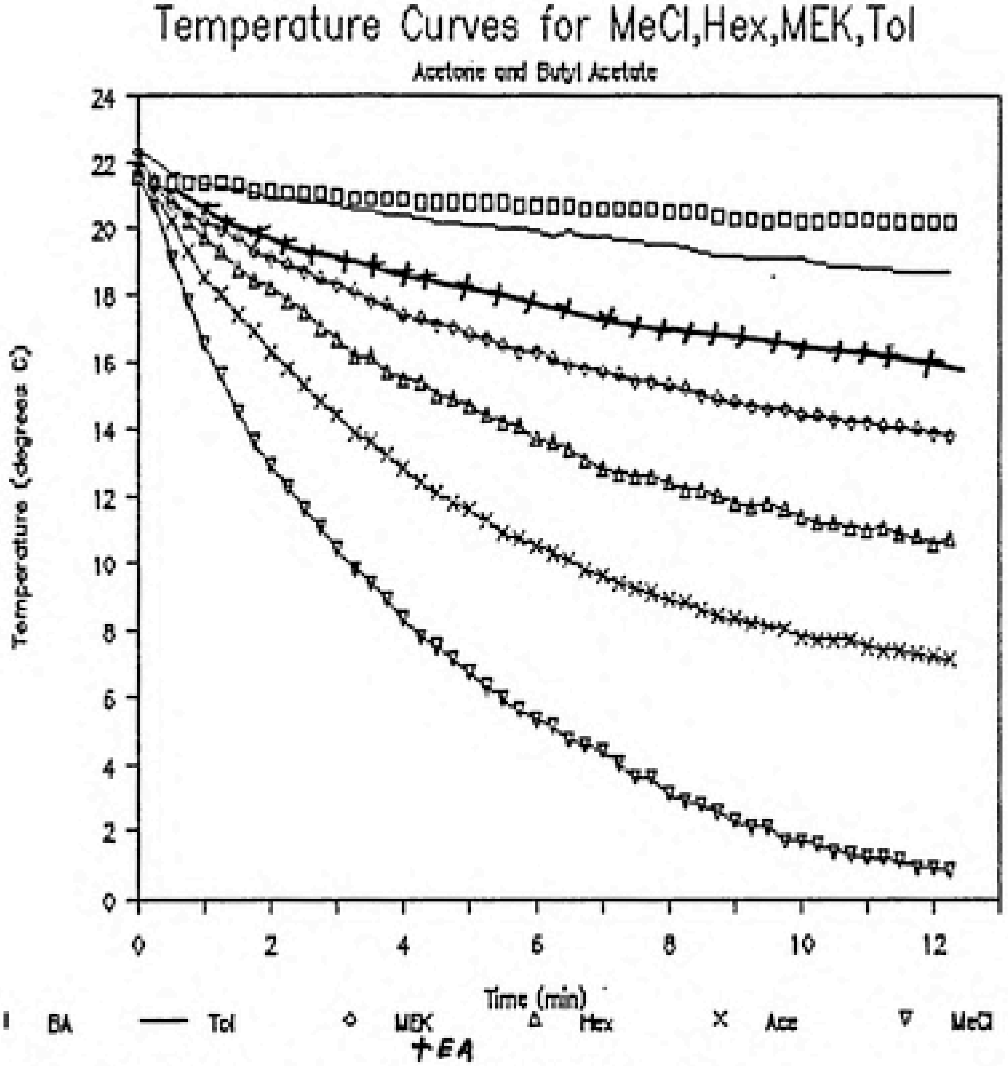


Figure 15. Plot of temperature curves for velocity tests.

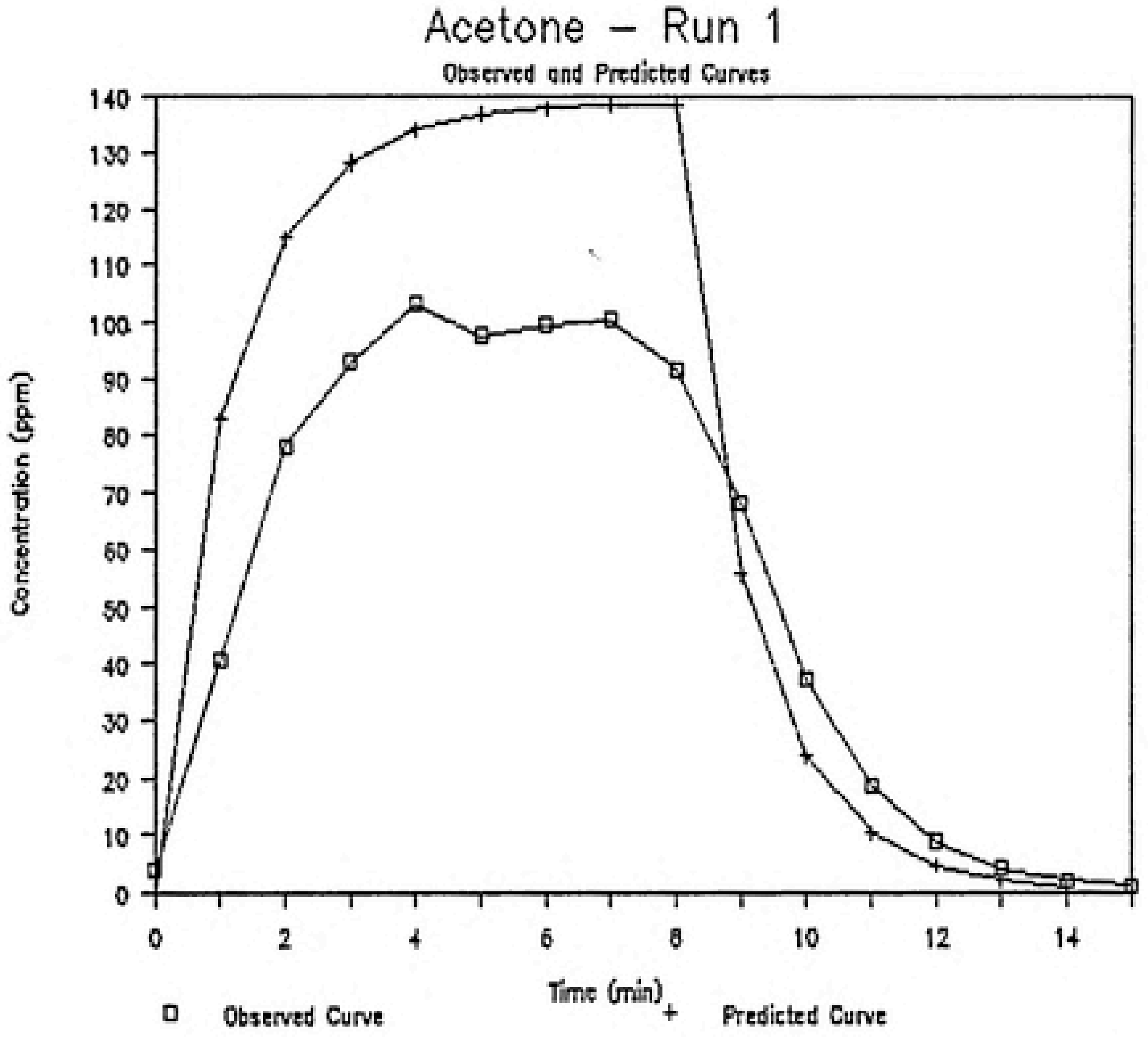


Figure 16. Comparison of measured concentration curve to Reist predicted using a measured evaporation rate.

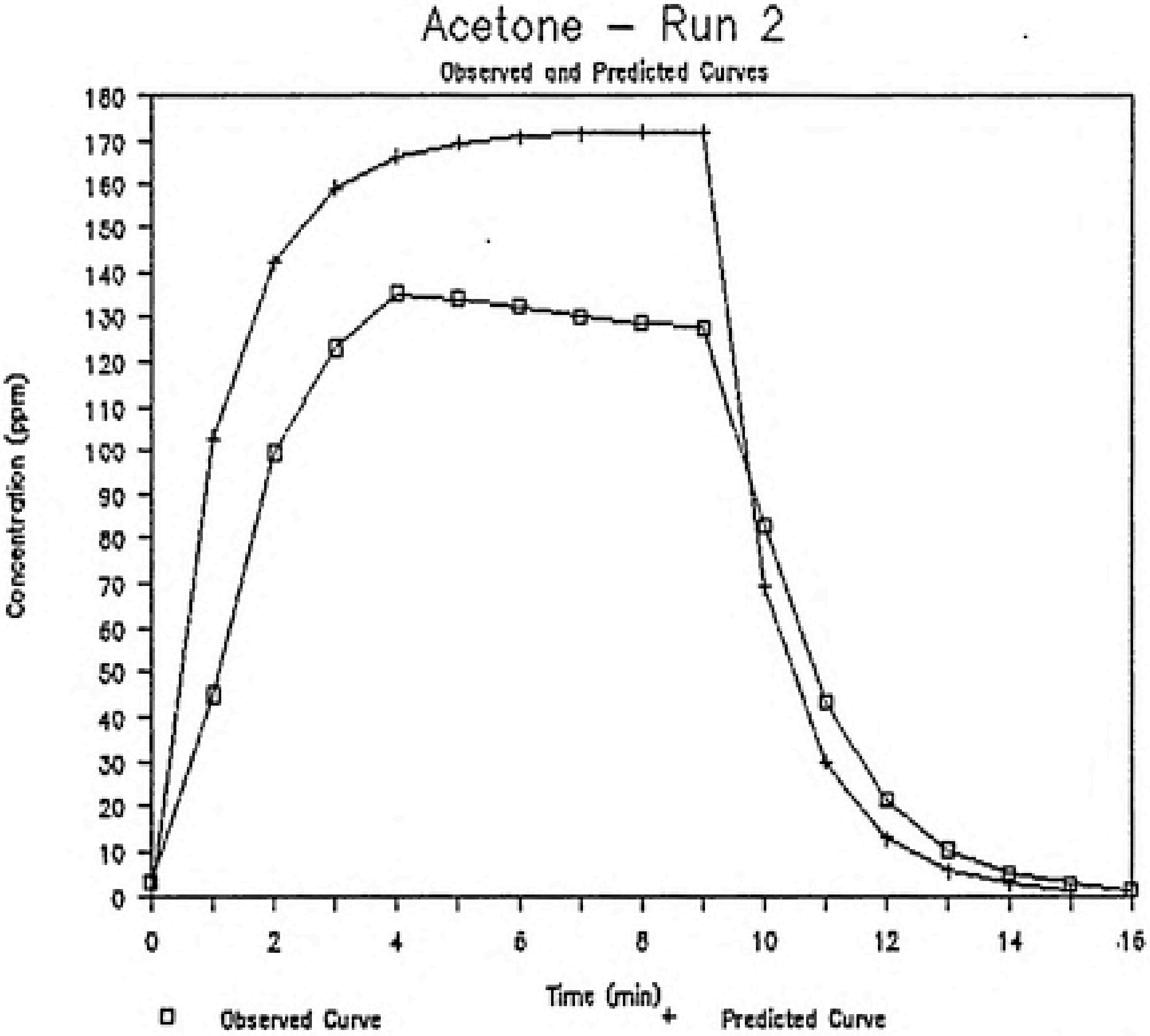


Figure 17._Comparison of measured concentration curve to Reist predicted using a measured evaporation rate.

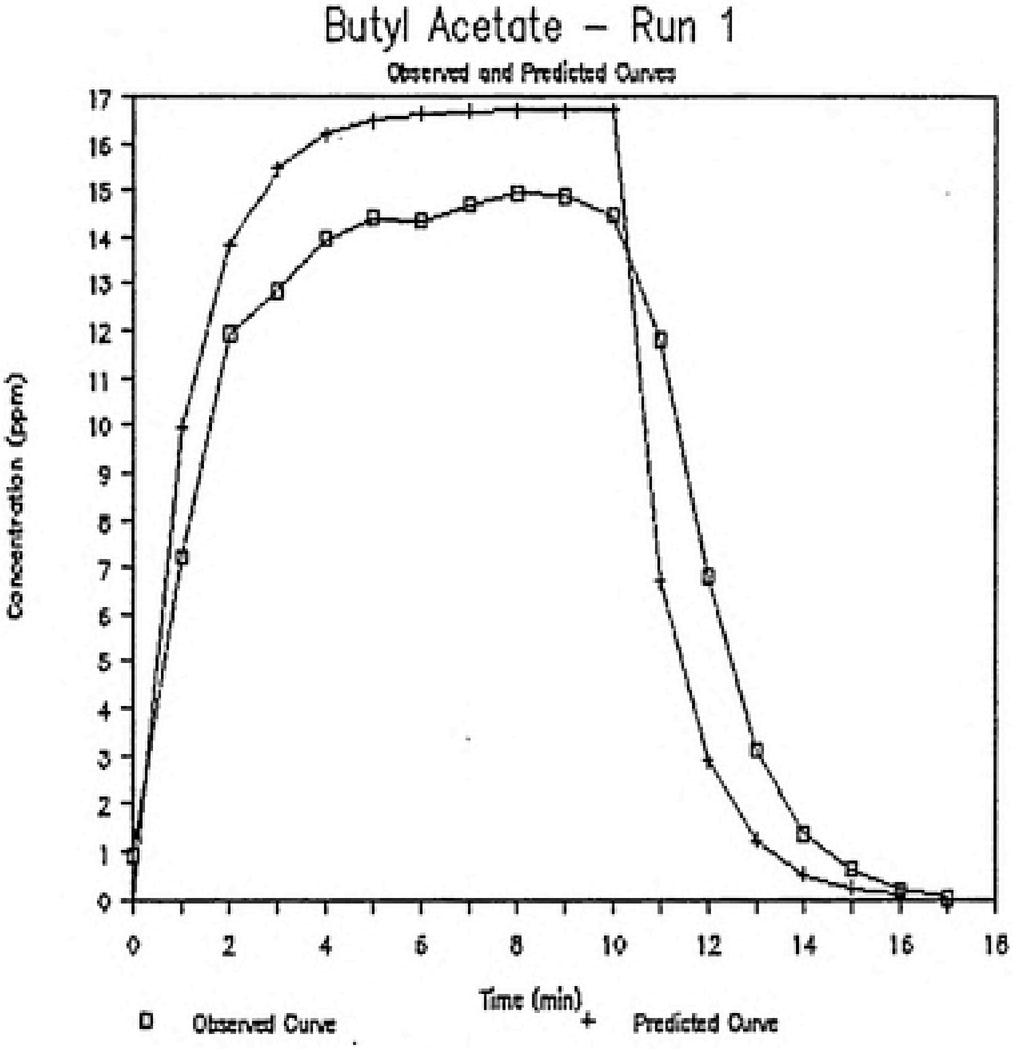


Figure 18. Comparison of measured concentration curve to Reist predicted using a measured evaporation rate.

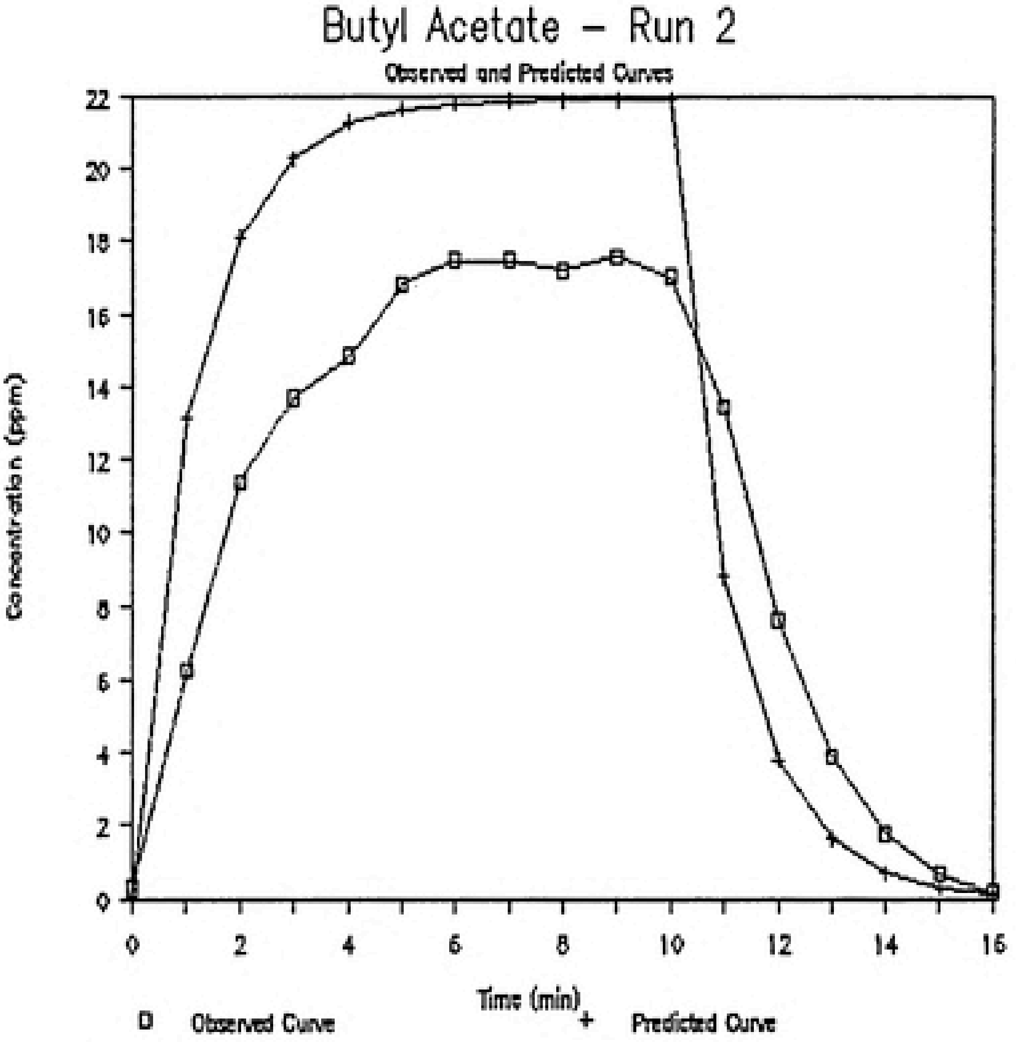


Figure 19. Comparison of measured concentration curve to Reist predicted using a measured evaporation rate.

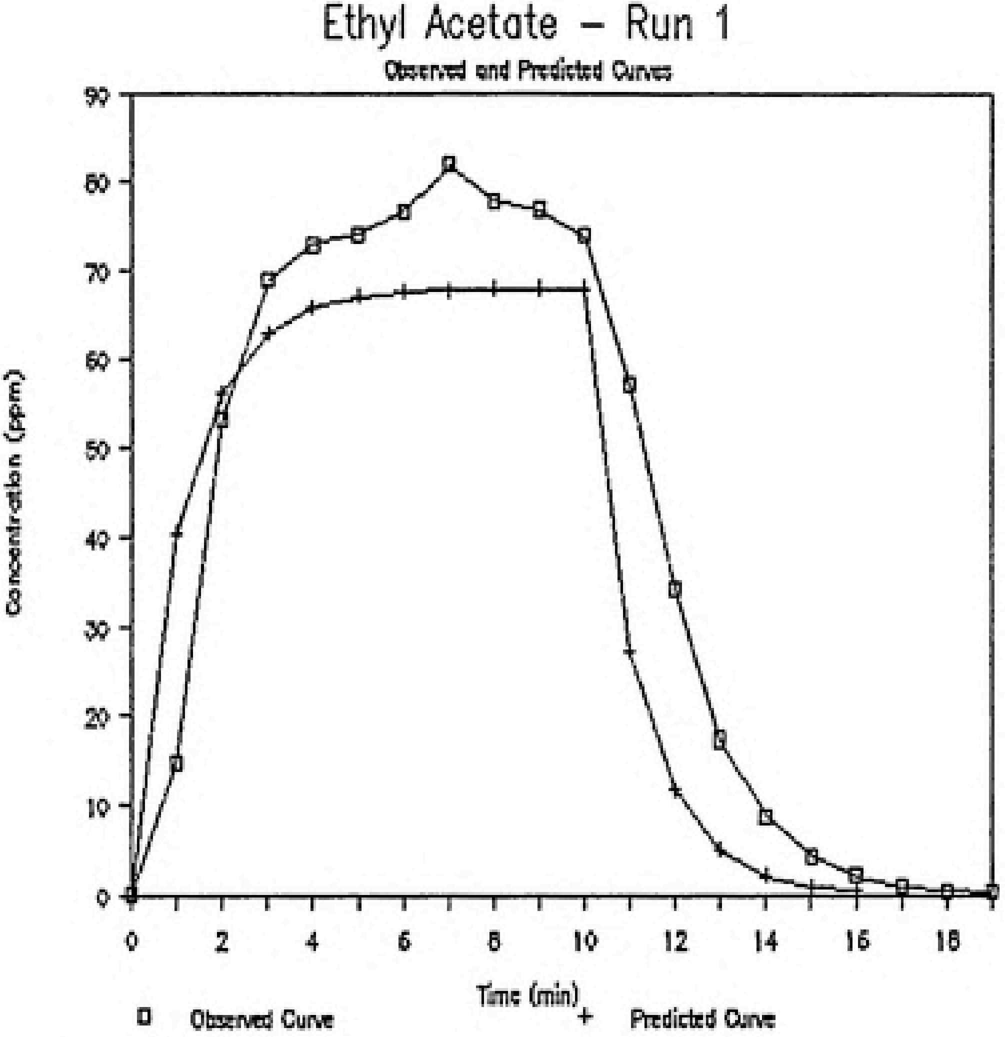


Figure 20. Comparison of measured concentration curve to Reist predicted using a measured evaporation rate.

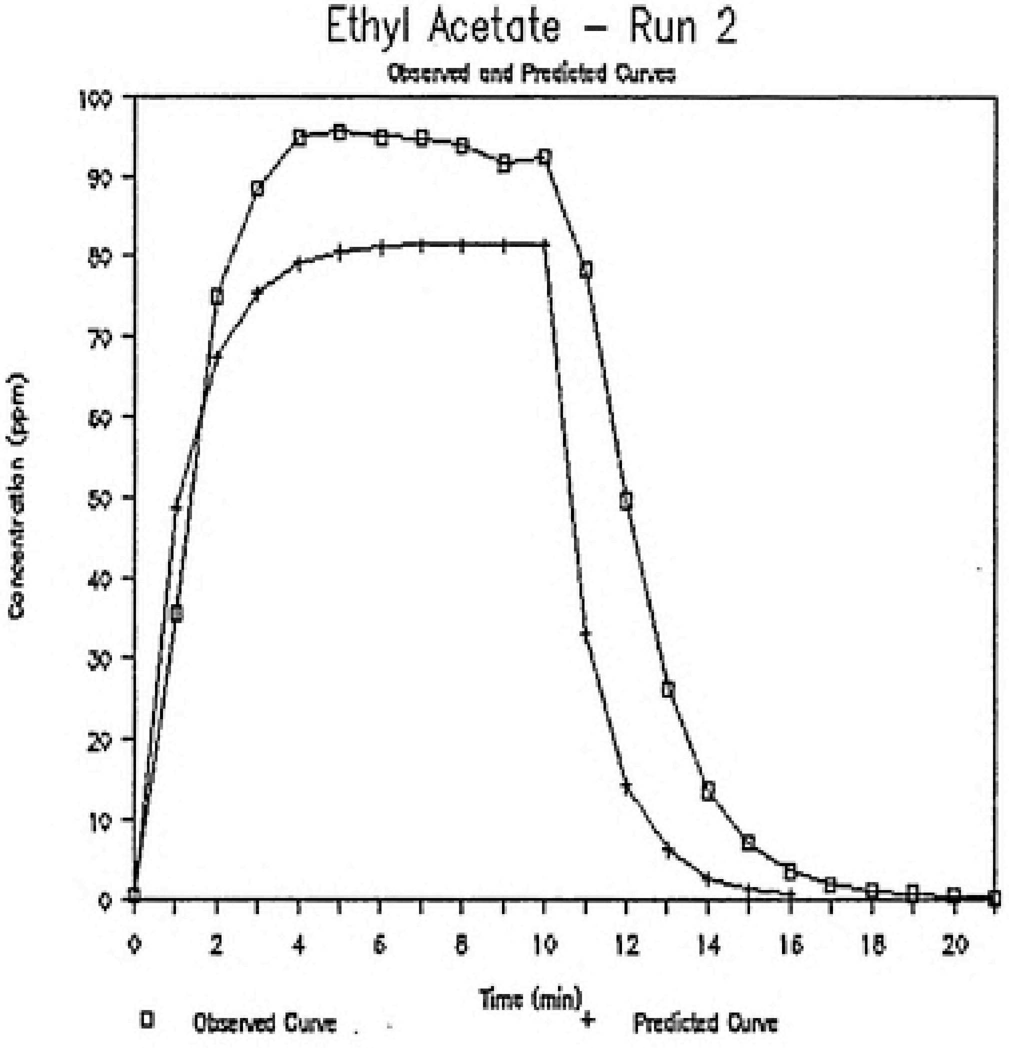


Figure 21. Comparison of measured concentration curve to Reist predicted using a measured evaporation rate.

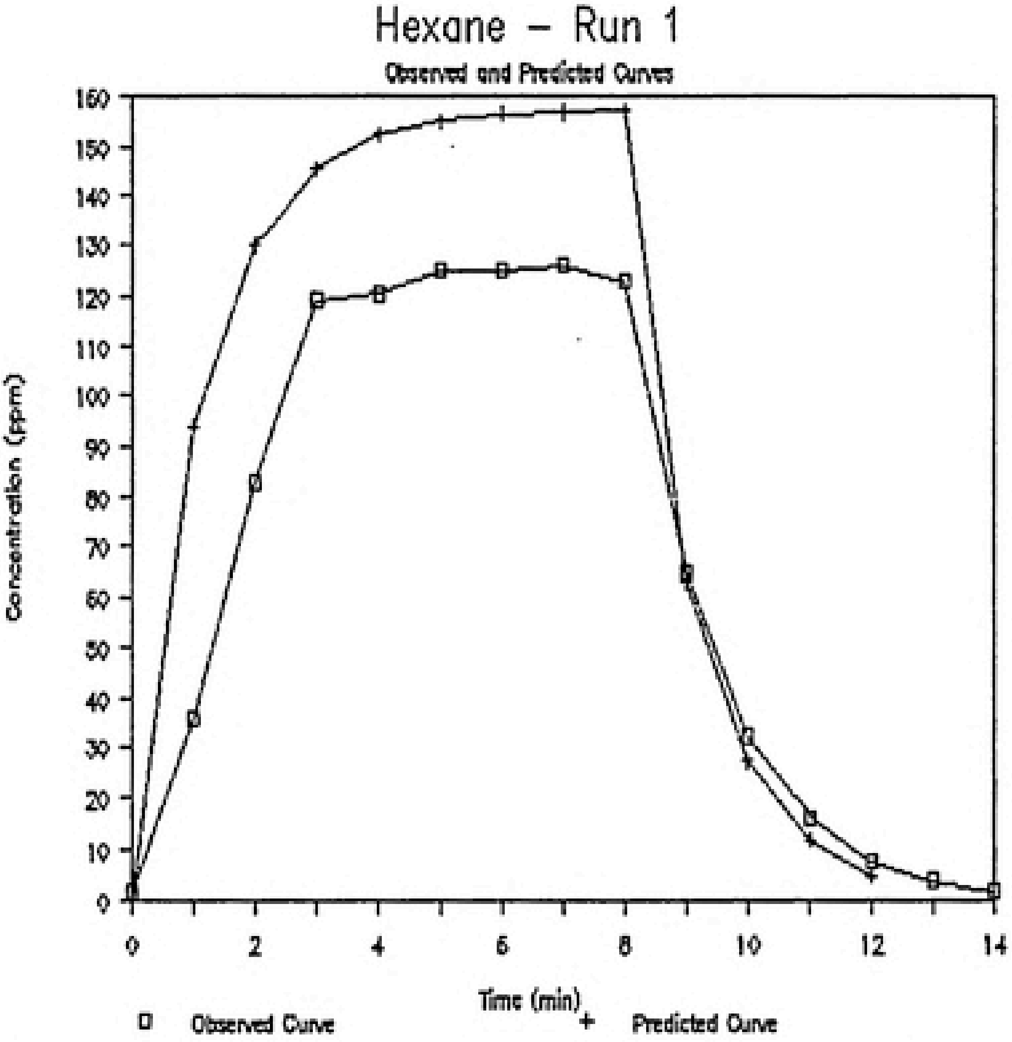


Figure 22. Comparison of measured concentration curve to Reist predicted using a measured evaporation rate.

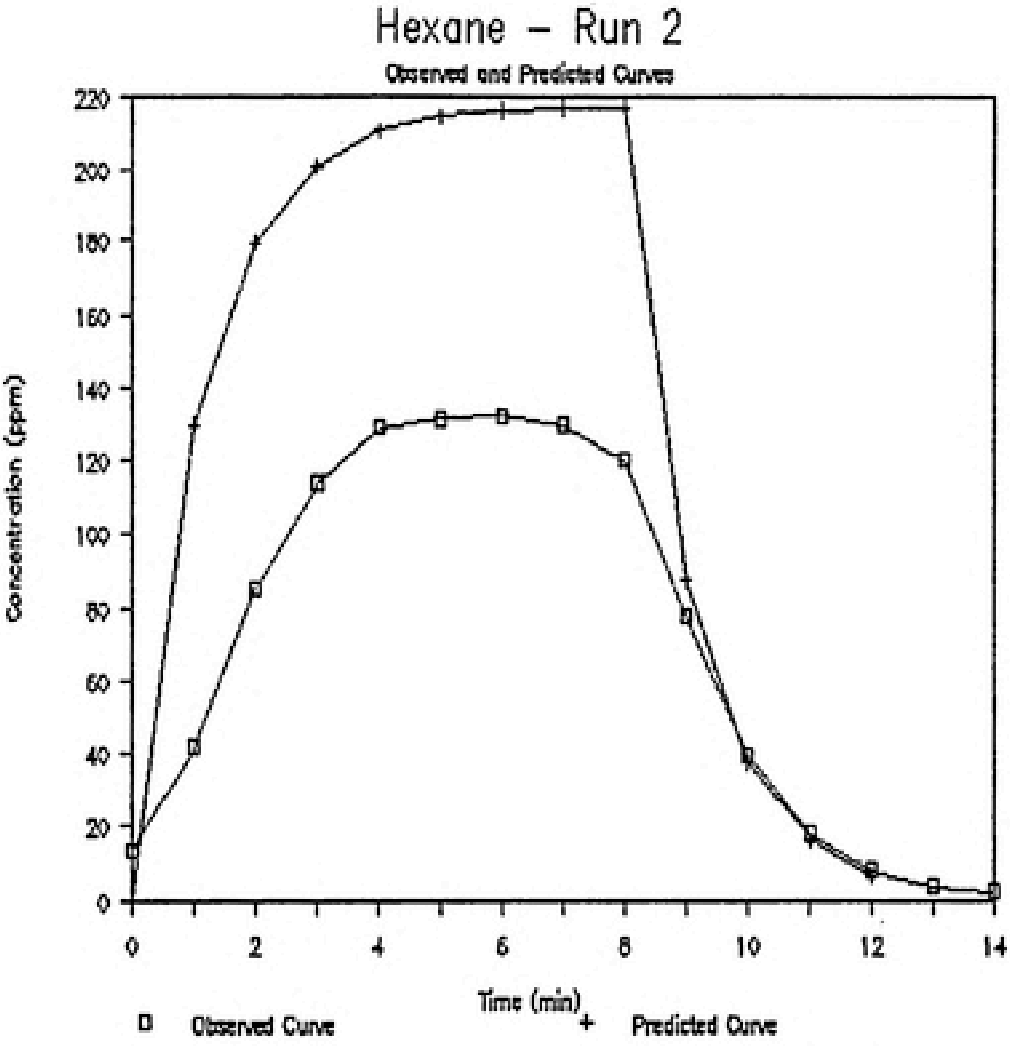


Figure 23. Comparison of measured concentration curve to Reist predicted using a measured evaporation rate.

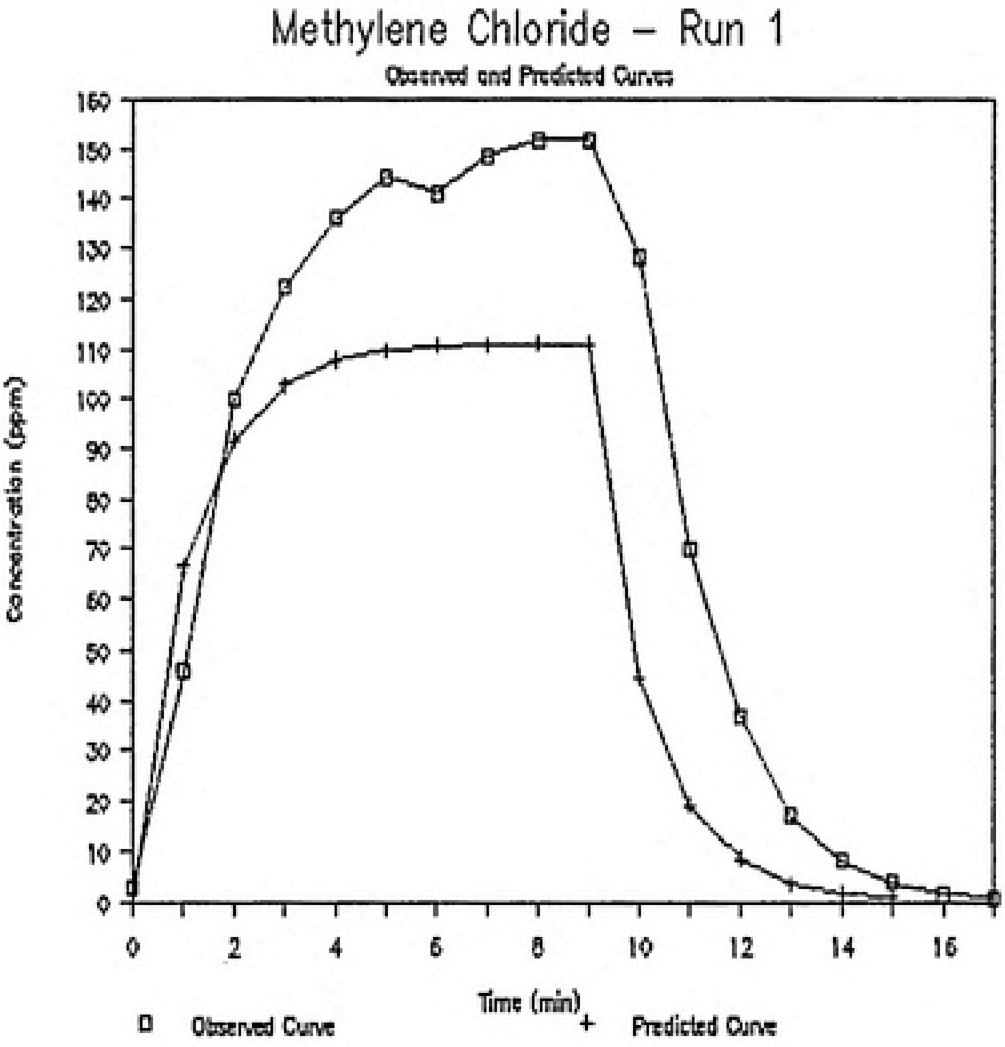


Figure 24. Comparison of measured concentration curve to Reist predicted using a measured evaporation rate.

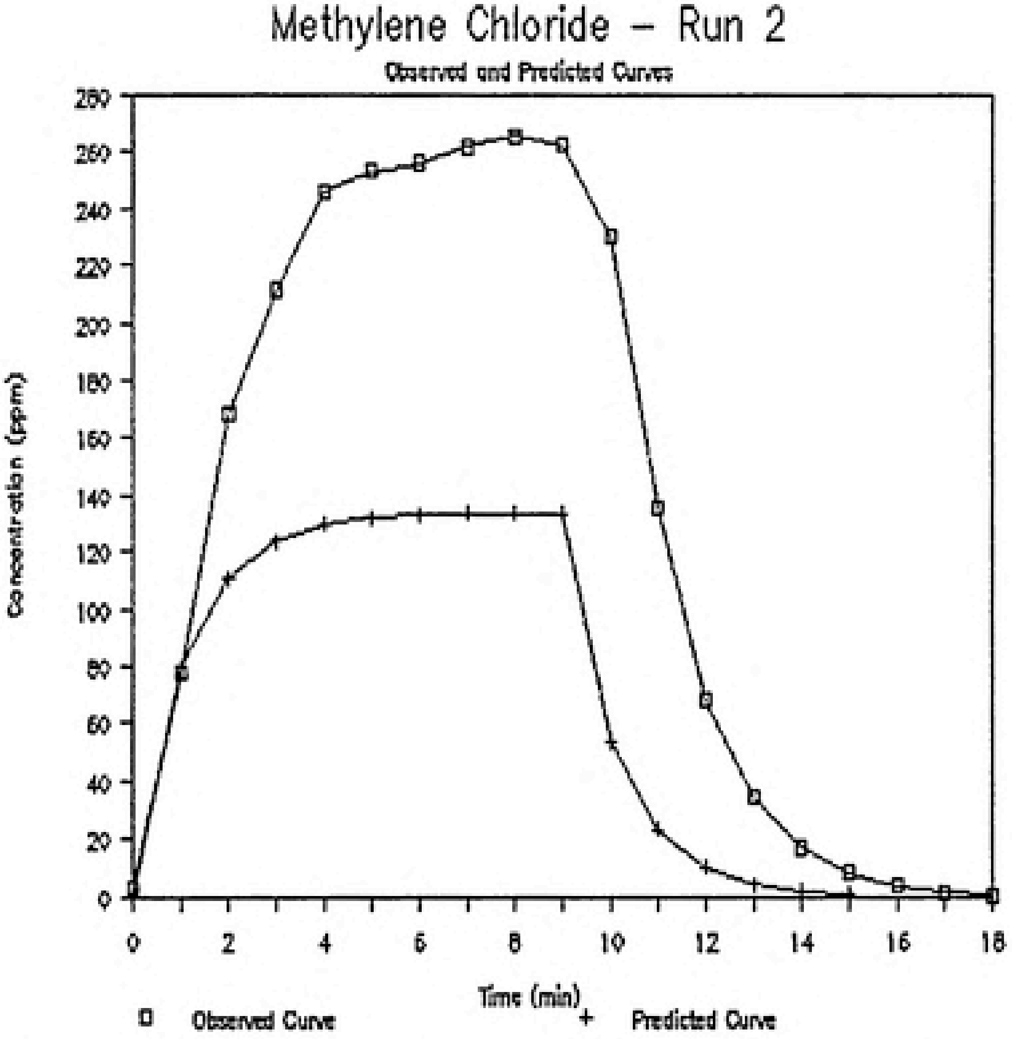


Figure 25. Comparison of measured concentration curve to Reist predicted using a measured evaporation rate.

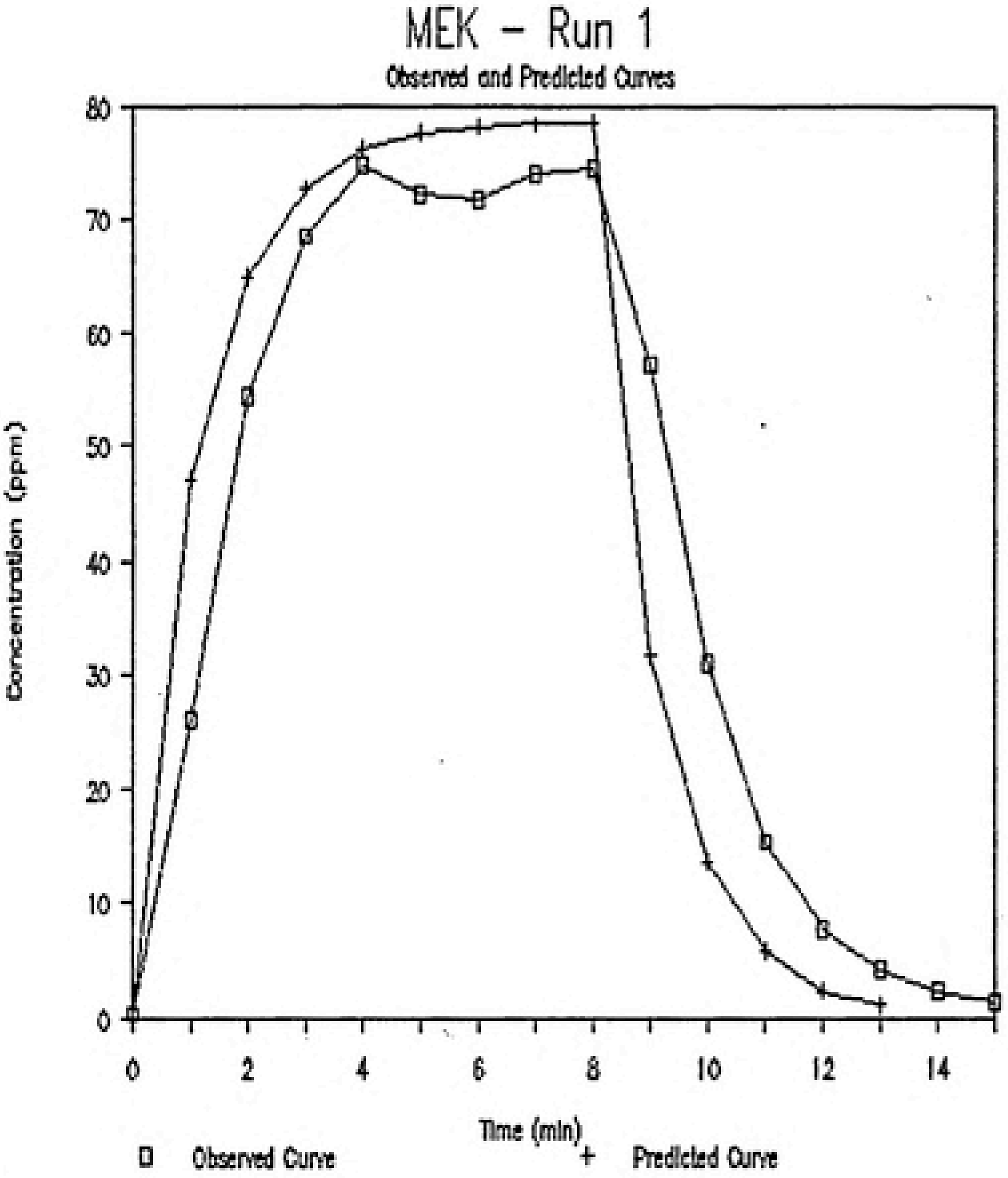


Figure 26. Comparison of measured concentration curve to Reist predicted using a measured evaporation rate.

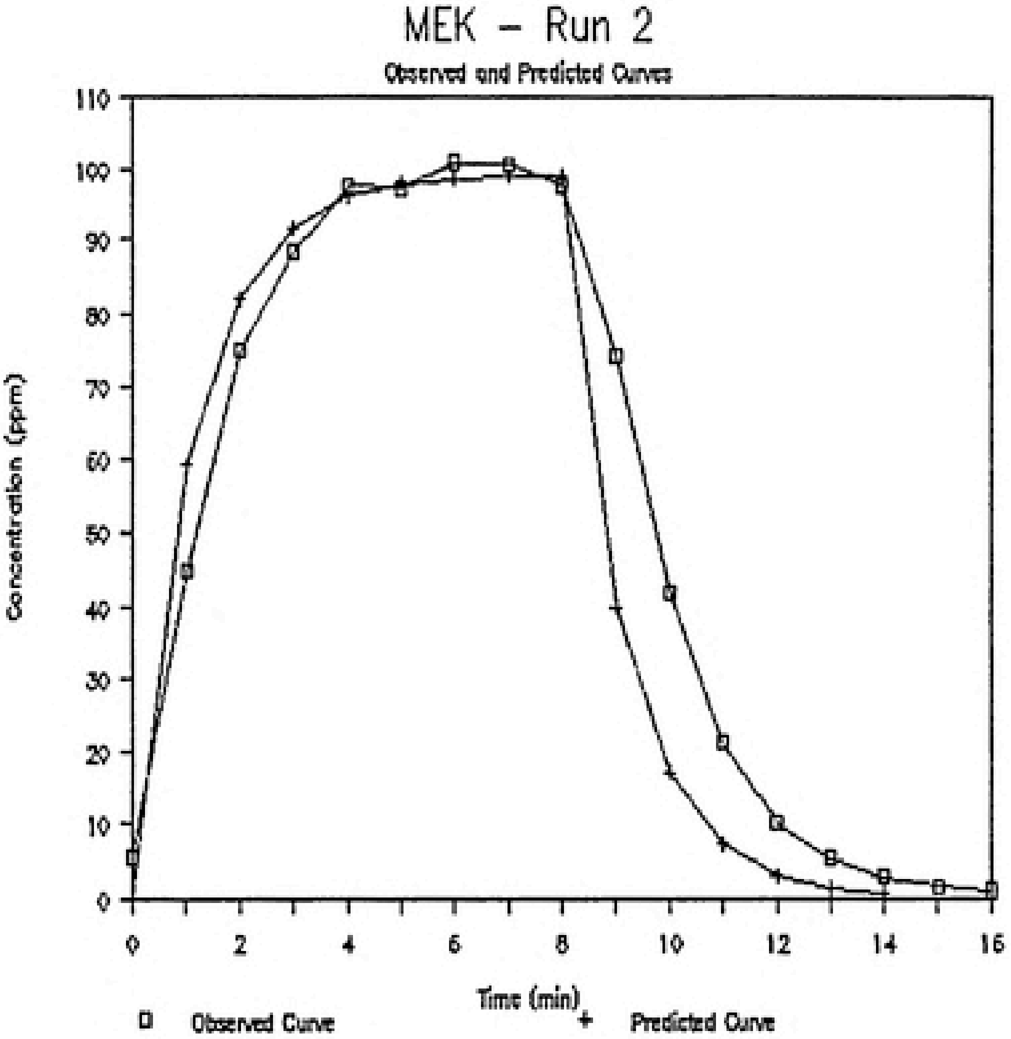


Figure 27. Comparison of measured concentration curve to Reist predicted using a measured evaporation rate.

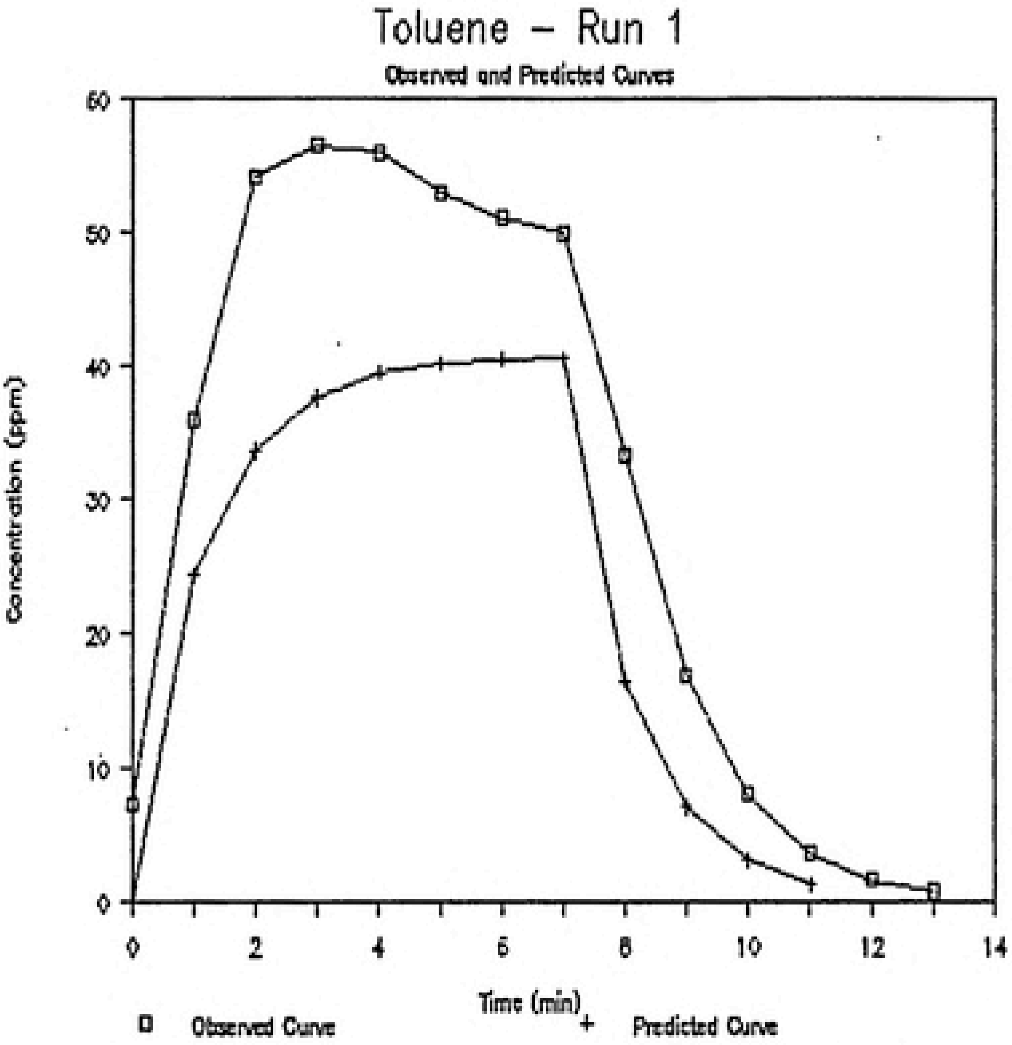


Figure 28. Comparison of measured concentration curve to Reist predicted using a measured evaporation rate.

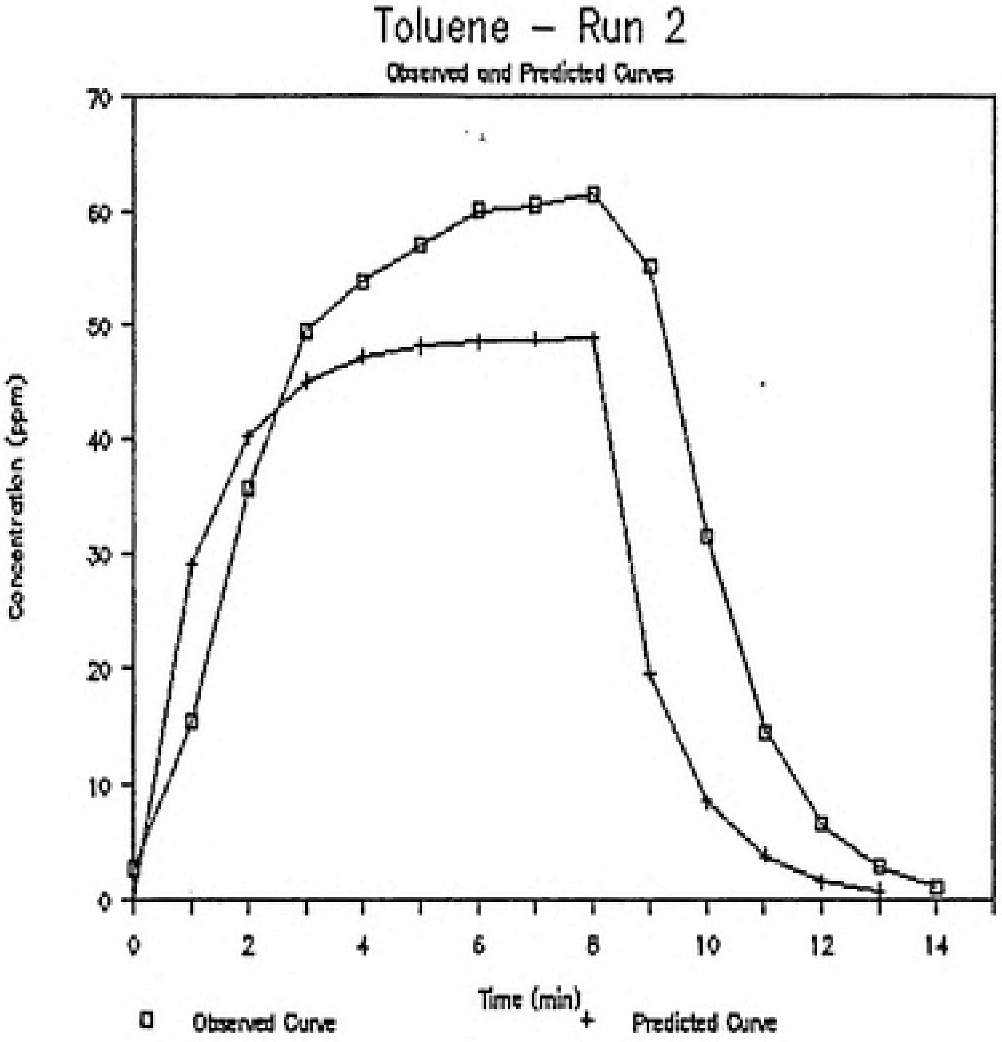


Figure 29. Comparison of measured concentration curve to Reist predicted using a measured evaporation rate.

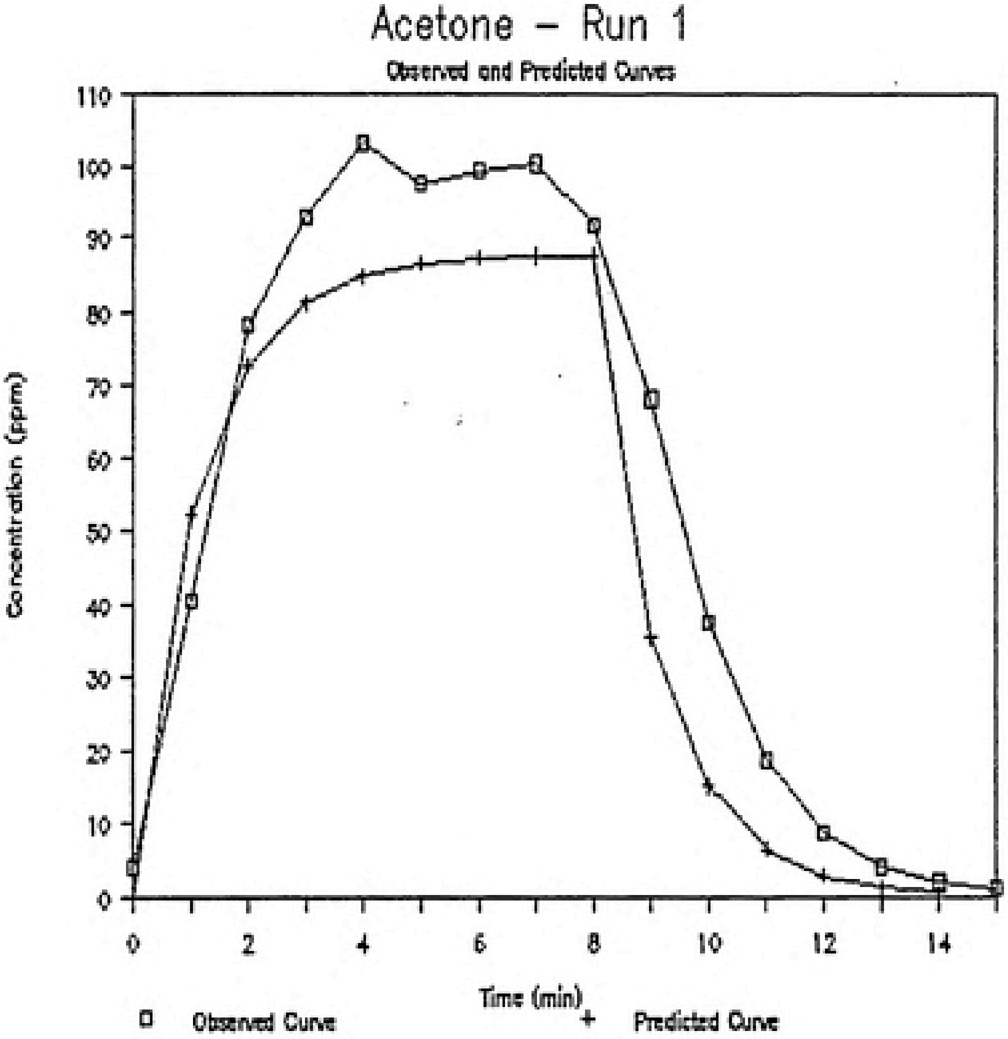


Figure 30. Comparison of measured concentration curve to Reist predicted using Kawamura-Mackay predicted evaporation rate.

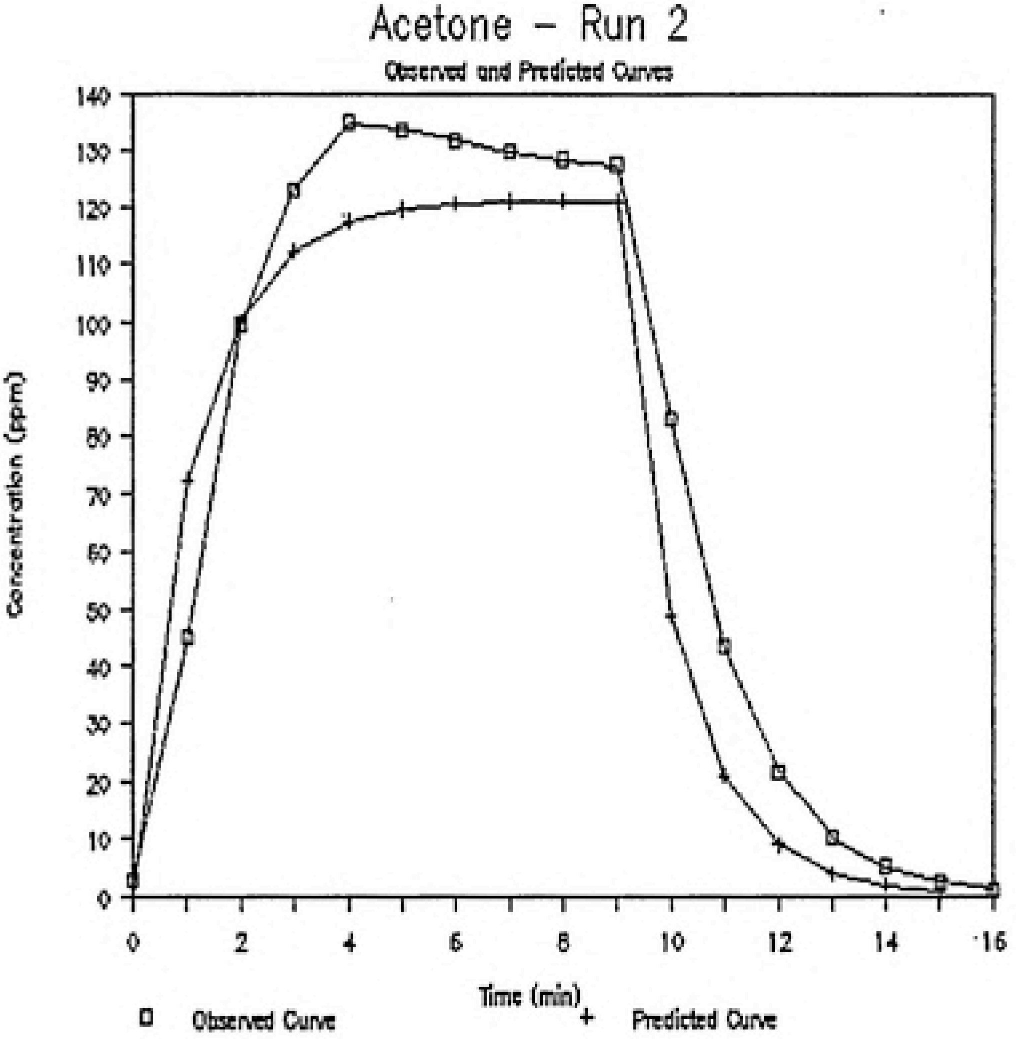


Figure 31. Comparison of measured concentration curve to Reist predicted using Kawamura-Mackay predicted evaporation rate.

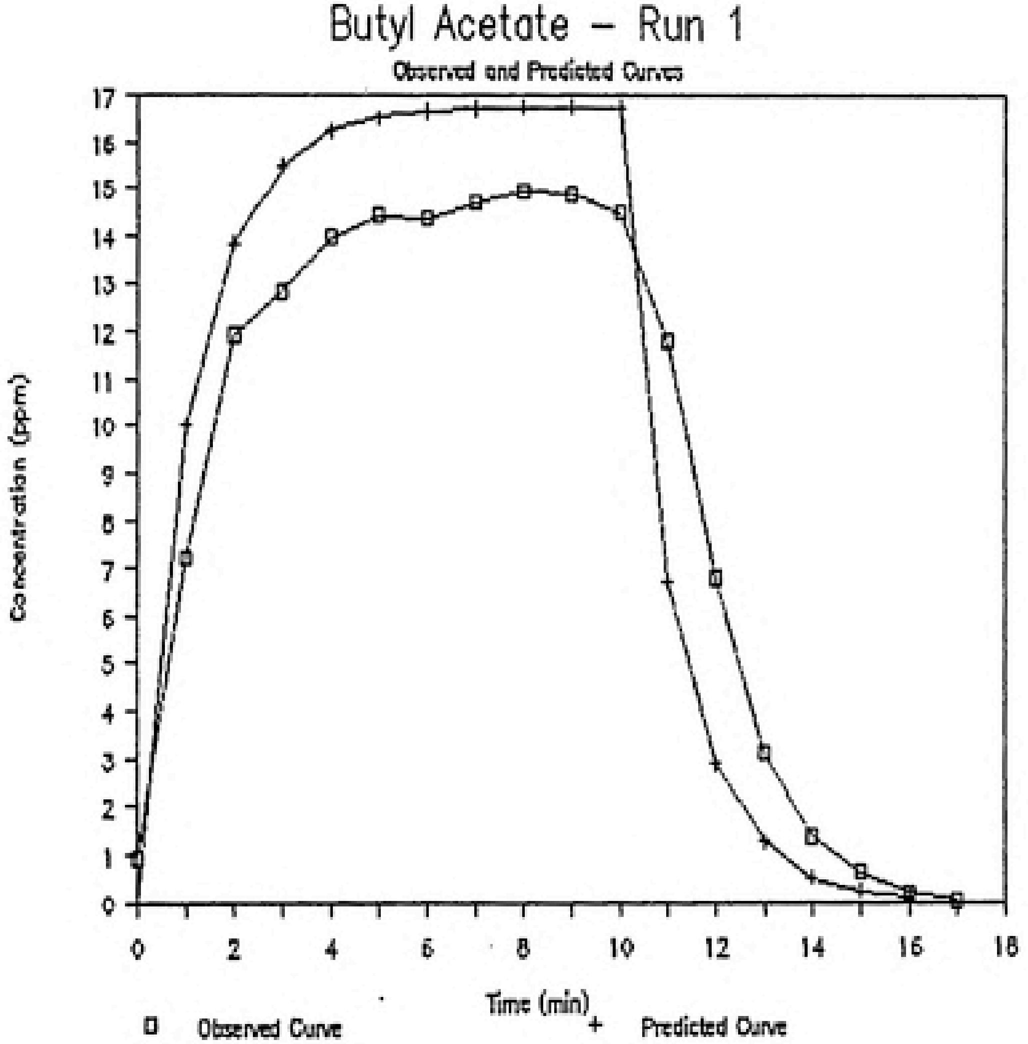


Figure 32. Comparison of measured concentration curve to Reist predicted using Kawamura-Mackay predicted evaporation rate.

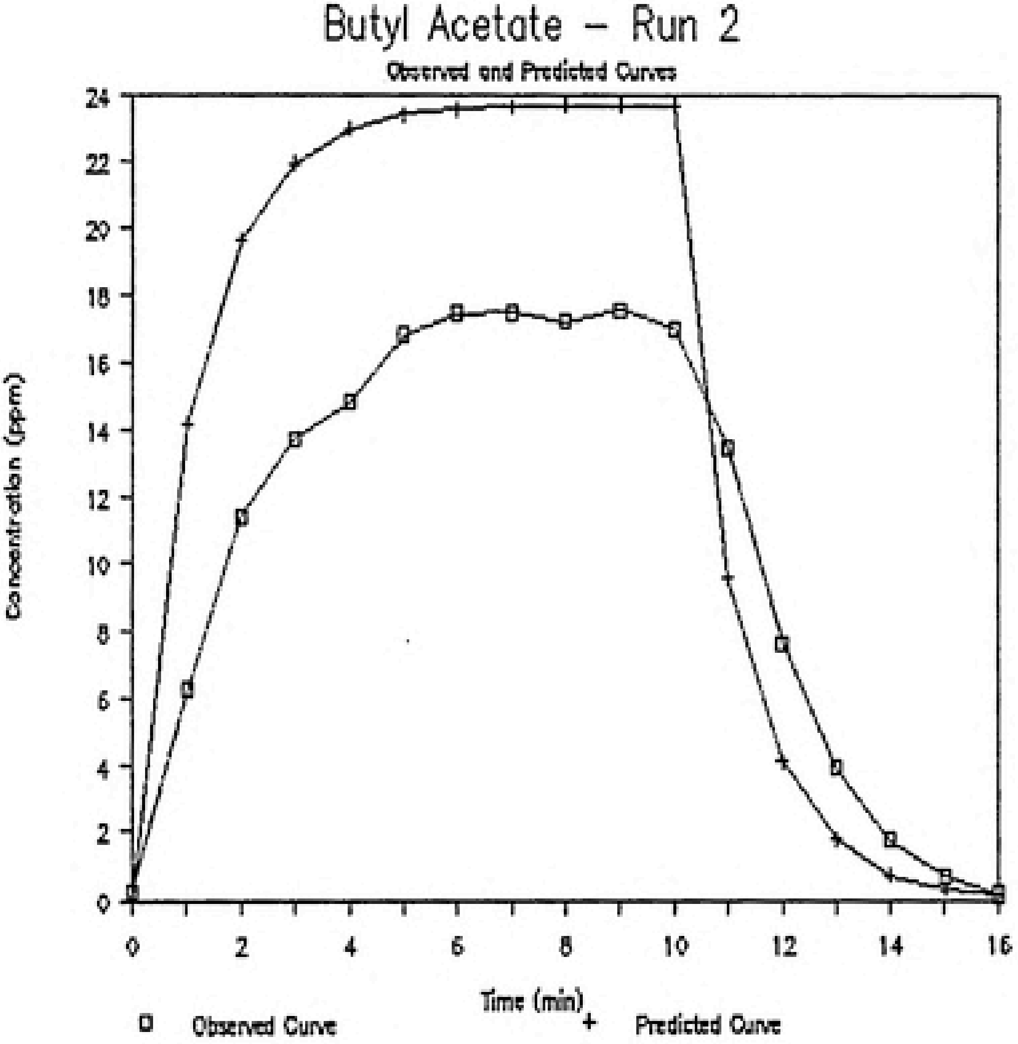


Figure 33. Comparison of measured concentration curve to Reist predicted using Kawamura-Mackay predicted evaporation rate.

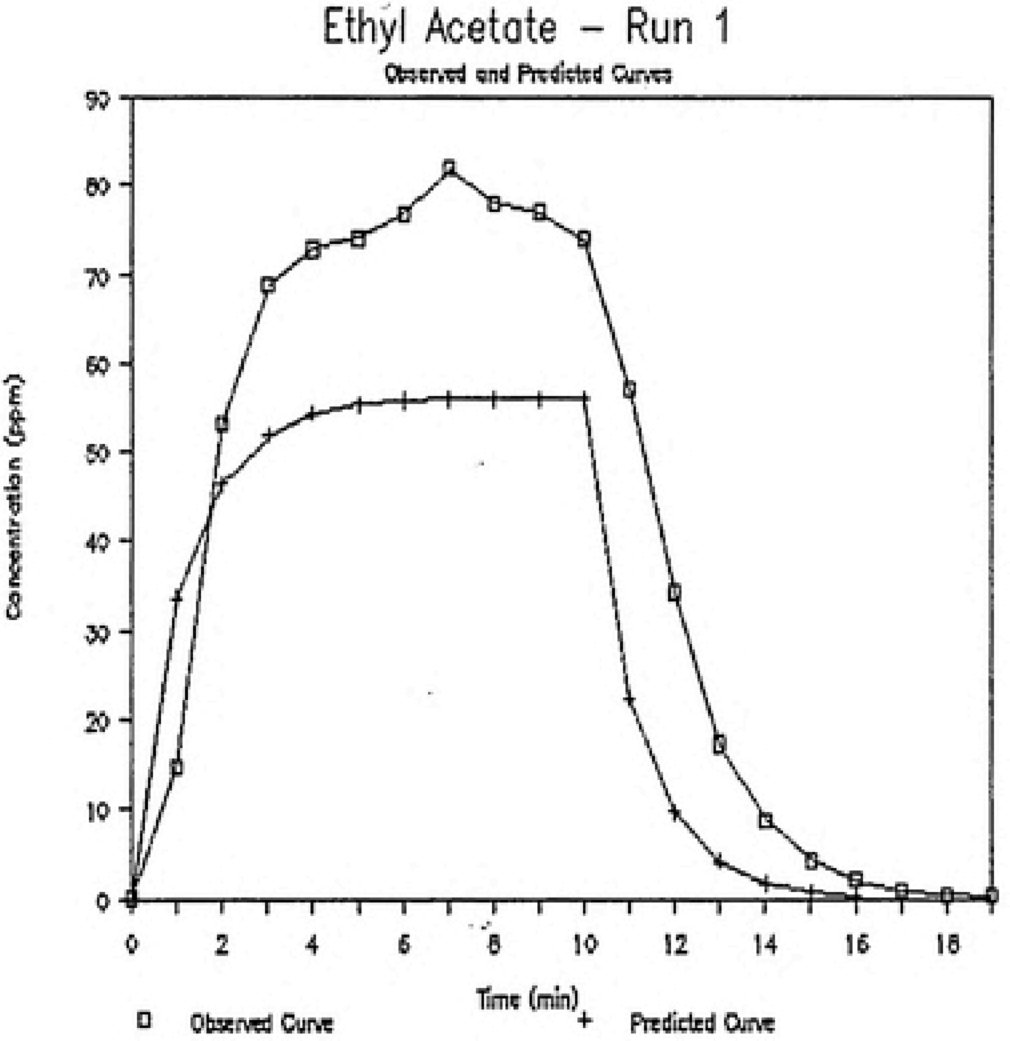


Figure 34. Comparison of measured concentration curve to Reist predicted using Kawamura-Mackay predicted evaporation rate.

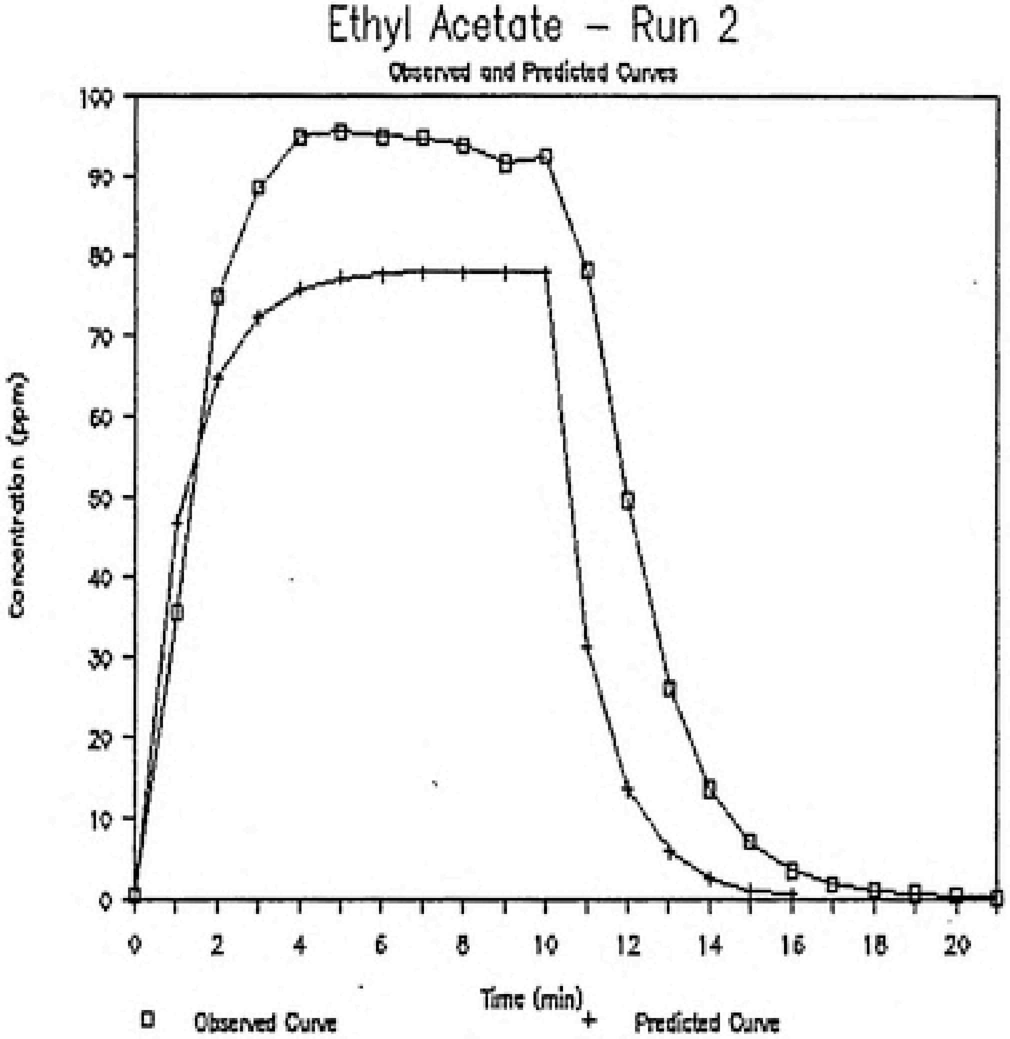


Figure 35. Comparison of measured concentration curve to Reist predicted using Kawamura-Mackay predicted evaporation rate.

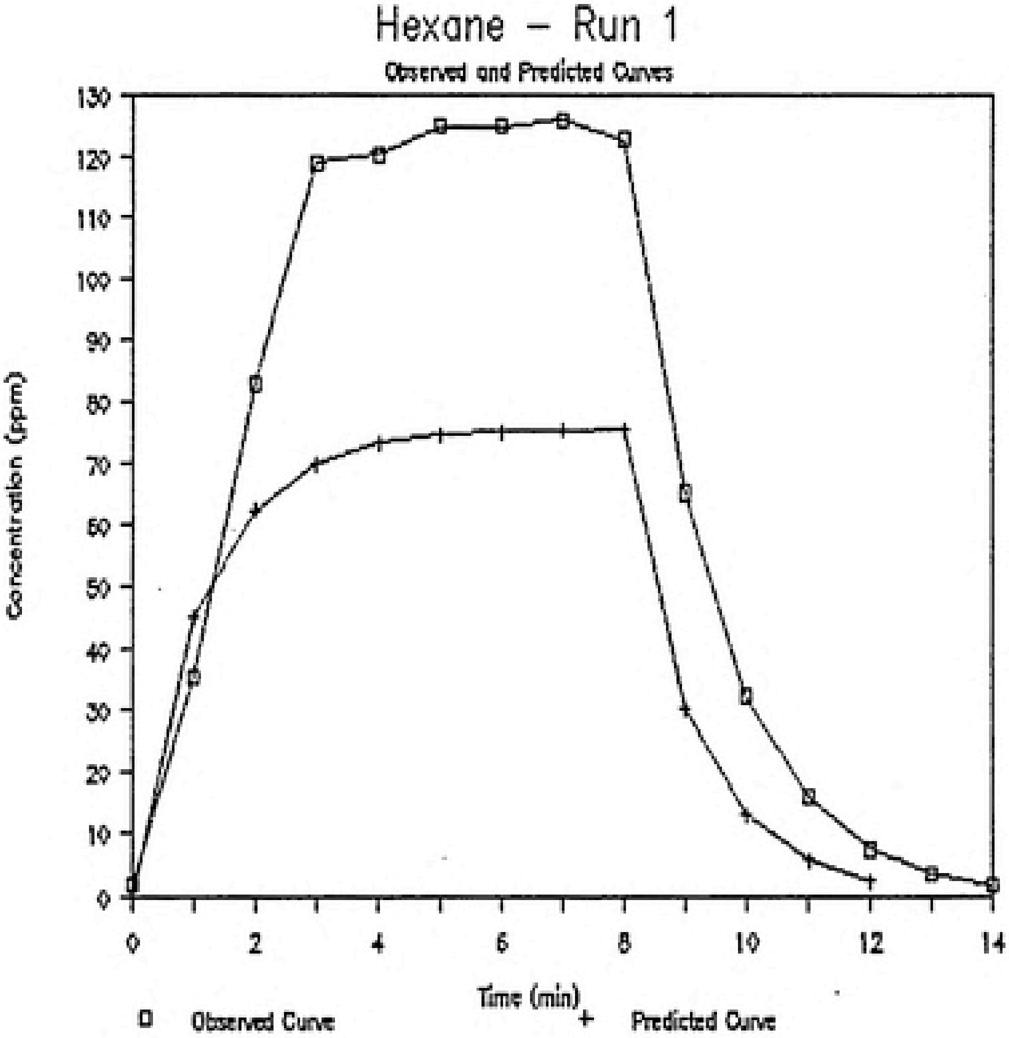


Figure 36. Comparison of measured concentration curve to Reist predicted using Kawamura-Mackay predicted evaporation rate.

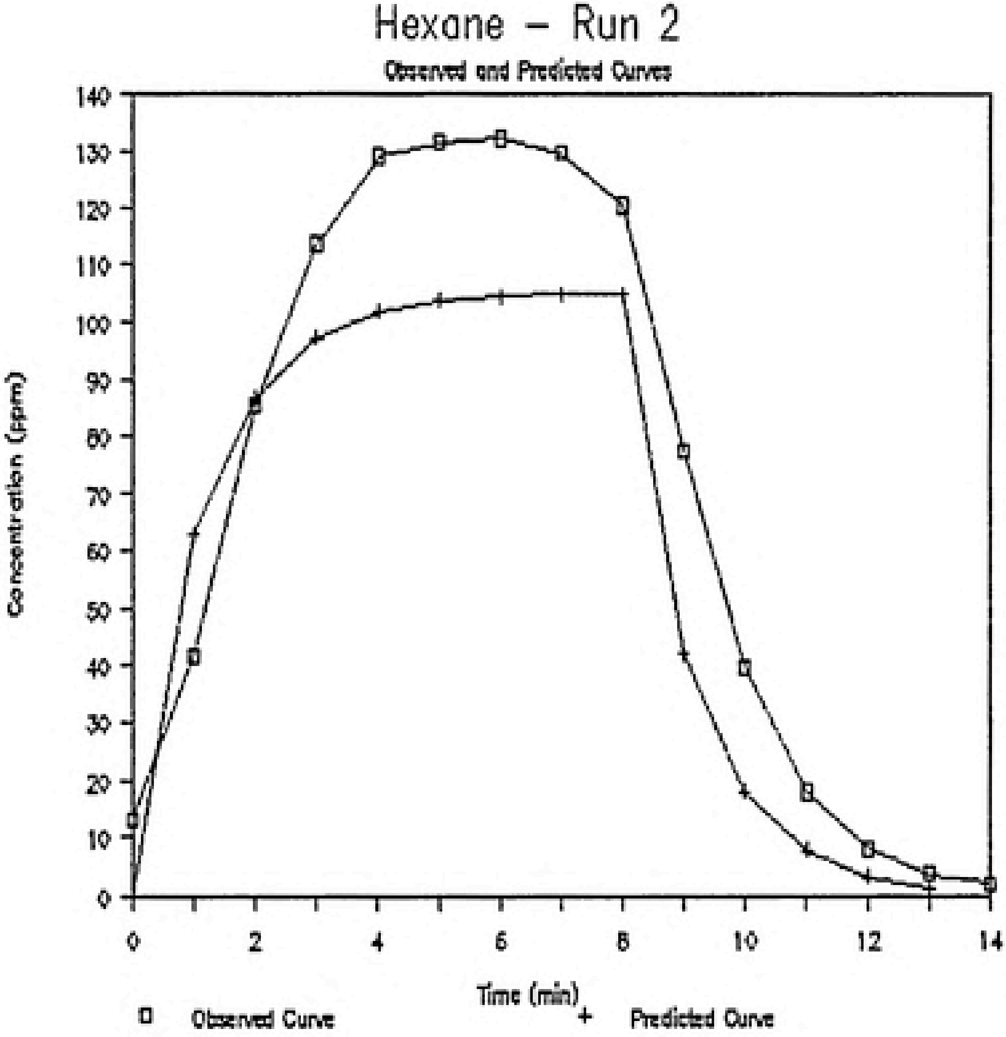


Figure 37. Comparison of measured concentration curve to Reist predicted using Kawamura-Mackay predicted evaporation rate.

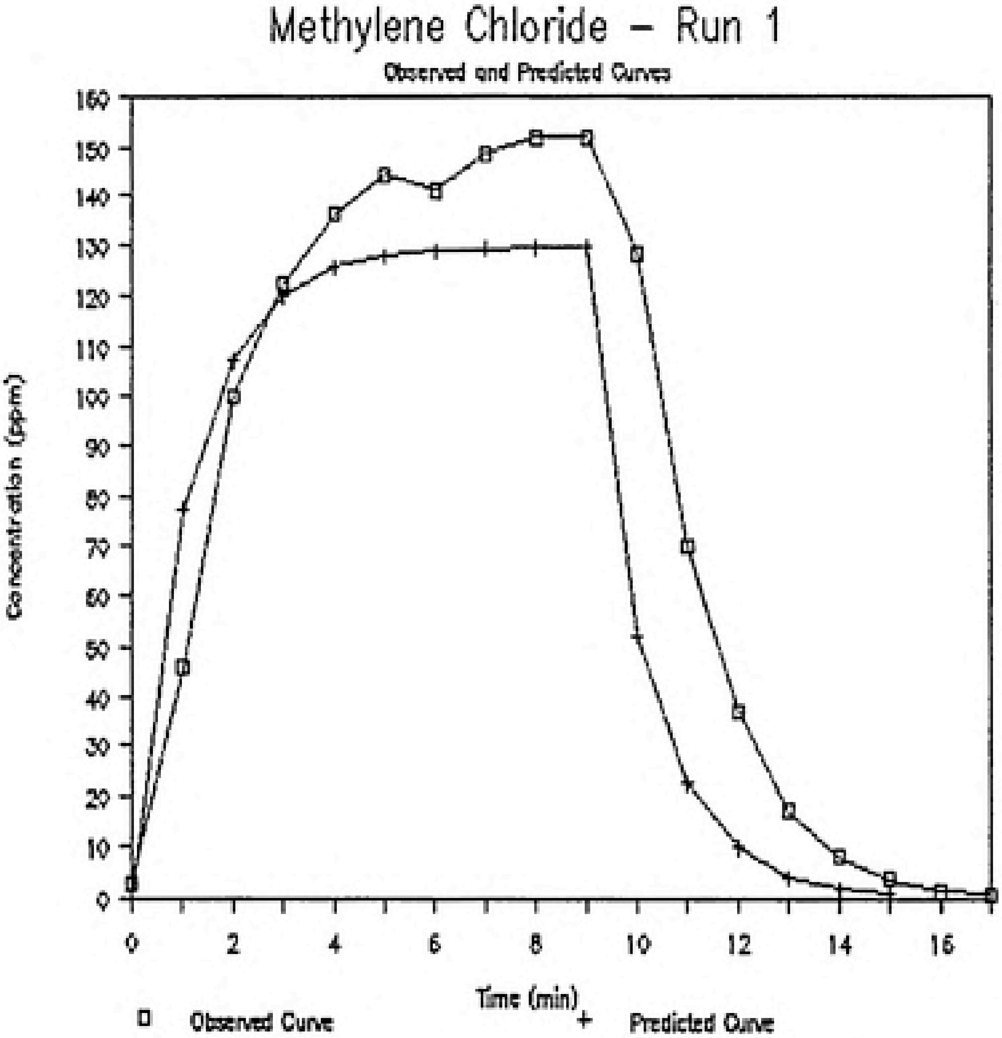


Figure 38. Comparison of measured concentration curve to Reist predicted using Kawamura-Mackay predicted evaporation rate.

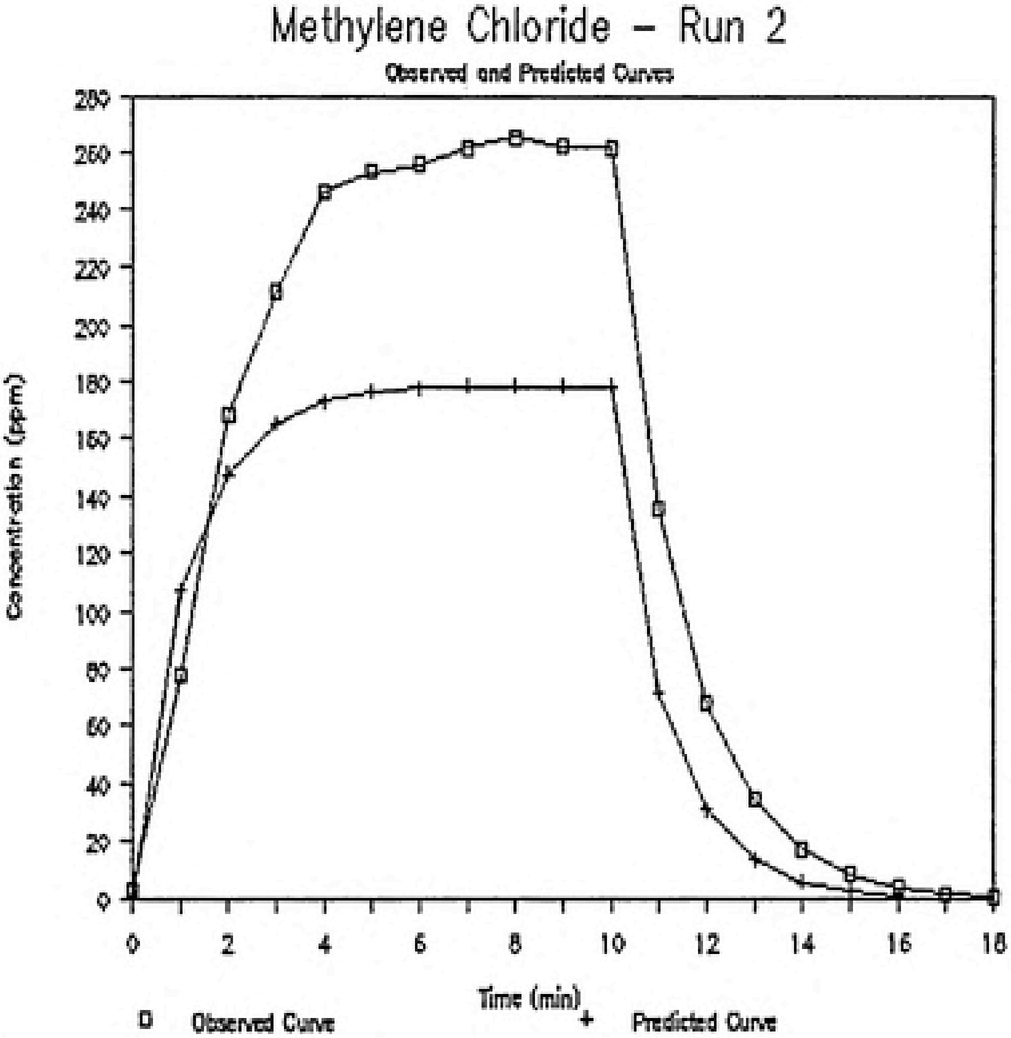


Figure 39. Comparison of measured concentration curve to Reist predicted using Kawamura-Mackay predicted evaporation rate.

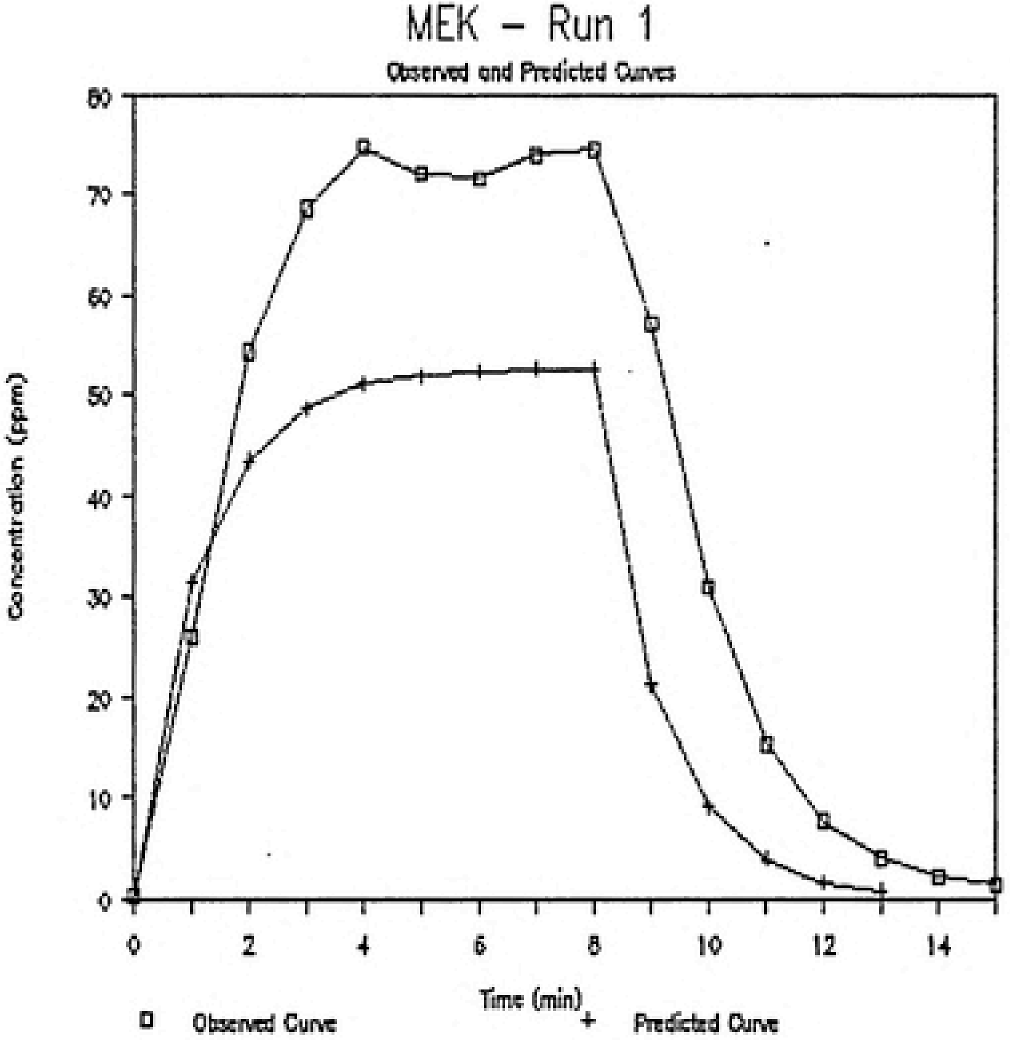


Figure 40. Comparison of measured concentration curve to Reist predicted using Kawamura-Mackay predicted evaporation rate.

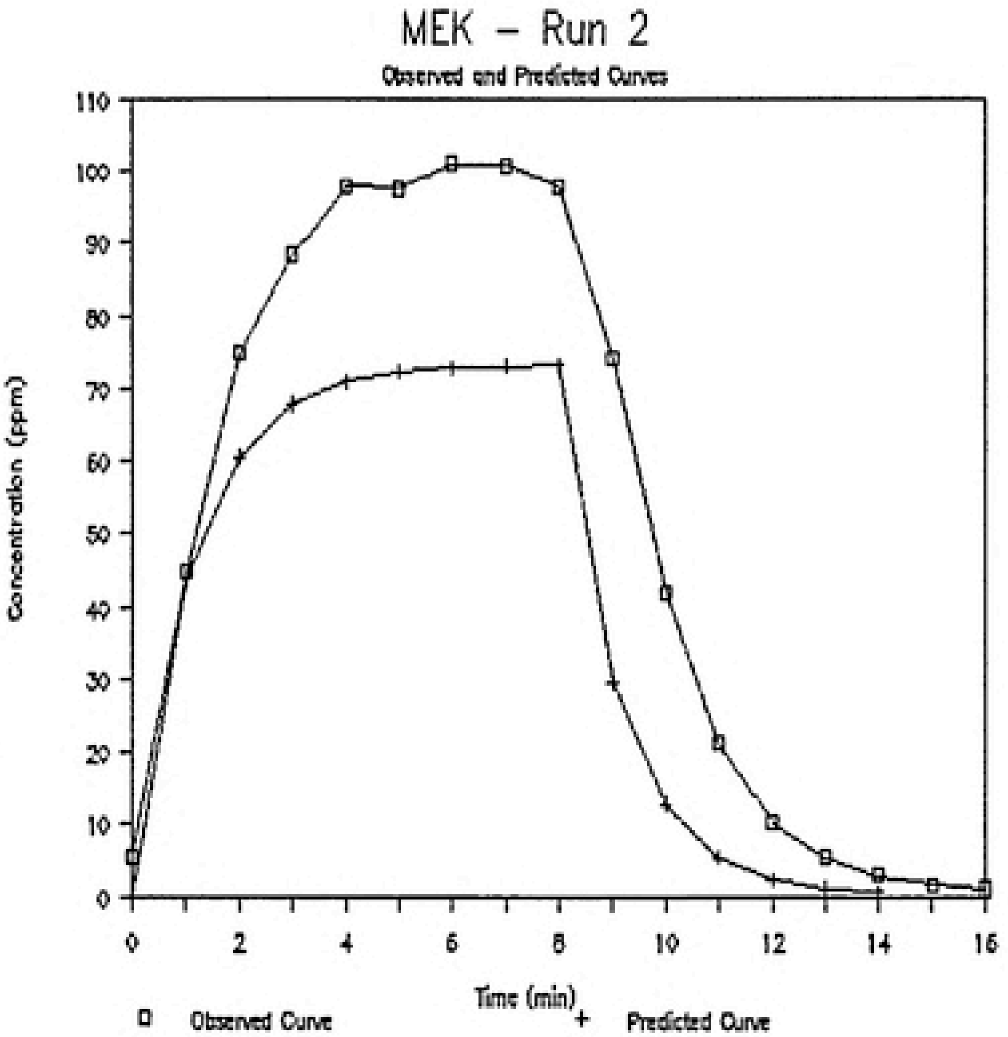


Figure 41. Comparison of measured concentration curve to Reist predicted using Kawamura-Mackay predicted evaporation rate.

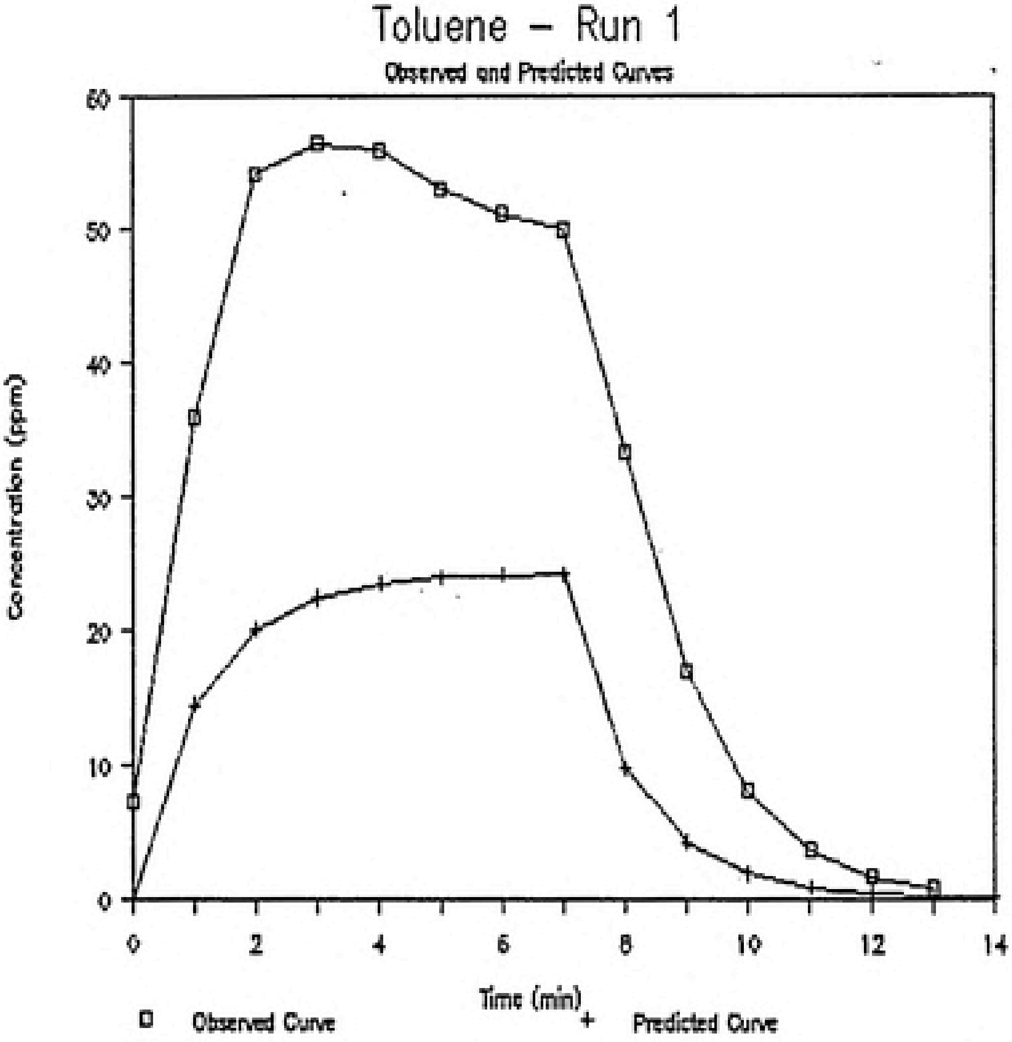


Figure 42. Comparison of measured concentration curve to Reist predicted using Kawamura-Mackay predicted evaporation rate.

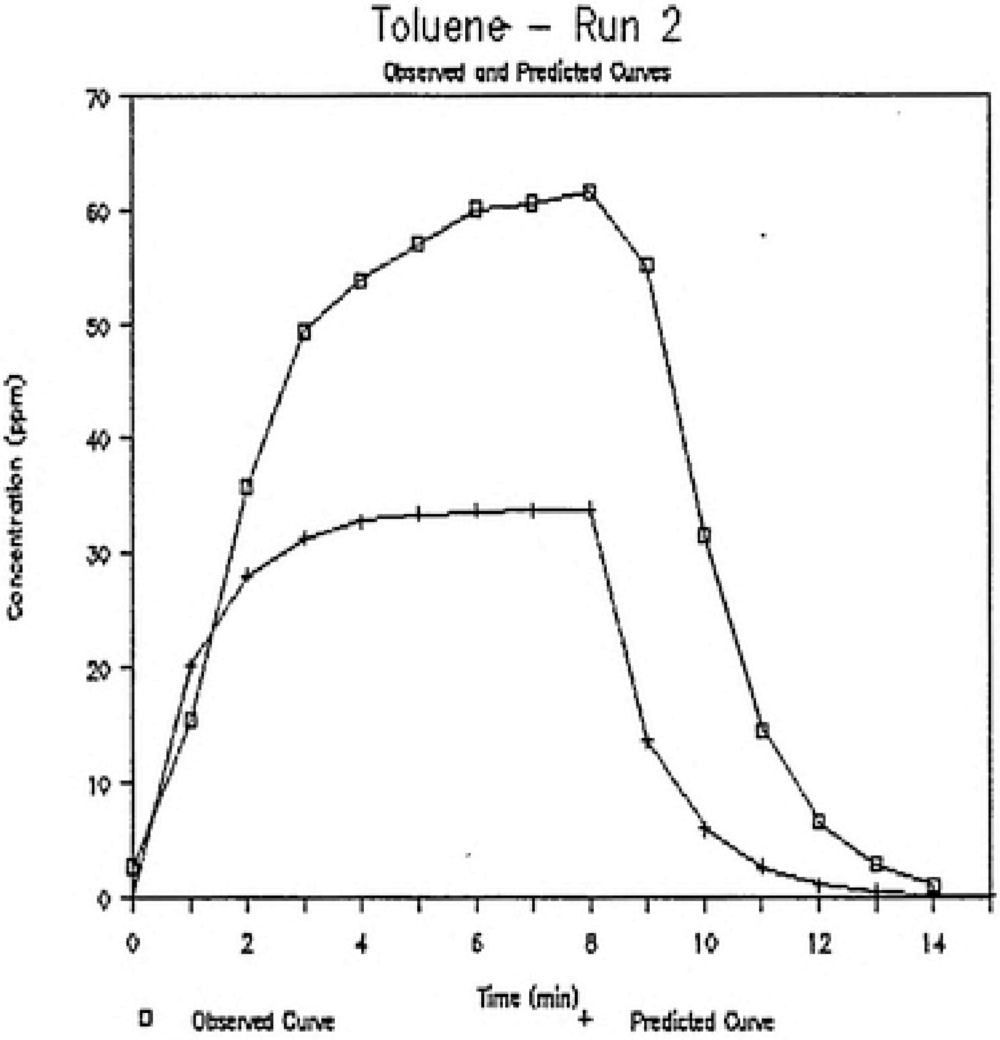


Figure 43. Comparison of measured concentration curve to Reist predicted using Kawamura-Mackay predicted evaporation rate.

DISCUSSION

The data and regression analyses confirm that the evaporation rate for each chemical is uniform over time. These rates were measured under ambient conditions with no unusual external influences. Therefore, the predominant influence governing the evaporation rate was, as expected, the vapor pressure. Figure 44 (using data from Table 3) illustrates this relationship between the vapor pressure and the evaporation rate. Evaporative cooling apparently did not play a significant role, even for methylene chloride, which has the highest vapor pressure, since the rate of evaporation did not decrease over time.

When the velocity over the liquid surface is increased, the evaporation rate curves do not remain uniform. Additional factors come into play which also affect the rate of evaporation. The movement of air across the surface of the liquid reduces the vapor concentration over the liquid. This, in turn, reduces the partial pressure of the vapor over the liquid surface and increases the evaporation rate. The greater the velocity, the greater the effect. An increase in the velocity also reduces the surface temperature, which has the effect of retarding the evaporation rate. Apparently, the reduction in surface temperature is not as significant as the reduction of the partial pressure over the liquid surface, since the overall effect of increased surface velocity is to

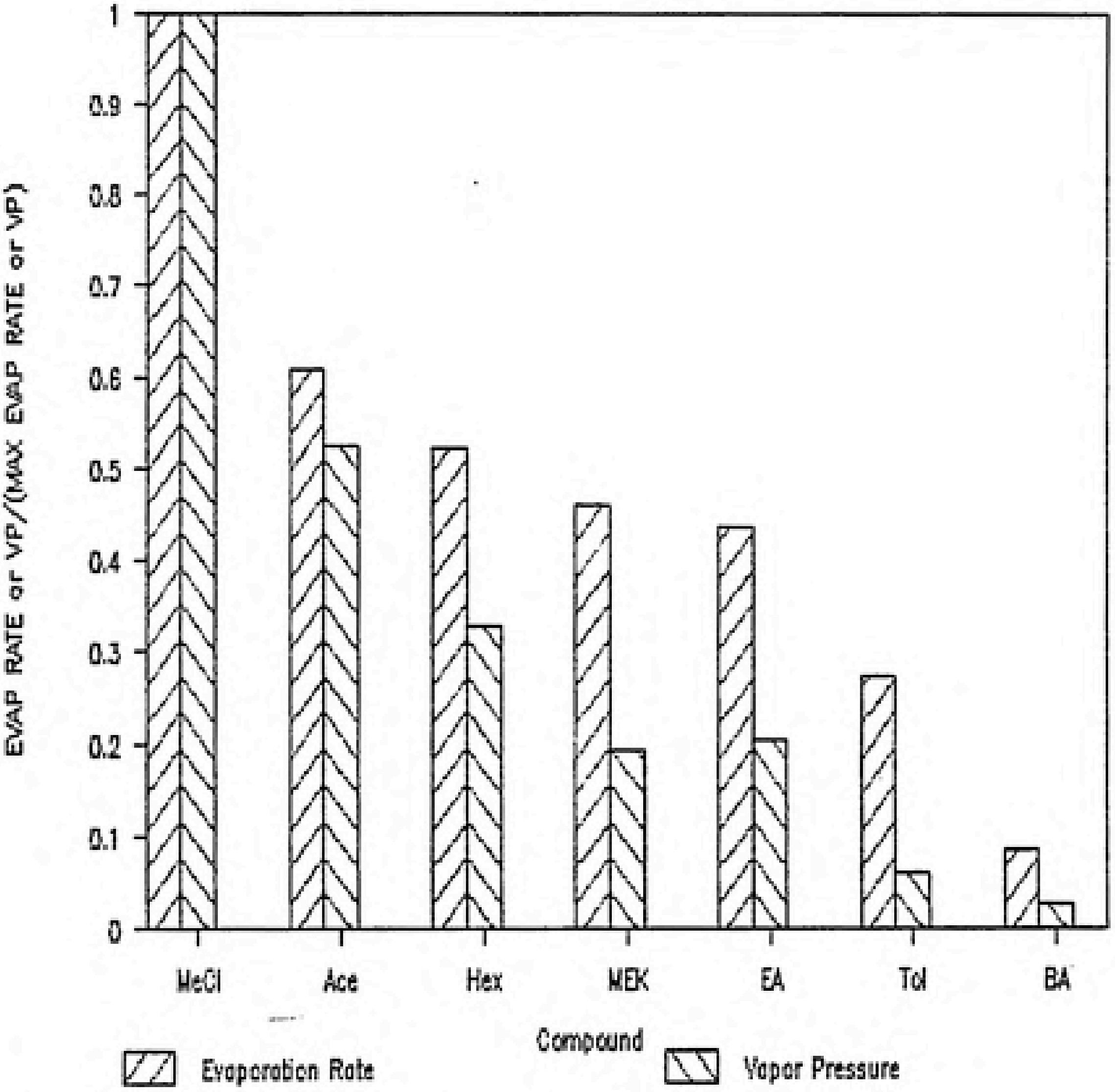


Figure 44. Comparison of measured evaporation rate and vapor pressure.

increase the evaporation rate. These influences on the evaporation rate may account for the irregularities noted in the velocity test curves.

The evaporation rate curves generated from the measured evaporation rates and the rates predicted using the Kawamura-Mackay model are, in general, similar (Figures 45-51). Both the measured and predicted evaporation rates increase with an increase in velocity. The predicted rates, except for methylene chloride, fall below the measured rates. This suggests that factors which affect evaporation rates may be present, but are not accounted for in the Kawamura-Mackay model. The predicted evaporation rates begin to exceed the measured evaporation rates for methylene chloride above 250 fpm. This may be due to surface temperature effects which are greater than those anticipated by Kawamura and Mackay for liquids with high vapor pressures.

Concentration curves were generated using both the measured and the Kawamura-Mackay evaporation rates in the Reist model. Both predicted concentration curves were generally similar in shape to the measured concentration curves. The shape of the predicted concentration curve is controlled by the time constant (T) in the Reist model. This constant is a function only of the fixed room volume and the flow through the room. Had the air flow through the room been incorrectly measured, the shape of the predicted and measured concentration curves would not have been similar. Based on the shape of the observed and predicted curves, the Reist model accurately predicts the time required for the concentration to build-up to equilibrium and the time required for the concentration to decay.

The model, however, does not consistently predict the equilibrium concentration, and the build-up and decay portions of the predicted curves slope more steeply than those of the measured curves. The reason for the differences in the build-up and decay slopes is explained by the fact that the MIRAN and data logger average the input data and produce a smoother curve than the predicted model.

Why the model does not consistently predict the measured equilibrium concentration is not so clear. One possible answer is the potential for error during the process of calibrating the MIRAN. However, all of the MIRAN calibration curves were constructed using the same technique and equipment. Errors in the calibration would, if all other factors were constant, cause measured concentrations to be consistently high or consistently low. Since the predictions were split equally between over and under-estimation of the measured values, this would seem to rule out calibration errors.

Factors which affect the predicted equilibrium concentration in the Reist model are the flow through the chamber and the evaporation rate. The flow through the chamber was determined to be correct, so the only remaining factor that can effect a difference is the evaporation rate. The surface velocities are based on evaporation rates measured in the chamber for each chemical. As stated earlier, the velocities found on the velocity test curves using these evaporation rates were averaged to obtain the surface velocity of Runs 1 and 2. These velocities (400 fpm and 600 fpm) were then used to determine the evaporation rates for each chemical and used in the Reist model to predict the equilibrium concentrations. Thus, individual fluctuations in velocity were not taken into account. This could explain why many of the predicted concentrations did not match the measured concentrations.

With the Kawamura-Mackay evaporation rates, the predicted equilibration concentrations fall below the measured equilibration concentrations. Why this is so is unclear. As stated above, for predictions using measured evaporation rates, errors in determining the surface velocity could be a factor. However, the effects of velocity are significantly reduced in the Kawamura-Mackay model as shown in equation (11). Temperature plays a larger role in the Kawamura-Mackay model, equation (12). Each degree error in air temperature measurement can cause as much as 2.5% error in the evaporation rate prediction. But, since the temperature varied no more than 1 degree, and since the same temperatures measured during the chamber tests were used in these predictions, temperature would not be a source of error.

The differences between the experimental and predicted equilibrium concentrations are acceptable. The Kawamura-Mackay model is a viable alternative to experimentally determining evaporation rates for use in the Reist model. Because the Reist-Kawamura-Mackay model under-estimates actual concentrations, the predicted results should be multiplied by a factor of two. Then, the predicted results either over-estimate or closely approximate the measured concentrations, giving an acceptable and consistent margin of safety. This is critical for the confident application of the model to industrial situations.

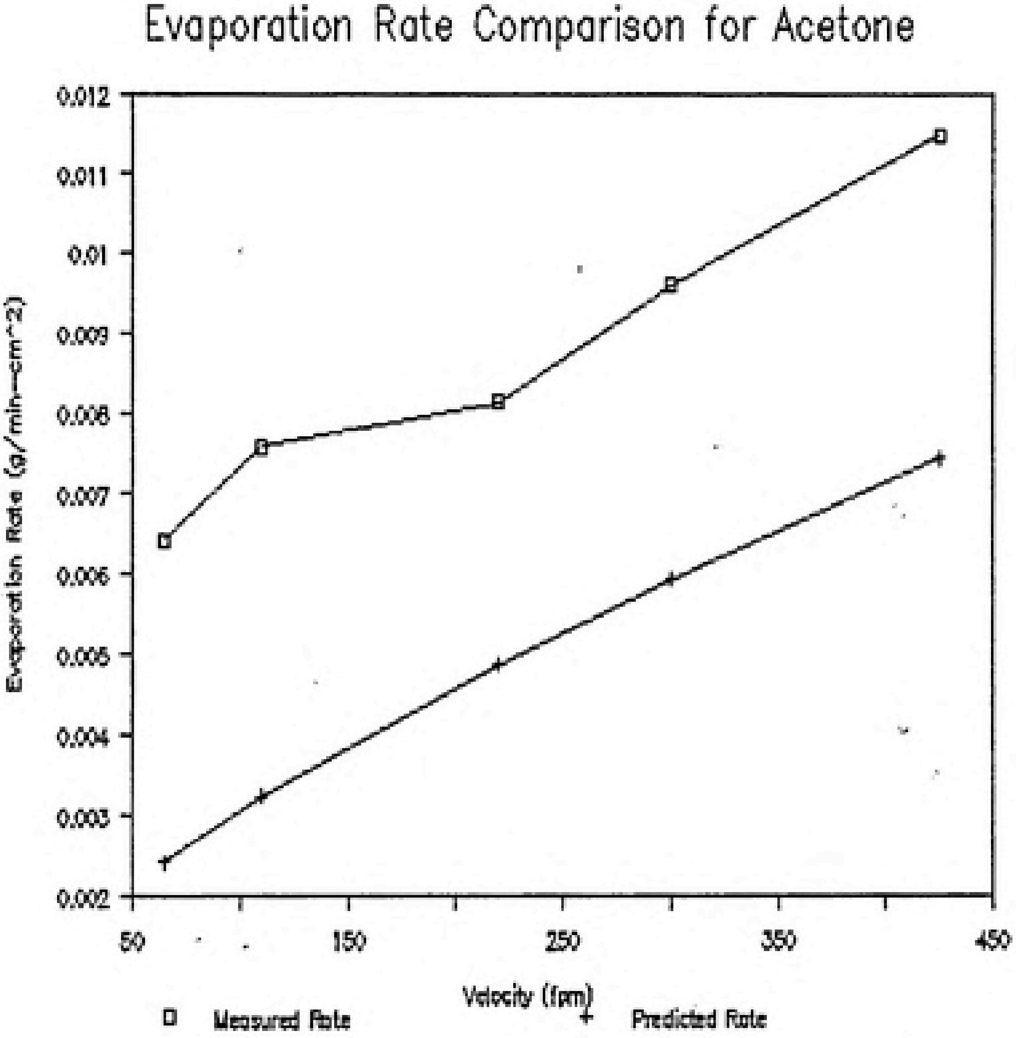


Figure 45. Comparison of measured evaporation rates to those predicted by the Kawamura-Mackay model.

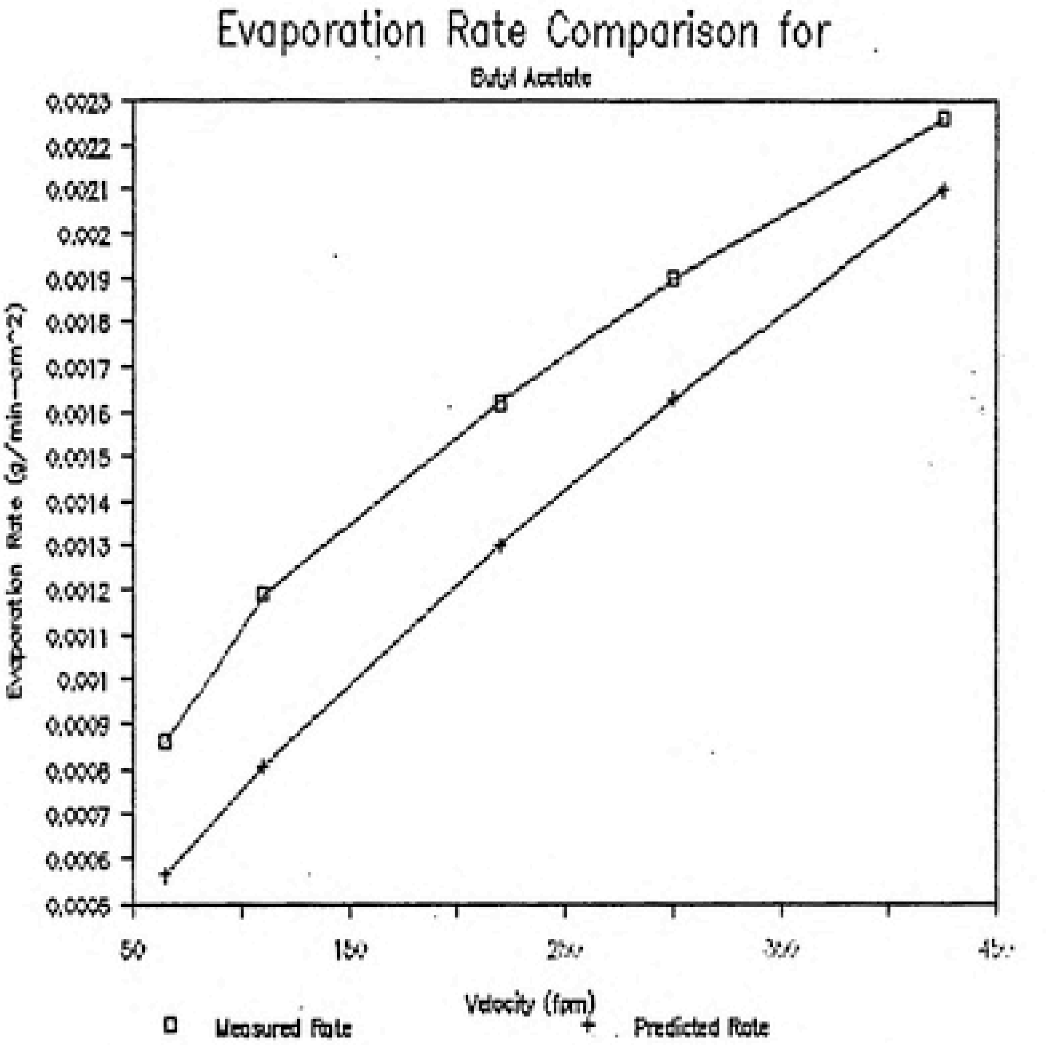


Figure 46. Comparison of measured evaporation rates to those predicted by the Kawamura-Mackay model.

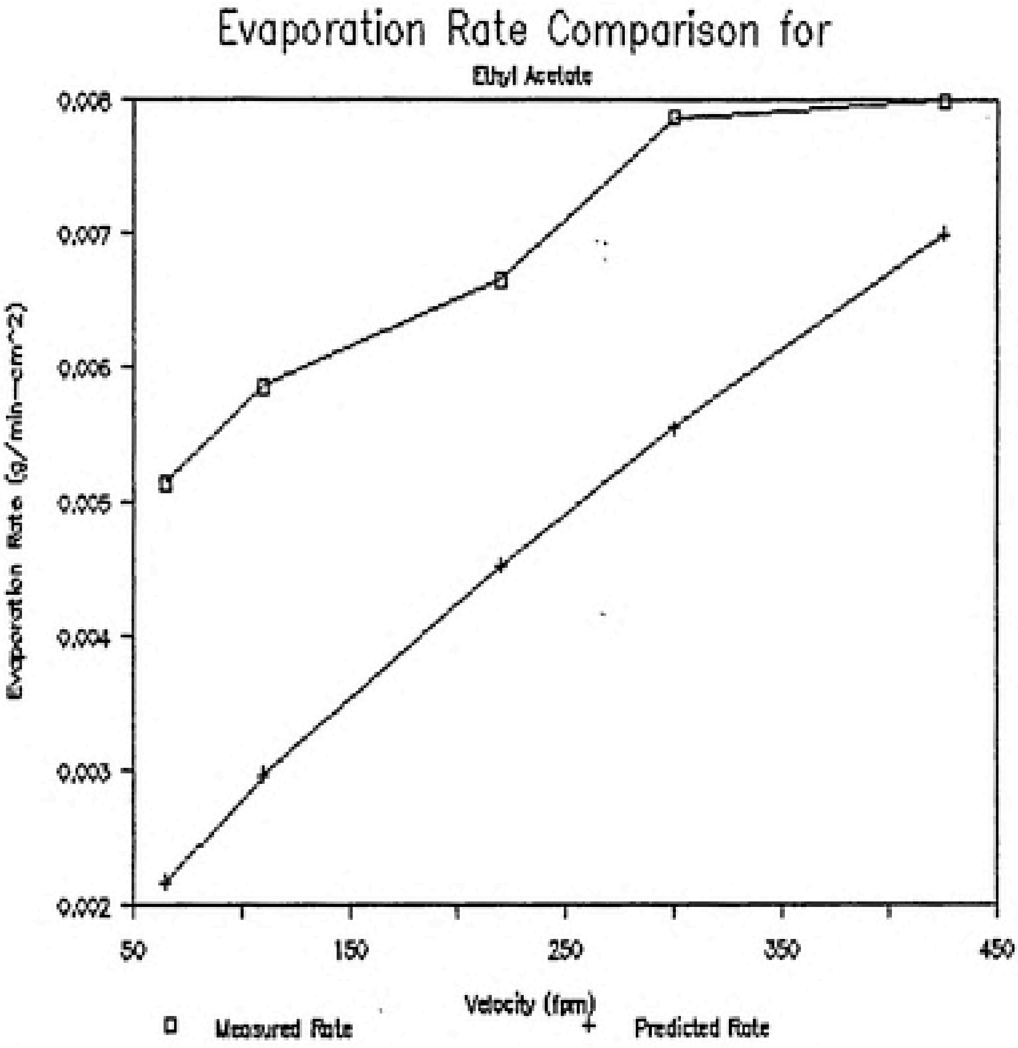


Figure 47. Comparison of measured evaporation rates to those predicted by the Kawamura-Mackay model.

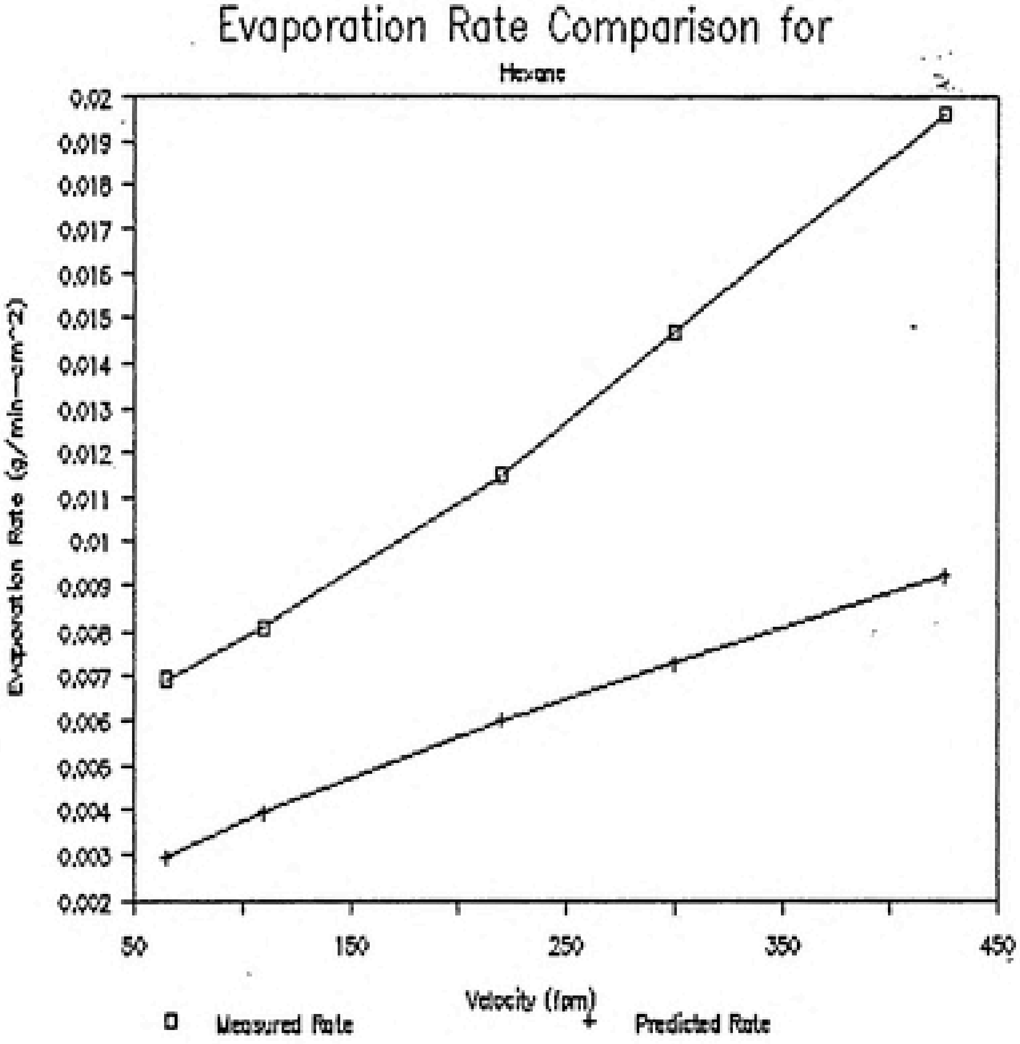


Figure 48. Comparison of measured evaporation rates to those predicted by the Kawamura-Mackay model.

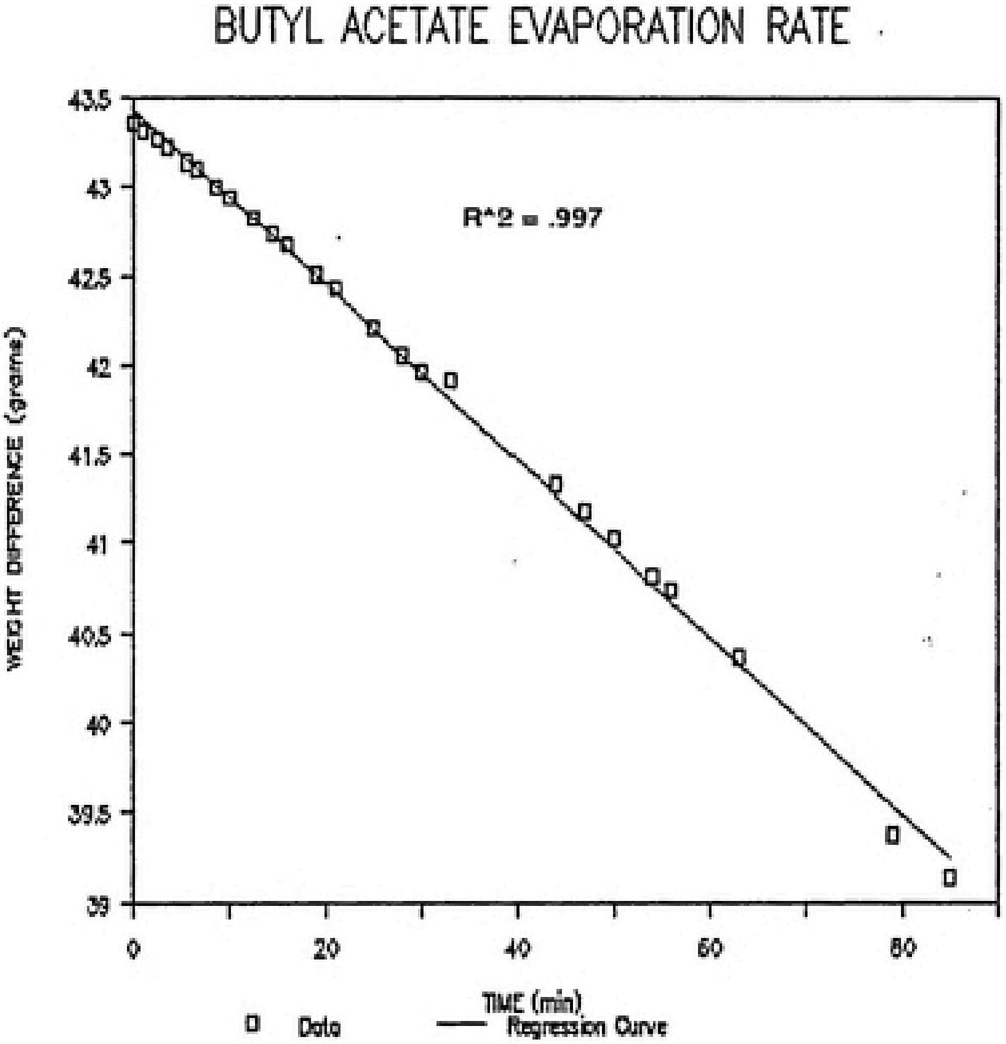


Figure 2A.–Evaporation rate test and regression curves.

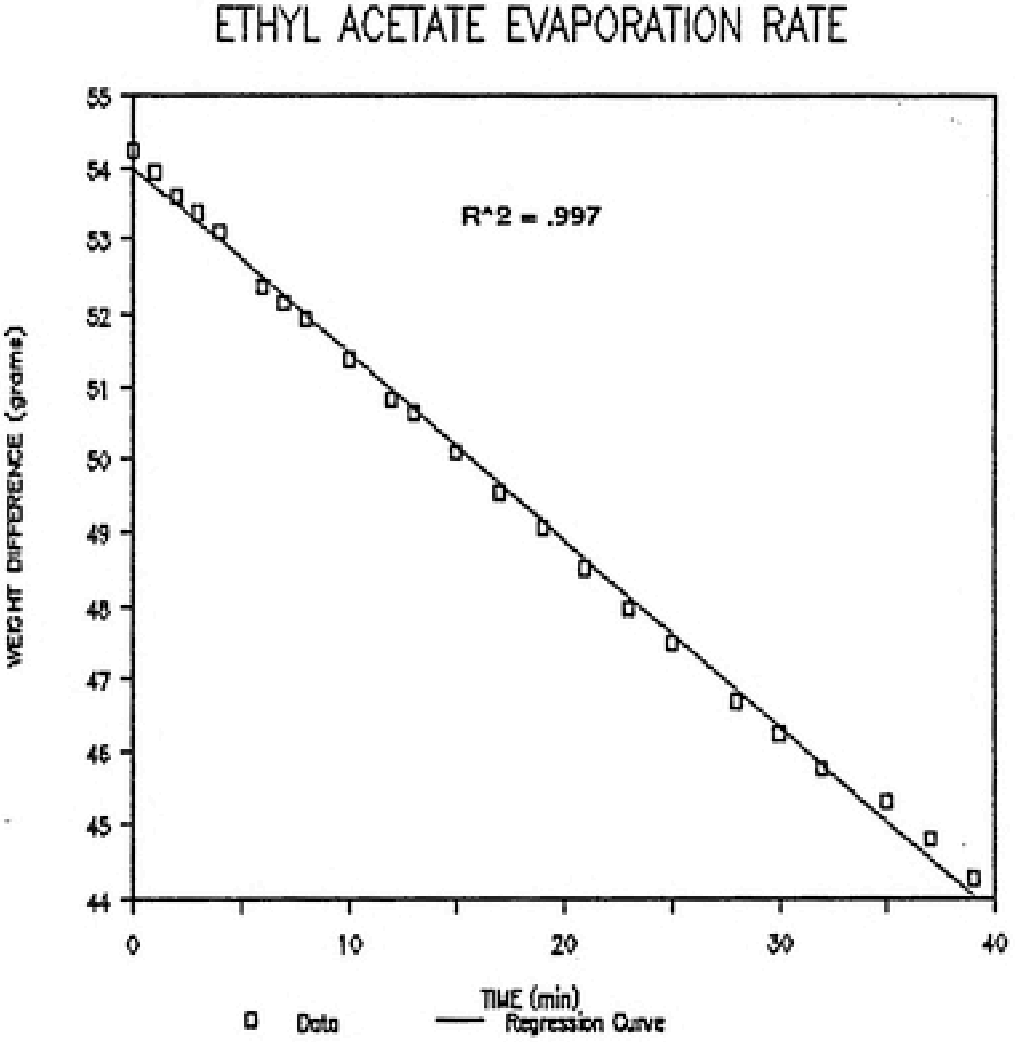


Figure 3A. Evaporation rate test and regression curves.

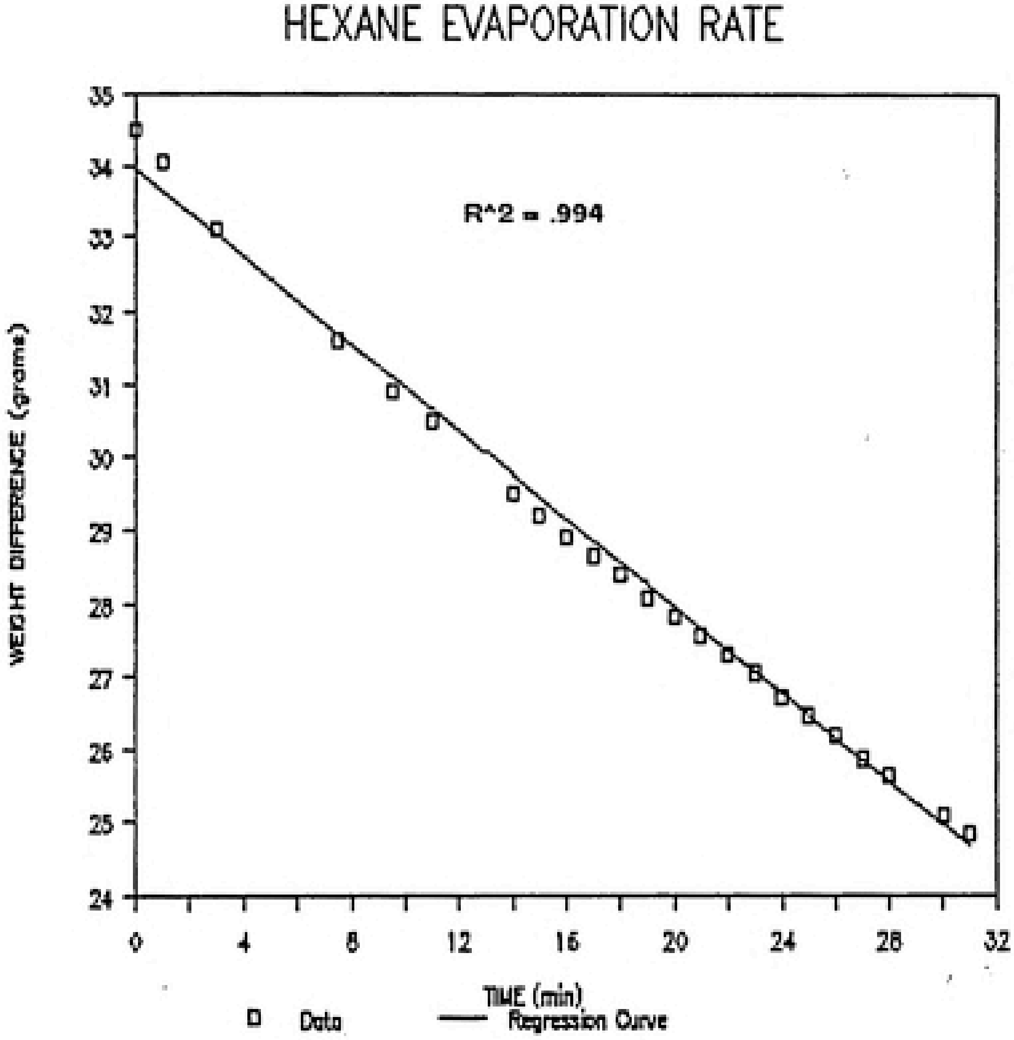


Figure 4A. Evaporation rate test and regression curves.

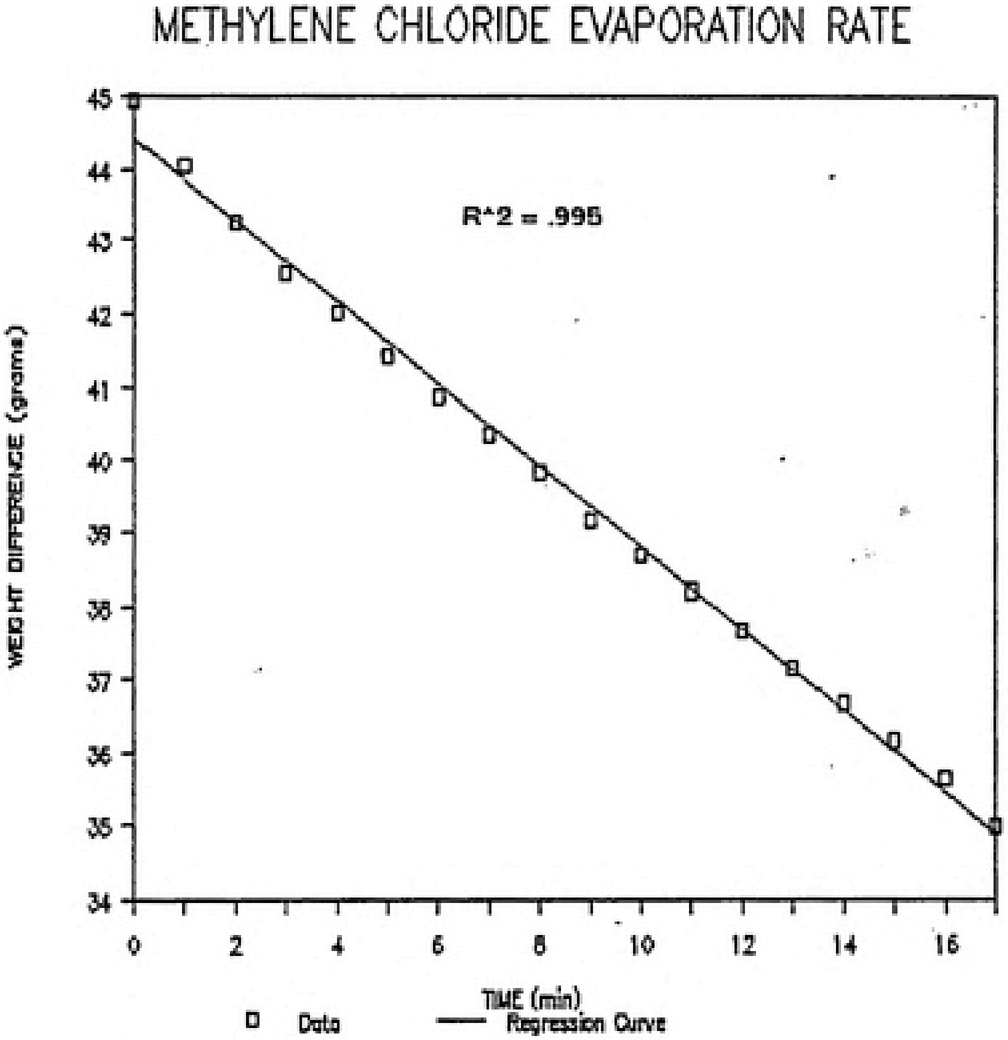


Figure 5A. Evaporation rate test and regression curves.

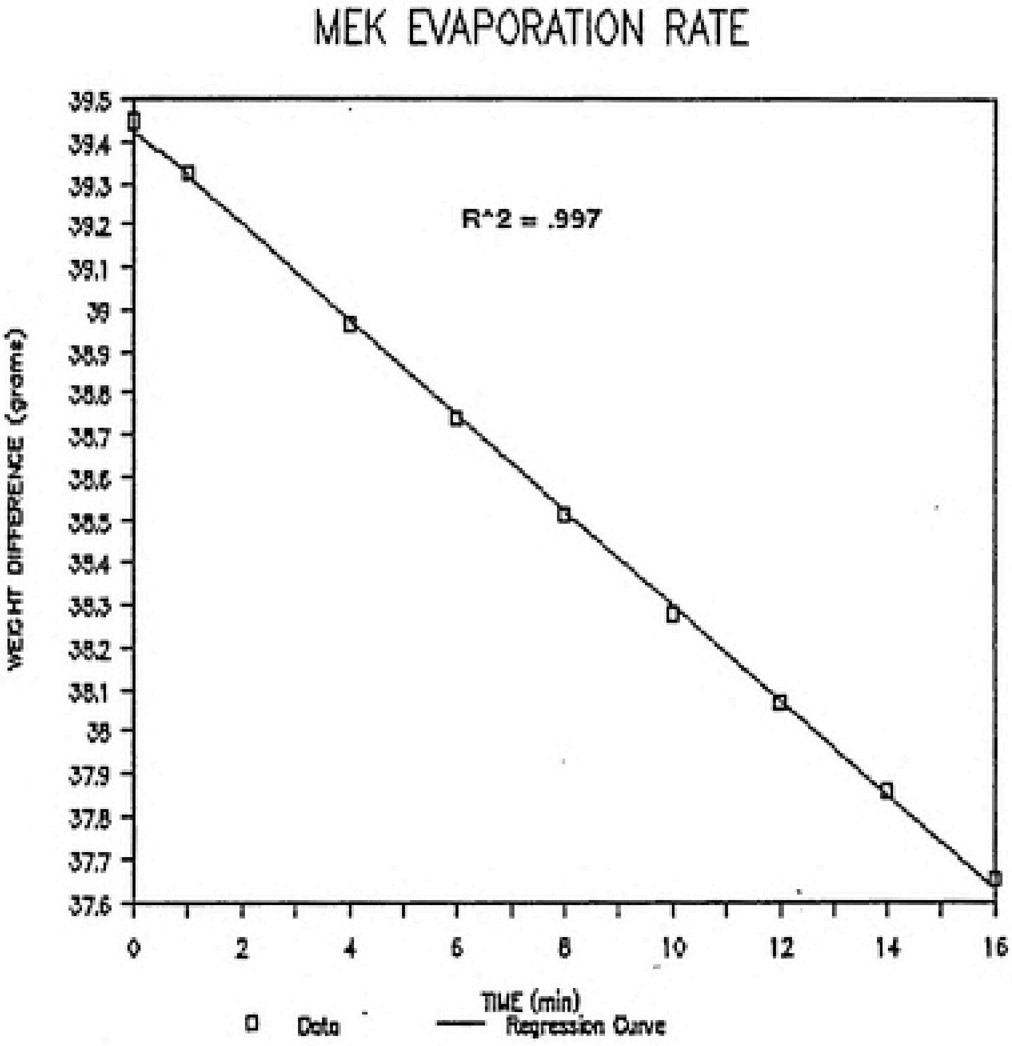


Figure 6A. Evaporation rate test and regression curves.

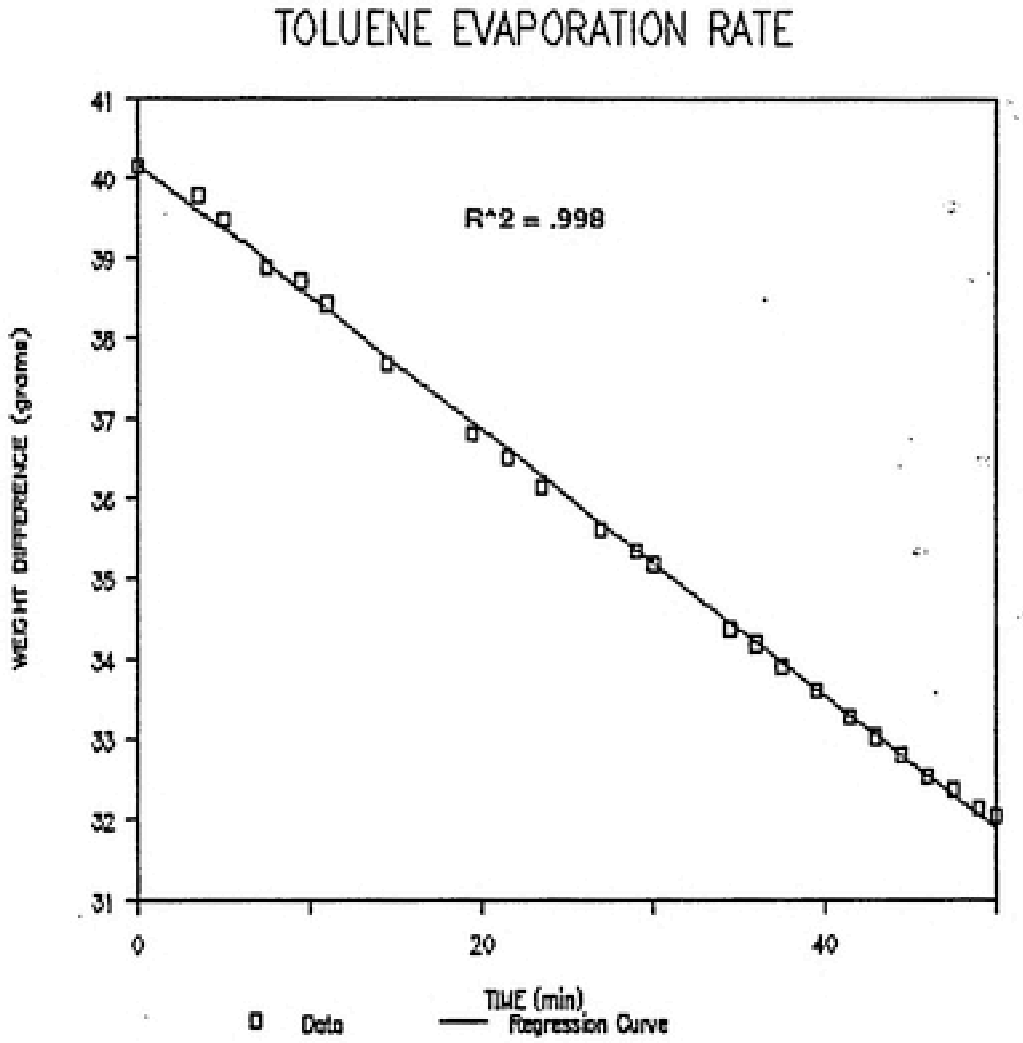


Figure 7A. Evaporation rate test and regression curves.

TABLE 8A: VELOCITY TEST DATA – ACETONE

Raw Data – Weight of liquid in grams, Temp in degrees Centigrade

Time (min)	20 fpm	Temp	50 fpm	Temp
0	123.95	22	132.05	22
2	123.135	22	131.115	22
4	122.44	22	130.24	22
6	121.78	22	129.445	22

Time (min)	80 fpm	Temp	120 fpm	Temp	180 fpm	Temp
0	128.5	22	129.48	22	131.1	22
2	127.5	22	128.318	22	129.72	22
4	126.57	22	127.2	22	128.36	22
6	125.68	22	126.11	22	127.03	22

Initial weight minus remaining weight = weight evaporated

20 fpm	50 fpm	80 fpm	120 fpm	180 fpm
0	0	0	0	0
0.815	0.935	1	1.162	1.38
1.51	1.81	1.93	2.28	2.74
2.17	2.605	2.82	3.37	4.07

Weight evaporated divided by time interval = evap rate (g/min)

20 fpm	50 fpm	80 fpm	120 fpm	180 fpm
0.4075	0.4675	0.5	0.581	0.69
0.3775	0.4525	0.4825	0.57	0.685
0.361666	0.434166	0.47	0.561666	0.678333

Evaporation Rate divided by surface area (59.45 cm^2) = Evaporation Rate (g/min-cm^2)

20 fpm	50 fpm	80 fpm	120 fpm	180 fpm
0.006854	0.007864	0.008410	0.009773	0.011607
0.006350	0.007611	0.008116	0.009588	0.011522
0.006083	0.007303	0.007906	0.009448	0.011410

Velocity (fpm)	Average Evaporation Rate (g/min-cm^2)
65	0.006429
110	0.007593
220	0.008144
300	0.009603
425	0.011513

Regression Output:

Constant		0.005677
Std Err of Y Est		0.000394
R Squared		0.969763
No. of Observations		5
Degrees of Freedom		3
X Coefficient(s)	0.000013	
Std Err of Coef.	0.000001	

TABLE 9A: VELOCITY TEST DATA - BUTYL ACETATE

Raw Data - Weight of liquid in grams, Temp in degrees Centigrade

Time (min)	20 fpm	Temp	50 fpm	Temp
0	96.21	22.9	95.17	23.2
2	96.107	23.2	95.023	23.4
4	95.988	23.2	94.86	23.3
6	95.866	23.2	94.707	23.2

Time (min)	80 fpm	Temp	120 fpm	Temp	180 fpm	Temp
0	103.95	23.2	101.98	23.1	99.67	23
2	103.748	23.2	101.75	23.1	99.393	23.2
4	103.535	23	101.487	23.1	99.095	23.1
6	103.321	23.2	101.231	23.2	98.768	23

20 fpm	50 fpm	80 fpm	120 fpm	180 fpm
Initial weight minus remaining weight = weight evaporated				
0	0	0	0	0
0.103	0.147	0.202	0.23	0.277
0.222	0.31	0.415	0.493	0.575
0.344	0.463	0.629	0.749	0.902

Weight evaporated divided by time interval = evap rate (g/min)

0.0515	0.0735	0.101	0.115	0.1385
0.0555	0.0775	0.10375	0.12325	0.14375
0.057333	0.077166	0.104833	0.124833	0.150333

Evaporation Rate divided by surface area (63.6172 cm^2) = Evaporation Rate (g/min-cm^2)

0.000809	0.001155	0.001587	0.001807	0.002177
0.000872	0.001218	0.001630	0.001937	0.002259
0.000901	0.001212	0.001647	0.001962	0.002363

Velocity (fpm)	Average Evaporation Rate (g/min-cm^2)
65	0.000861
110	0.001195
220	0.001622
300	0.001902
425	0.002266

Regression Output:

Constant	0.000719
Std Err of Y Est	0.000091
R Squared	0.979563
No. of Observations	5
Degrees of Freedom	3
X Coefficient(s)	0.000003
Std Err of Coef.	0.000000

TABLE 10A: VELOCITY TEST DATA - ETHYL ACETATE

Raw Data - Weight of liquid in grams, Temp in degrees Centigrade

Time (min)	20 fpm	Temp	50 fpm	Temp
0	93.5	23	98.4	23.2
2	92.84	23	97.672	23.1
4	92.2	23.1	96.897	23.2
6	91.55	23	96.138	23.1

Time (min)	80 fpm	Temp	120 fpm	Temp	180 fpm	Temp
0	91.64	23.2	95.57	23	95.6	22.7
2	90.833	23.2	94.58	23	94.48	22.9
4	89.922	23.1	93.57	23	93.593	23
6	89.004	23.2	92.52	23	92.729	23.1

Initial weight minus remaining weight = weight evaporated

20 fpm	50 fpm	80 fpm	120 fpm	180 fpm
0	0	0	0	0
0.66	0.728	0.807	0.99	1.12
1.3	1.503	1.718	2	2.007
1.95	2.262	2.636	3.05	2.871

Weight evaporated divided by time interval = evap rate (g/min)

0.33	0.364	0.4035	0.495	0.56
0.325	0.37575	0.4295	0.5	0.50175
0.325	0.377	0.439333	0.508333	0.4785

Evaporation Rate divided by surface area (63.6172 cm^2) = Evaporation Rate

0.005187	0.005721	0.006342	0.007780	0.008802	(g/min-cm^2)
0.005108	0.005906	0.006751	0.007859	0.007887	
0.005108	0.005926	0.006905	0.007990	0.007521	

Velocity	Average Evaporation Rate (g/min-cm^2)
65	0.005134
110	0.005851
220	0.006666
300	0.007876
425	0.008070

Regression Output:

Constant	0.004835
Std Err of Y Est	0.000388
R Squared	0.929460
No. of Observations	5
Degrees of Freedom	3

X Coefficient(s)	0.000008
Std Err of Coef.	0.000001

TABLE 11A: VELOCITY TEST DATA - HEXANE

Raw Data - Weight of liquid in grams, Temp in degrees Centigrade

Time (min)	20 fpm	Temp	50 fpm	Temp
0	75.15	22.7	79.4	22.8
2	74.255	22.8	78.41	22.8
4	73.36	22.9	77.3	22.8
6	72.55	22.8	76.26	22.8

Time (min)	80 fpm	Temp	120 fpm	Temp	180 fpm	Temp
0	80.8	22.9	83.2	22.9	86.85	22.9
2	79.325	22.8	81.34	22.9	84.18	22.7
4	77.853	22.8	79.395	22.9	81.874	22.7
6	76.46	22.9	77.55	22.8	79.8	22.6

Initial weight minus remaining weight = weight evaporated

20 fpm	50 fpm	80 fpm	120 fpm	180 fpm
0	0	0	0	0
0.895	0.99	1.475	1.86	2.67
1.79	2.1	2.947	3.805	4.976
2.6	3.14	4.34	5.65	7.05

Weight evaporated divided by time interval = evap rate (g/min)

0.4475	0.495	0.7375	0.93	1.335
0.4475	0.525	0.73675	0.95125	1.244
0.433333	0.523333	0.723333	0.941666	1.175

Evaporation Rate divided by surface area of 63.6172 cm^2 = Evaporation Rate (g/min-cm^2)

0.007034	0.007780	0.011592	0.014618	0.020984
0.007034	0.008252	0.011580	0.014952	0.019554
0.006811	0.008226	0.011370	0.014802	0.018469

Velocity	Evaporation Rate (g/min-cm^2)
65	0.006960
110	0.008086
220	0.011514
300	0.014791
425	0.019669

Regression Output:

Constant	0.004240
Std Err of Y Est	0.000442
R Squared	0.994540
No. of Observations	5
Degrees of Freedom	3

X Coefficient(s)	0.000035
Std Err of Coef.	0.000001

TABLE 12A: VELOCITY TEST DATA – METHYLENE CHLORIDE

Raw Data – Weight of liquid in grams, Temp in degrees Centigrade

Time (min)	20 fpm	Temp	50 fpm	Temp
0	105.704	23.1	123.219	23.3
2	104.583	23.1	122.118	23.3
4	103.5	23.2	120.965	23.3
6	102.452	23.2	119.845	23.3

Time (min)	80 fpm	Temp	120 fpm	Temp	180 fpm	Temp
0	126.705	23.2	123.766	23.3	130.06	23.4
2	125.37	23.3	122.312	23.4	128.325	23.1
4	124.062	23.4	120.858	23.3	126.612	23.4
6	122.767	23.3	119.417	23.2	124.89	23.4

20 fpm	50 fpm	80 fpm	120 fpm	180 fpm
Initial weight minus remaining weight = weight evaporated				
0	0	0	0	0
1.121	1.101	1.335	1.454	1.735
2.204	2.254	2.643	2.908	3.448
3.252	3.374	3.938	4.349	5.17

Weight evaporated divided by time interval = evap rate (g/min)

0.5605	0.5505	0.6675	0.727	0.8675
0.551	0.5635	0.66075	0.727	0.862
0.542	0.562333	0.656333	0.724833	0.861666

Evaporation Rate divided by surface area of 63.6172 cm^2 = Evaporation Rate (g/min-cm^2)

0.008810	0.008653	0.010492	0.011427	0.013636
0.008661	0.008857	0.010386	0.011427	0.013549
0.008519	0.008839	0.010316	0.011393	0.013544

Average Evaporation Rate:

0.008663	0.008783	0.010398	0.011416	0.013576

Velocity	Evaporation Rate (g/min-cm^2)
65	0.008663
110	0.008783
220	0.010398
300	0.011416
425	0.013576

Regression Output:

Constant	0.007448
Std Err of Y Est	0.000280
R Squared	0.985796
No. of Observations	5
Degrees of Freedom	3

X Coefficient(s)	0.000013
Std Err of Coef.	0.000000

TABLE 13A: VELOCITY TEST DATA - MEK

Raw Data - Weight of liquid in grams, Temp in degrees Centigrade

Time (min)	20 fpm	Temp	50 fpm	Temp
0	118.82	22.1	117.29	22.2
2	118.45	22.1	116.66	22.2
4	117.87	22.1	116.08	22.2
6	117.53	22.1	115.54	22.2

Time (min)	80 fpm	Temp	120 fpm	Temp	180 fpm	Temp
0	115.42	22.3	113.11	22.3	110.66	22.3
2	114.625	22.3	112.245	22.3	109.725	22.3
4	113.88	22.3	111.42	22.3	108.868	22.3
6	113.14	22.3	110.68	22.3	108.09	22.3

20 fpm	50 fpm	80 fpm	120 fpm	180 fpm
Initial weight minus remaining weight = weight evaporated				
0	0	0	0	0
0.37	0.63	0.795	0.865	0.935
0.95	1.21	1.54	1.69	1.792
1.29	1.75	2.28	2.43	2.57

Weight evaporated divided by time interval = evap rate (g/min)

0.185	0.315	0.3975	0.4325	0.4675
0.2375	0.3025	0.385	0.4225	0.448
0.215	0.291666	0.38	0.405	0.428333

Evaporation Rate divided by surface area of 59.45 cm^2 = Evaporation Rate (g/min-cm^2)

0.003112	0.005298	0.006686	0.007275	0.007864
0.003995	0.005088	0.006476	0.007107	0.007536
0.003616	0.004906	0.006392	0.006812	0.007205

Velocity	Evaporation Rate (g/min-cm^2)
65	0.003574
110	0.005097
220	0.006518
300	0.007065
425	0.007535

Regression Output:

Constant		0.003635
Std Err of Y Est		0.000674
R Squared		0.869387
No. of Observations		5
Degrees of Freedom		3
X Coefficient(s)	0.000010	
Std Err of Coef.	0.000002	

TABLE 14A: VELOCITY TEST DATA - TOLUENE

Raw Data - Weight of liquid in grams, Temp in degrees Centigrade

Time (min)	20 fpm	Temp	50 fpm	Temp
0	87.3	22.8	82.85	22.7
2	86.874	22.8	82.395	22.8
4	86.454	22.8	81.913	22.9
6	86.053	22.7	81.43	22.9

Time (min)	80 fpm	Temp	120 fpm	Temp	180 fpm	Temp
0	90.51	22.9	85.35	22.8	85.3	22.7
2	89.95	22.8	84.77	23	84.61	22.8
4	89.353	22.8	84.184	23	83.924	22.8
6	88.753	22.8	83.56	23	83.239	22.8

Initial weight minus remaining weight = weight evaporated

20 fpm	50 fpm	80 fpm	120 fpm	180 fpm
0	0	0	0	0
0.426	0.455	0.56	0.58	0.69
0.846	0.937	1.157	1.166	1.376
1.247	1.42	1.757	1.79	2.061

Weight evaporated divided by time interval = evap rate (g/min)

0.213	0.2275	0.28	0.29	0.345
0.2115	0.23425	0.28925	0.2915	0.344
0.207833	0.236666	0.292833	0.298333	0.3435

Evaporation Rate divided by surface area of 63.6172 cm^2 = Evaporation Rate (g/min-cm^2)

0.003348	0.003576	0.004401	0.004558	0.005423
0.003324	0.003682	0.004546	0.004582	0.005407
0.003266	0.003720	0.004603	0.004689	0.005399

Velocity (fpm)	Average Evaporation Rate (g/min-cm^2)
65	0.003313
110	0.003659
220	0.004517
300	0.004610
425	0.005409

Regression Output:

Constant		0.003040
Std Err of Y Est		0.000163
R Squared		0.970963
No. of Observations		5
Degrees of Freedom		3
X Coefficient(s)	0.000005	
Std Err of Coef.	0.000000	

TABLE 15A: Velocity Test Temperatures

Time (min)	Acetone	Butyl Acetate	Ethyl Acetate	Hexane	Methylene Chloride	MEK	Toluene
0	21.8	21.6	21.6	22.1	21.5	22.3	22.4
0.25	21.1	21.4	21.2	21.5	20.7	21.4	22.1
0.5	20.2	21.4	20.9	21	19.1	20.7	21.7
0.75	19.3	21.4	20.6	20.2	17.8	20.4	21.6
1	18.5	21.4	19.8	19.7	16.5	20.2	21.4
1.25	18	21.4	19.8	19.3	15.6	20	21.3
1.5	17.4	21.3	19.6	18.8	14.5	19.7	21.2
1.75	16.9	21.2	19.2	18.4	13.6	19.3	21.1
2	16.3	21.2	18.9	18.2	12.9	19.1	20.9
2.25	15.8	21.1	18.6	17.8	12.3	18.9	20.9
2.5	15.3	21.1	18.4	17.5	11.6	18.7	20.8
2.75	14.8	21.1	18.2	17	11.1	18.5	20.8
3	14.4	21	17.9	16.7	10.4	18.3	20.7
3.25	13.9	20.9	17.8	16.2	9.8	18.1	20.6
3.5	13.6	20.9	17.5	16.2	9.4	17.8	20.6
3.75	13.2	20.9	17.4	15.7	8.9	17.7	20.4
4	12.8	20.9	17.2	15.5	8.3	17.4	20.4
4.25	12.4	20.8	17.1	15.4	7.8	17.3	20.3
4.5	12.1	20.8	17.1	15	7.5	17.1	20.2
4.75	11.8	20.8	16.8	14.9	7.1	17	20.2
5	11.6	20.8	16.7	14.7	6.7	16.8	20.1
5.25	11.3	20.8	16.6	14.4	6.3	16.7	20.1
5.5	10.9	20.8	16.4	14.2	5.9	16.5	20
5.75	10.7	20.7	16.3	14.1	5.6	16.3	20
6	10.5	20.7	16.1	13.7	5.3	16.3	19.9
6.25	10.3	20.7	15.8	13.6	5.1	16.1	19.8
6.5	10.1	20.7	15.8	13.4	4.7	15.9	19.9
6.75	9.8	20.6	15.7	13.1	4.6	15.8	19.8
7	9.6	20.6	15.6	12.8	4.4	15.7	19.8
7.25	9.4	20.6	15.5	12.7	4	15.6	19.7
7.5	9.2	20.6	15.4	12.6	3.6	15.4	19.6
7.75	9.1	20.6	15.3	12.6	3.6	15.4	19.5
8	8.9	20.5	15.2	12.4	3.1	15.3	19.5
8.25	8.8	20.5	15.1	12.2	2.9	15.2	19.4
8.5	8.6	20.5	15.1	12.2	2.8	15	19.3
8.75	8.4	20.4	14.9	12	2.6	14.9	19.2
9	8.3	20.3	14.7	11.8	2.3	14.8	19.2
9.25	8.2	20.3	14.6	11.7	2.1	14.7	19.1
9.5	8.1	20.2	14.6	11.8	2.1	14.6	19.1
9.75	8	20.3	14.5	11.6	1.7	14.6	19.1
10	7.8	20.2	14.3	11.4	1.7	14.4	19.1
10.25	7.7	20.2	14.3	11.2	1.6	14.4	19
10.5	7.7	20.3	14.3	11.2	1.4	14.3	18.9
10.75	7.7	20.3	14.3	11.1	1.3	14.2	18.9
11	7.5	20.3	14.2	11	1.2	14.2	18.8
11.25	7.4	20.2	14.2	11.1	1.2	14.1	18.8
11.5	7.4	20.2	14.1	10.9	1.1	14.1	18.7
11.75	7.3	20.2	13.9	10.8	0.9	14	18.7
12	7.2	20.2	13.9	10.6	0.9	13.9	18.7
12.25	7.1	20.2	13.9	10.7	0.8	13.8	18.7

TABLE 16A: MIRAN CALIBRATION CURVE DATA – ACETONE

Miran Reading A	Concentration in MIRAN in ppm:	Corrected Miran Reading A–Ao
0.108	0	0
0.163	26.13929	0.055
0.2125	52.26688	0.1045
0.2636	78.38274	0.1556
0.331	130.5910	0.223
0.387	182.7525	0.279
0.4575	260.9247	0.3495
0.513	338.9917	0.405
0.5712	442.9411	0.4632
0.6304	572.6451	0.5224
0.68	702.0585	0.572

TABLE 17A: MIRAN CALIBRATION CURVE DATA - BUTYL ACETATE

Miran Reading A	Concentration in MIRAN in ppm:	Corrected Miran Reading A-Ao
0.0142	0	0
0.084	7.271758	0.0698
0.148	14.52723	0.1338
0.206	21.76645	0.1918
0.305	36.21247	0.2908
0.383	50.59385	0.3688
0.446	64.91089	0.4318

TABLE 18A: MIRAN CALIBRATION CURVE DATA – ETHYL ACETATE

Miran Reading %A	Concentration in MIRAN in ppm:	Corrected Miran Reading A–Ao
0.0314	0	0
0.134	9.867570	0.1026
0.311	29.58501	0.2796
0.445	49.26713	0.4136
0.566	73.82568	0.5346
0.654	98.32923	0.6226
0.716	122.7778	0.6846

TABLE 19A: MIRAN CALIBRATION CURVE DATA - HEXANE

Miran Reading Absorbance (A)	Concentration in MIRAN in ppm:	Corrected Miran Reading A-Ao
0.0114	0	0
0.019	14.76108	0.0076
0.0246	29.50894	0.0132
0.0309	44.24357	0.0195
0.0387	66.32571	0.0273
0.0481	95.72898	0.0367
0.0577	125.0795	0.0463
0.0659	154.3775	0.0545
0.0733	183.6230	0.0619

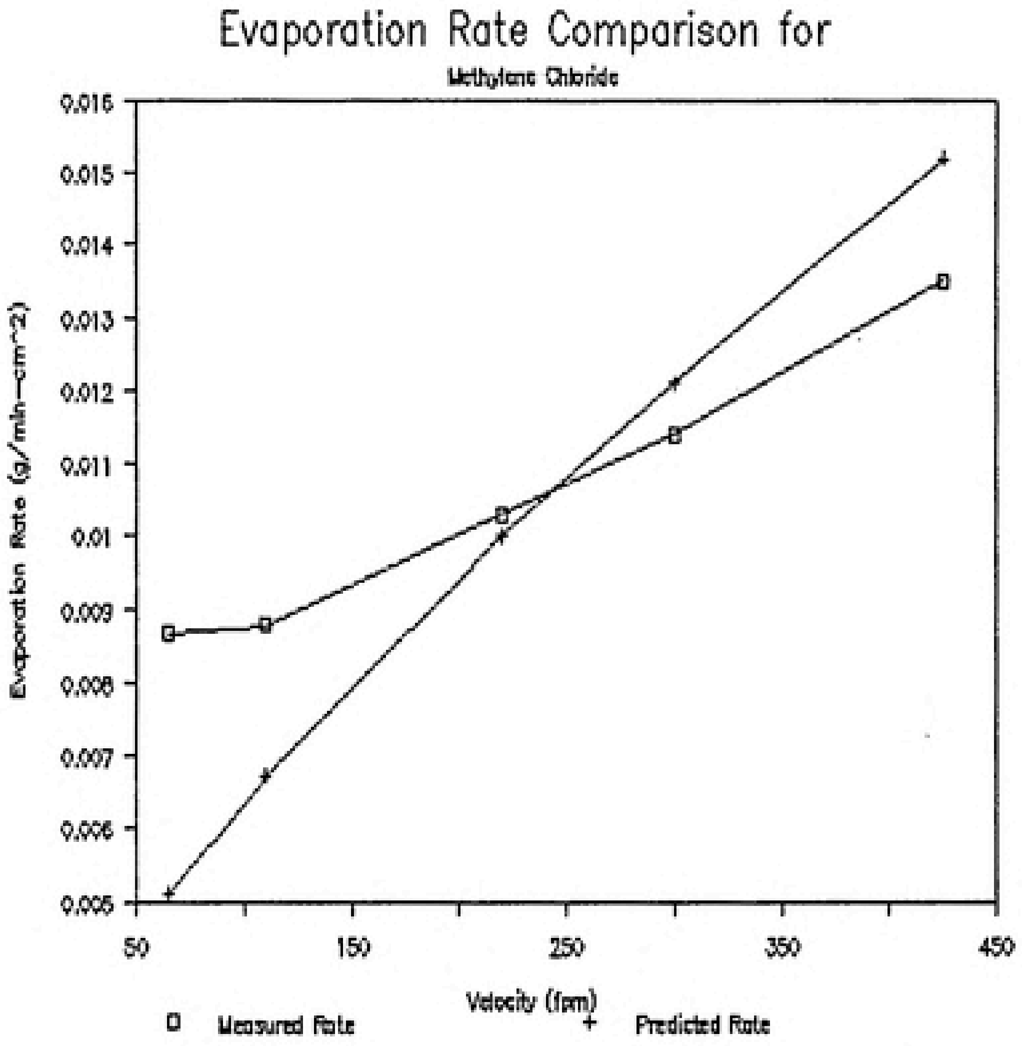


Figure 49. Comparison of measured evaporation rates to those predicted by the Kawamura-Mackay model.

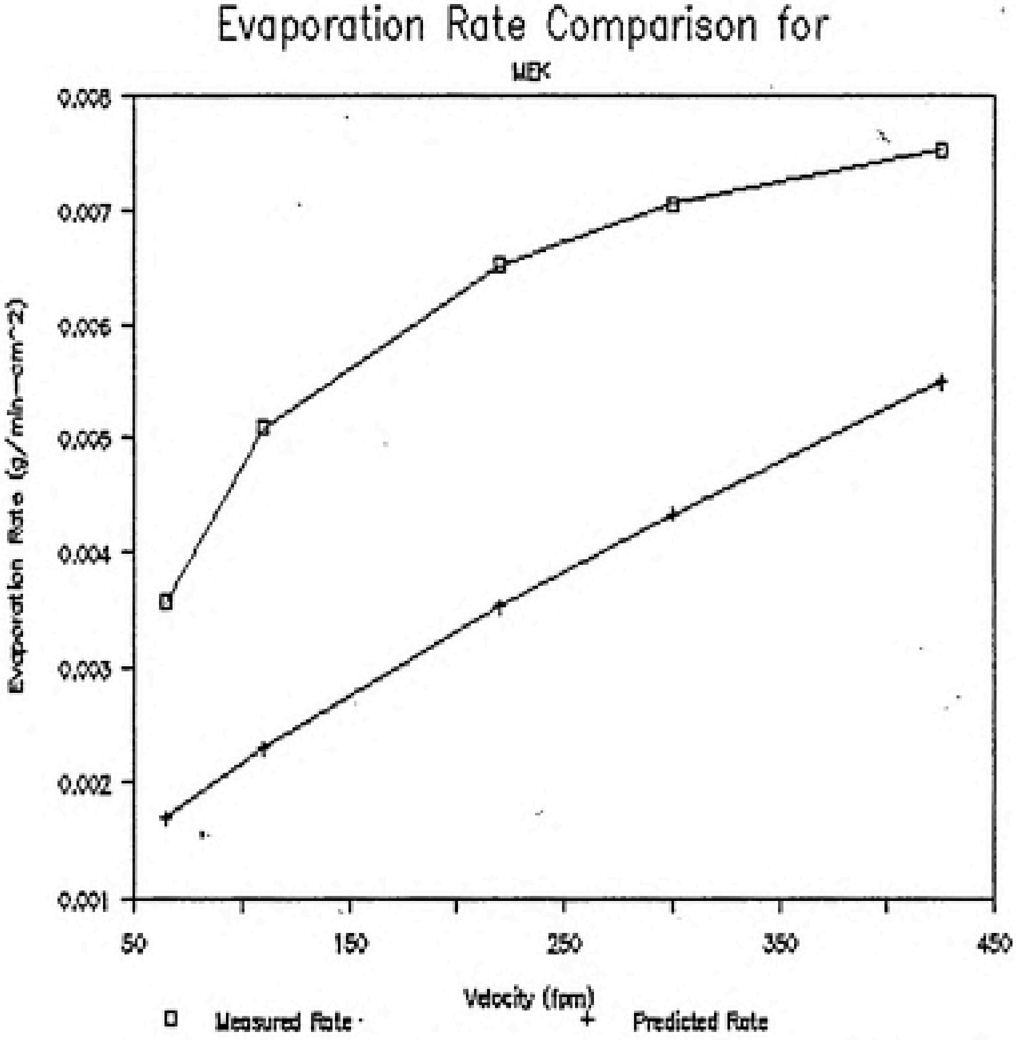


Figure 50. Comparison of measured evaporation rates to those predicted by the Kawamura-Mackay model.

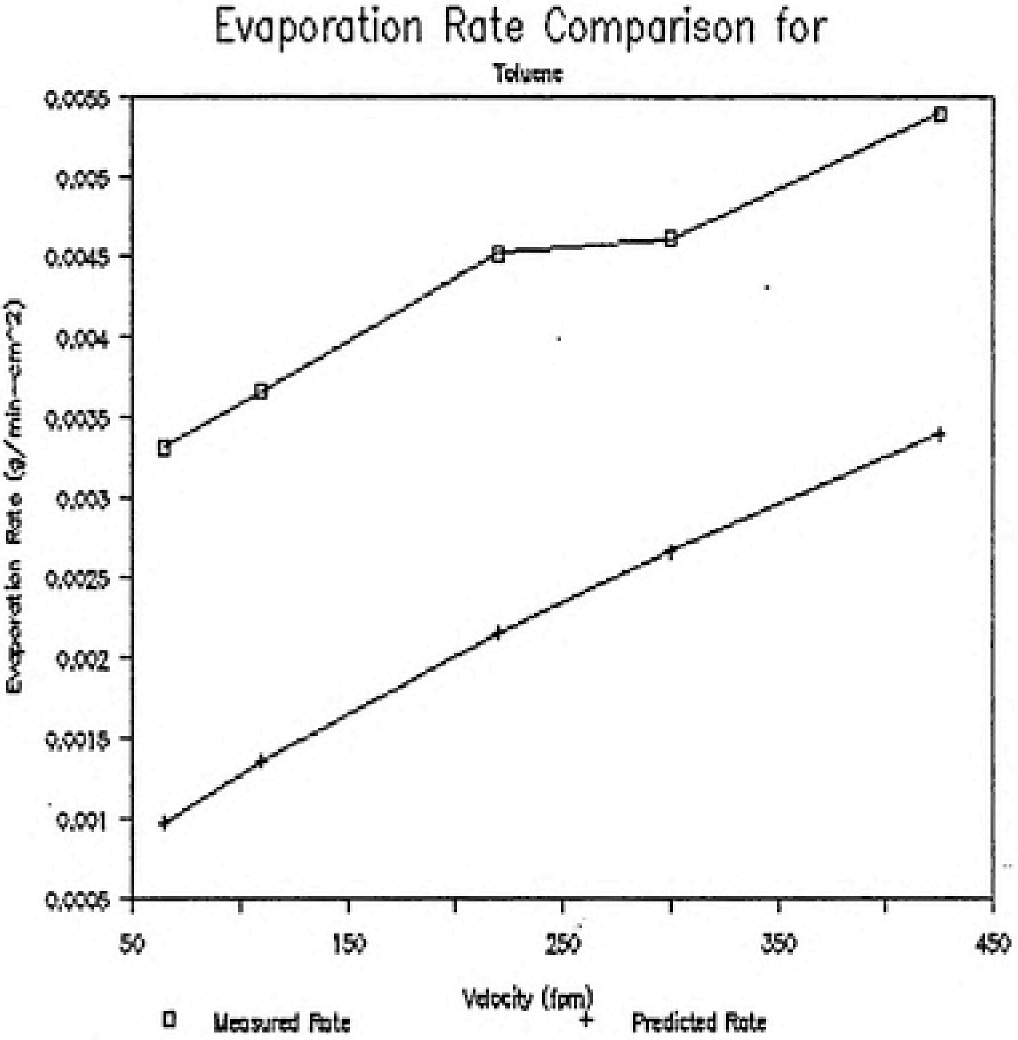


Figure 51. Comparison of measured evaporation rates to those predicted by the Kawamura-Mackay model.

CONCLUSIONS AND RECOMMENDATIONS

The models presented could prove to be invaluable to the industrial hygienist concerned with chemical spills or evaporation of solvents from open surface tanks or other containers in a workplace. If he or she has determined the air flow characteristics of the room, volume of the room, physical properties of the chemical, and can estimate the spill area, and air velocity across the surface of the spill, he or she can accurately predict the time required to reach the equilibrium concentration in the room. The resultant concentration value can be a good approximation but should be multiplied by a factor of two to ensure that the expected concentration is over-estimated, providing a safety margin. Investigation into the basis for the consistent under-prediction of the expected air concentration is needed.

The results obtained using the Reist model and the Kawamura-Mackay model were calculated using LOTUS 1-2-3. Without the use of a program such as this, calculating concentrations, especially in an emergency situation, could be difficult. The prudent industrial hygienist could prepare a spreadsheet, for each workplace and the chemicals used there, from information gathered during surveys. Then, concentration curves could be developed for a particular chemical within minutes of a spill.

The major factors affecting vapor concentration over a liquid according to the models are: air flow through the room, surface area of the spill, air velocity over the liquid, and the liquid surface temperature. Increasing air flow through the room both increases the removal of airborne vapors and increases the velocity over the liquid surface which increases the evaporation rate. Reducing the surface area reduces the evaporation rate reducing the concentration in the air. Increasing the air velocity over the liquid increases the evaporation rate but also lowers the liquid surface temperature which helps reduce the evaporation rate.

This knowledge can be put to use in the event of a spill. The most important thing to do is to first cover the spill with an inert absorbing material to reduce the vapor pressure over the liquid. Enough material must be used to ensure the liquid does not soak through. If this happened, the surface area would increase and the evaporation rate would escalate. Next, the flow through the room should be increased to ensure rapid removal of any airborne contaminant. Finally, clean up the spill as soon as possible.

The results of this research are good only for the chemicals tested. Further research in the application of these models to other classes of chemicals and chemical mixtures would have significant industrial applications.

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APPENDIX A

SAMPLE CALCULATION FOR ACETONE USING REIST MODEL

A. Spill & Chemical Data

Chemical	Acetone
Spill Area, A	619 cm^2
Velocity over surface of liquid	400 fpm
Air temperature	22.4 C
Molecular weight, MW	58.08
Mixing factor, K	1
Room volume, X	830 ft^3
Air flow through room, Q	713 ft^3/min
Elapsed time, t	8 min
Rate of generation, m	.006859 $g/min\text{-}cm^2$ (from Kawamura-Mackay model)

B. Model Calculations for Build-up Concentration

Since there is no filter and no incoming concentration of contaminant, equation (7) reduces to:

$$C = (m/Q)(1-\exp^{-t/T})$$

where $T = X/(KQ)$

$$C = (m/713)(1-\exp^{((-8)(1)(713)/830)}$$

Converting m to units of ft^3/min:

$$m = (.006859)(619)(22.4)(273+22.4)/$$
$$(58.08)(28.3)(273)$$

$$m = .0626\ ft^3/min$$

and $$C = (8.8 \text{ X } 10^{-5})(.9989) = 8.8 \text{ X } 10^{-4}$$

to get ppm $$C = (8.8^{-5})(10^6) = 88 \text{ ppm}$$

EXPERIMENTAL METHODS

I. Determination of Evaporation Rates.

  A. Apparatus set up (Equipment List 1):

    1. Open fume hood sash fully.
    2. Place balance inside fume hood.
    3. Attach temperature probe to side of balance. Ensure that the end of the probe extends into balance door area but does not contact any part of the balance.

  B. Procedure:

    1. Measure cross-draft through the balance with anemometer and record the velocity.
    2. Zero the balance.
    3. Weigh petri dish bottom and record the weight.
    4. Fill petri dish to within several mm from the top with the chemical to be tested and place on balance pan.
    5. Close balance doors and weigh petri dish and chemical, note the weight, start the stopwatch, and record the weight noted and temperature. Open balance doors.
    6. Record weight at regular time intervals.
    7. Repeat the procedure in lines 5 and 6 until enough measurements have been taken to ensure an accurate curve.

8. To plot the evaporation rate curve, subtract the weight of the petri dish from each measured weight and plot the difference vs time interval.

II. Determination of Evaporation Rates as a Function of Time, Surface Area, and Weight at Various Velocities.

   A. Apparatus Setup (Equipment List 2):

      1. Place the balance on a laboratory workbench near a flexible exhaust hood with blast gate.

      2. Position the exhaust hood near a door opening in the balance and secure the hood to the bench. Ensure the hood is positioned to allow airflow across the top of the petri dish when placed on the balance pan.

      3. Tape cardboard squares over the door areas to reduce the area. Ensure that there is enough space between the bottom of the cardboard squares and the top of the petri dish when on the pan to allow for air flow across the top of the dish, and that the doors close easily. Also, the space must be wide enough to allow for easy removal from and placement of the petri dish on the balance pan.

      4. Tape the thermoanemometer probe to the door opposite the exhaust hood. Ensure that the probe sensor is positioned at the same height as the top of the petri dish and that it is properly

aligned to measure the maximum velocity.

5. Attach the temperature probe so probe extends into the airstream but does not contact any part of the balance.

B. Procedure:

1. Zero the balance.
2. Weigh the petri dish and record the weight.
3. Turn on the exhaust and adjust the blast gate to achieve the desired velocity across the top of the petri dish.
4. Fill petri dish to within several mm of the top but not completely full and place on the balance pan.
5. Close the balance doors, weigh the chemical and petri dish, start the stopwatch, open doors, and record weight and temperature.
6. Leaving the stopwatch running, take and record measurements as described in line 5 at 2, 4, and 6 minute intervals.
7. Following the procedures outlined in lines 3-6 above and record measurements for each chemical at velocities of 20, 50, 80, 120, and 180 feet per minute.
8. Plot of evaporation rate curves:
    a. For each velocity run done, subtract the weight of the petri dish from the measured

weight and divide the difference by: the time interval in minutes, the area of the petri dish in square centimeters, and the number of time runs done (3). This yields one data point on the curve.

b. Repeat the procedure in 8.a. for each velocity run and plot the results (evaporation rate in g/min-cm^2) vs velocity.

III. Chamber Data Collection.

A. MIRAN Calibration (Equipment List 3). Calibrate the MIRAN using the following technique:

1. First, a known concentration of vapor of the chemical to be used must be made. To do this:

a. Determine the maximum vapor concentration of the chemical at equilibrium at the present temperature using the following equation:

$Cm = VP/14.7 \times 10^6$

Where: Cm = Maximum concentration in parts per million (ppm)

VP = Vapor Pressure in pounds per square inch absolute (psia)

14.7 = Atmospheric Pressure in psia

VP is obtained using the following equation:

$\log VP = (A - (B/C + T))/760 \times 14.7$

Where: A, B, and C are constants obtained from Lange's Handbook of Chemistry [5]

T = Temperature in degrees Centigrade (C)

b. Once the maximum concentration has been determined, a known concentration can be made in the calibration flask using the following equation (note: the known concentration should be less than the maximum concentration to ensure that the liquid chemical that is injected into the calibration flask totally evaporates).

$$Cf = Vi \times p \times N \times (T + 273)/273 \times 10^6/(MW \times Vf)$$

Where:

Cf = Concentration in flask in ppm

Vi = Volume of liquid injected into flask in milliliters (ml)

p = Density in grams per milliliter (g/ml)

N = Molar volume at 0 degrees C (22.4 g/g mole)

T = Temperature in degrees C

MW = Molecular Weight in g/g mole

Vf = Volume of flask in liters (l)

c. Pick a value for Cf (must be $<$ Cm) and solve the above equation for Vi. This will give the amount of liquid that must be injected into the calibration flask to produce the desired concentration (Cf).

4. Extract the amount of chemical determined for Vi using a syringe and inject into the calibration flask through the septum.
5. Hold the flask in a horizontal position in both hands and gently rock the flask to allow the glass beads to spread the liquid across the interior of the flask. Then vigorously shake the flask to allow the liquid adhering to the beads to evaporate. Repeat this process until <u>all</u> the liquid has evaporated.

b. Next, determine the analytical wavelength, pathlength, and slit width required for the chemical used.

1. Make a strip chart record of the MIRAN in % Transmission and Scan mode for ambient air. Compare to a scan made after injecting a small amount of chemical into the MIRAN. Peak differences will determine the best wavelength to use.
2. Pathlength and slit width will depend on the sensitivity required for the

detection of the chemical used.

c. Connect the Metal Bellows pump to the MIRAN as shown in Figure 4 (note: the MIRAN should be turned on at least 24 hours prior to use). Set the MIRAN to the proper wavelength, pathlength, slit width, and set scale to absorbance (1A). Connect Data Logger to output terminals.

d. To calibrate the MIRAN, known volumes must be extracted from the calibration flask and injected into the MIRAN. As extractions are made from the flask, the concentration in the flask changes. And, as injections are made into the MIRAN, the concentration there also changes. To account for these changes in concentration, the following equations are required:

For change in concentration in the flask:

$C = Co \; X \; e^{-W/Vf}$ [8]

Where: C = Concentration in flask after extraction in ppm

Co = Concentration before extraction in ppm

W = Volume extracted in l

Vf = Volume of flask in l

For change in concentration in the MIRAN:

Cm = W X Co/Vm

Where: Cm = Concentration in MIRAN after injection in ppm

W = Volume injected in l

Co = Concentration in volume injected in ppm

Vm = Volume of MIRAN in l

e. Extractions from the calibration flask are injected into the MIRAN. The change in absorbance is noted after each injection by reading the output on the data logger. Record the absorbance after each injection (allowing 30 seconds between injection and reading to allow for mixing in the MIRAN cell). Each injection equals one data point on the calibration curve. Ensure enough points are taken to get a good curve.

f. Plot concentration vs absorbance to get the calibration curve.

B. Characterization of Chamber (Equipment List 4).

1. Measure and record the inside dimensions of the chamber.

2. Determine the air flow through the chamber.

C. Chemical Buildup and Decay Measurements.

1. Apparatus set up (Figures 5-7 and Equipment List 5):

a. Program data logger.

   1. Two channels are required. Program one channel for input from the MIRAN to record absorbance. Program the second channel to record temperature using a Type J thermocouple.

   2. Program the system for:

      1 sample/second

      input length = 1 minute

      # periods to combine = 1

      baud rate = 9600

b. Connect the MIRAN and the thermocouple to the appropriate data logger terminals.

c. Connect tubing with diffuser to MIRAN inlet.

d. Connect MIRAN pump to MIRAN outlet and turn on pump.

e. Turn on chamber ventilation system.

f. Position cart in chamber.

g. Tape tubing to cart with probe positioned over pan area.

h. Place fan on cart in front of pan area.

i. Place pan on cart.

2. Procedure:

   a. Determine the air velocity over the liquid surface either by direct measurement, by calculation using empirical data from evaporation rate tests in the chamber, or by prediction using the Kawamura-Mackay model.

b. Set data logger to log mode, and pour chemical into pan, filling to height approximated during velocity measurements.

c. Close chamber door.

d. Observe the input from the MIRAN channel on the data logger. When the absorbance peaks or appears to decline remove pan containing chemical from the chamber and place in chemical fume hood.

e. When the input from the MIRAN returns to zero terminate the log mode on the data logger.

f. Repeat lines c through f above with the fan on.

CHEMICAL LIST

All chemicals were from the Aldrich Chemical Company

Acetone 99 + %

2-Butanone (MEK) 99 + %

Butyl Acetate 99 + %

Ethyl Acetate 99.5 + %

Hexane HPLC 96.9%

Methylene Chloride 99.6% ACS Reagent

Toluene 99 + % ACS Reagent

EQUIPMENT LIST 1

Mettler Balance - Type H4, Capacity 160g, SN 127526

YSI Digital Thermometer - Model 49Ta, SN 820

YSI Probe - Series 400

TSI Air Velocity Meter - Model 1650, SN 058, Calibrated May 89

Heuer Microsplit Stopwatch - Model 1020

Glass Petri Dish Bottom - 9cm diameter

Kewaunee Scientific Corporation Laboratory Fume Hood

EQUIPMENT LIST 2

Mettler Balance - Type H4, Capacity 160g, SN 127526

YSI Digital Thermometer - Model 49Ta, SN 820

YSI Probe - Series 400

TSI Air Velocity Meter - Model 1650, SN 058, Calibrated May 89

Heuer Microsplit Stopwatch - Model 1020

Glass Petri Dish Bottom - 9cm diameter and 8.7cm diameter

Flexible Exhaust Hood with Blast Gate

EQUIPMENT LIST 3

Wilks MIRAN - Model 1A-CVF, SN 2833

Metrosonics Data Logger - Model dl-714, SN 001222

OMEGA Type J Iron Constantan Thermocouple

2.23 Liter Flask with Rubber Stopper

Heuer Microsplit Stopwatch - Model 1020

Metal Bellows Pump - Model MB-41, SN 11630

Glass Beads

Modeling Clay

Hamilton Gastight 5ml Syringe - Model 1005

Hamilton Gastight 1ml Syringe - Model 1001

EQUIPMENT LIST 4

TSI Air Velocity Meter – Model 1650, SN 059, Calibrated May 89

Stanley Powerlock II Tape Measure – Model PL312

EQUIPMENT LIST 5

Wilks MIRAN - Model 1A-CVF, SN 2833

Metrosonics Data Logger - Model dl-714, SN 001222

OMEGA Type J Iron Constantan Thermocouple

Fan - Axial Type, 3-Blade, 5.5in Diameter

Staco Variable Autotransformer - Model 3PN1010, SN 8935

Cart

830 Cubic Foot Chamber with Exhaust Ventilation = 418cfm

Modeling Clay

Imperial Eastman Nylo-seal "7" Tubing, C908-1/2" ID with Probe

Teflon coated pan measuring 8" X 12" X 2"

TABLE 1A: EVAPORATION RATE TEST – ACETONE

TEMP (deg C)	ELAPSED TIME (min)	WT OF ACETONE AND DISH (g)	WT OF ACETONE (g)	Regression Curve
22.9	0	70.6	43.36	43.08961
22.9	1	70.27	43.03	42.73387
22.8	2.5	69.56	42.32	42.20027
22.9	3.5	69.145	41.905	41.84454
23	4.5	68.75	41.51	41.48880
23	5.5	68.355	41.115	41.13307
22.9	7	67.7	40.46	40.59947
23	8	67.32	40.08	40.24373
23	9	66.96	39.72	39.88800
23	10	66.625	39.385	39.53227
23	11	66.255	39.015	39.17653
23	12	65.91	38.67	38.82080
23	13	65.56	38.32	38.46506
23	14	65.233	37.993	38.10933
23	16	64.524	37.284	37.39786
23	17	64.235	36.995	37.04213
23.1	18	63.913	36.673	36.68639
23	19	63.565	36.325	36.33066
23.1	20	63.297	36.057	35.97492
23	21.5	62.805	35.565	35.44132
22.9	24	61.97	34.73	34.55199
23	25	61.675	34.435	34.19625

Regression Output:

Constant		43.0896127
Std Err of Y Est		0.15576689
R Squared		0.99675796
No. of Observations		22
Degrees of Freedom		20
X Coefficient(s)	-0.355734146	
Std Err of Coef.	0.004536538	

TABLE 2A: EVAPORATION RATE TEST – BUTYL ACETATE

TEMP (deg C)	ELAPSED TIME (min)	WT OF BA & DISH (g)	WT OF BUTYL ACETATE (g)	REGRESSION CURVE
23.2	0	70.6	43.36	43.43104
23.1	1	70.558	43.318	43.38180
23.1	2.5	70.507	43.267	43.30795
23.1	3.5	70.463	43.223	43.25872
23.2	5.5	70.38	43.14	43.16025
23.2	6.5	70.34	43.1	43.11101
23.2	8.5	70.244	43.004	43.01254
23.3	10	70.172	42.932	42.93869
23.3	12.5	70.06	42.82	42.81561
23.4	14.5	69.965	42.725	42.71714
23.4	16	69.902	42.662	42.64328
23.4	19	69.75	42.51	42.49558
23.4	21	69.66	42.42	42.39711
23.3	25	69.439	42.199	42.20017
23.4	28	69.297	42.057	42.05247
23.4	30	69.2	41.96	41.95400
23.3	33	69.16	41.92	41.80630
23.5	44	68.567	41.327	41.26472
23.4	47	68.42	41.18	41.11702
23.4	50	68.265	41.025	40.96931
23.4	54	68.066	40.826	40.77237
23.5	56	67.98	40.74	40.67391
23.4	63	67.607	40.367	40.32926
23.3	79	66.616	39.376	39.54151
23.3	85	66.38	39.14	39.24611

Regression Output:

Constant		43.4310
Std Err of Y Est		0.06084
R Squared		0.997
No. of Observations		25
Degrees of Freedom		23
X Coefficient(s)	-0.0492344	
Std Err of Coef.	0.00050013	

TABLE 3A: EVAPORATION RATE TEST DATA – ETHYL ACETATE

TEMP (deg C)	ELAPSED TIME (min)	WT OF ETHYL ACETATE AND DISH (g)	WT OF ETHYL ACETATE (g)	Regression Curve
22.3	0	81.5	54.26	54.02618
22.2	1	81.19	53.95	53.76997
22.2	2	80.87	53.63	53.51376
22.2	3	80.628	53.388	53.25755
22.1	4	80.35	53.11	53.00134
22.2	6	79.615	52.375	52.48892
22.2	7	79.388	52.148	52.23271
22.1	8	79.17	51.93	51.97650
22.2	10	78.635	51.395	51.46408
22.1	12	78.09	50.85	50.95166
22.3	13	77.883	50.643	50.69545
22.3	15	77.333	50.093	50.18303
22.2	17	76.799	49.559	49.67061
22.2	19	76.293	49.053	49.15819
22.2	21	75.76	48.52	48.64577
22.3	23	75.225	47.985	48.13335
22.3	25	74.74	47.5	47.62093
22.2	28	73.928	46.688	46.85230
22.3	30	73.469	46.229	46.33988
22.3	32	73.012	45.772	45.82746
22.3	35	72.548	45.308	45.05883
22.2	37	72.043	44.803	44.54641
22.4	39	71.5	44.26	44.03399

Regression Output:

Constant		54.026185639
Std Err of Y Est		0.1504023898
R Squared		0.9978593266
No. of Observations		23
Degrees of Freedom		21
X Coefficient(s)	-0.2562099992	
Std Err of Coef.	0.0025895659	

TABLE 4A: EVAPORATION RATE TEST DATA – HEXANE

TEMP (deg C)	ELAPSED TIME (min)	WT OF HEXANE AND DISH (g)	WT OF HEXANE (g)	Regression Curve
22.3	0	61.75	34.51	33.95955
22.3	1	61.32	34.08	33.65976
22.2	3	60.36	33.12	33.06018
22.2	7.5	58.835	31.595	31.71112
22.2	9.5	58.153	30.913	31.11154
22.3	11	57.758	30.518	30.66186
22.1	14	56.743	29.503	29.76248
22.2	15	56.474	29.234	29.46269
22.2	16	56.172	28.932	29.16290
22.3	17	55.92	28.68	28.86311
22.3	18	55.655	28.415	28.56332
22.2	19	55.33	28.09	28.26353
22.2	20	55.07	27.83	27.96374
22.1	21	54.815	27.575	27.66395
22.2	22	54.545	27.305	27.36416
22.2	23	54.285	27.045	27.06437
22.2	24	53.968	26.728	26.76458
22.2	25	53.713	26.473	26.46479
22.2	26	53.444	26.204	26.16500
22.2	27	53.13	25.89	25.86521
22.2	28	52.899	25.659	25.56542
22.2	30	52.342	25.102	24.96583
22.2	31	52.08	24.84	24.66604
22.2	32	51.817	24.577	24.36625
22.2	33	51.61	24.37	24.06646

Regression Output:

Constant		33.959558867
Std Err of Y Est		0.2129180211
R Squared		0.9947479081
No. of Observations		25
Degrees of Freedom		23
X Coefficient(s)	-0.2997906378	
Std Err of Coef.	0.0045421742	

TABLE 5A: EVAPORATION RATE TEST DATA – METHYLENE CHLORIDE

TEMP (deg C)	ELAPSED TIME (min)	WT OF METH CHLORIDE AND DISH (g)	WT OF METH CHLORIDE (g)	Regression Curve
23.3	0	72.2	44.96	44.40135
23.3	1	71.32	44.08	43.84301
23.3	2	70.49	43.25	43.28467
23.3	3	69.79	42.55	42.72632
23.2	4	69.25	42.01	42.16798
23.1	5	68.66	41.42	41.60964
23.2	6	68.1	40.86	41.05130
23.2	7	67.6	40.36	40.49295
23.2	8	67.095	39.855	39.93461
23.2	9	66.44	39.2	39.37627
23.3	10	65.93	38.69	38.81793
23.2	11	65.448	38.208	38.25958
23.2	12	64.925	37.685	37.70124
23.2	13	64.398	37.158	37.14290
23.2	14	63.935	36.695	36.58456
23.2	15	63.42	36.18	36.02621
23.2	16	62.885	35.645	35.46787
23.1	17	62.232	34.992	34.90953

Regression Output:

Constant		44.401356725
Std Err of Y Est		0.2010422172
R Squared		0.9957367216
No. of Observations		18
Degrees of Freedom		16
X Coefficient(s)	-0.5583426213	
Std Err of Coef.	0.0091335661	

TABLE 6A: EVAPORATION RATE TEST – MEK

TEMP (deg C)	ELAPSED TIME (min)	WT OF MEK AND DISH (g)	WT OF MEK (g)	Regression Curve
22	0	125.75	39.45	39.42777
22	1	125.625	39.325	39.31514
22	4	125.265	38.965	38.97724
22	6	125.04	38.74	38.75197
22	8	124.815	38.515	38.52670
22	10	124.58	38.28	38.30144
22	12	124.368	38.068	38.07617
22	14	124.16	37.86	37.85090
22	16	123.95	37.65	37.62563

Regression Output:

Constant		39.42777592
Std Err of Y Est		0.017824717
R Squared		0.999307249
No. of Observations		9
Degrees of Freedom		7
X Coefficient(s)	-0.112633567	
Std Err of Coef.	0.0011208766	

TABLE 7A: EVAPORATION RATE TEST DATA – TOLUENE

TEMP (deg C)	ELAPSED TIME (min)	WT OF TOLUENE AND DISH (g)	WT OF TOLUENE (g)	Regression Curve
21.8	0	67.38	40.14	40.18532
21.6	3.5	67.032	39.792	39.60410
21.6	5	66.735	39.495	39.35501
21.6	7.5	66.14	38.9	38.93985
21.8	9.5	65.94	38.7	38.60773
21.7	11	65.67	38.43	38.35864
21.6	14.5	64.935	37.695	37.77742
21.7	19.5	64.06	36.82	36.94711
22	21.5	63.765	36.525	36.61498
21.8	23.5	63.4	36.16	36.28286
21.9	27	62.86	35.62	35.70164
21.8	29	62.575	35.335	35.36951
21.9	30	62.425	35.185	35.20345
21.8	34.5	61.63	34.39	34.45617
21.8	36	61.43	34.19	34.20707
21.8	37.5	61.158	33.918	33.95798
22	39.5	60.84	33.6	33.62586
22	41.5	60.52	33.28	33.29373
22.1	43	60.265	33.025	33.04464
21.9	44.5	60.04	32.8	32.79554
22.1	46	59.79	32.55	32.54645
22	47.5	59.6	32.36	32.29736
22.1	49	59.383	32.143	32.04826
22.1	50	59.29	32.05	31.88220

Regression Output:

Constant		40.1853284
Std Err of Y Est		0.08920984
R Squared		0.99892961
No. of Observations		24
Degrees of Freedom		22
X Coefficient(s)	-0.1660624667	
Std Err of Coef.	0.0011589451	

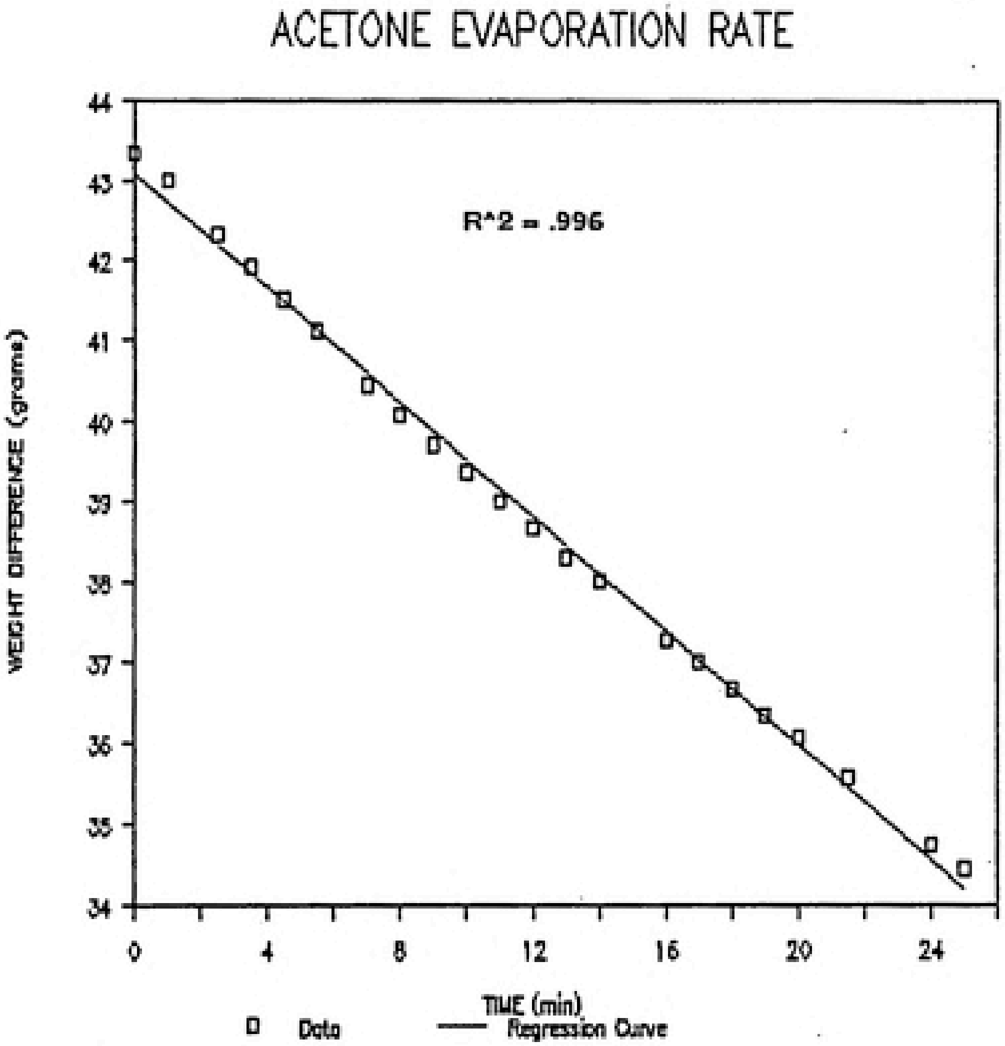

Figure 1A. Evaporation rate test and regression curves.

TABLE 20A: MIRAN CALIBRATION CURVE DATA – METHYLENE CHLORIDE

Miran Reading Absorbance (A)	Concentration in MIRAN in ppm:	Corrected Miran Reading A–Ao
0.016	0	0
0.0944	30.12644	0.0784
0.245	90.35231	0.229
0.388	150.5242	0.372
0.524	210.6421	0.508
0.706	300.7382	0.69
0.816	360.7215	0.8

TABLE 21A: MIRAN CALIBRATION CURVE DATA - MEK

Miran Reading Absorbance (A)	Concentration in MIRAN in ppm:	Corrected Miran Reading A–Ao
0.017	0	0
0.038	8.552987	0.021
0.081	25.65129	0.064
0.123	42.73427	0.106
0.162	59.80193	0.145
0.201	76.85429	0.184
0.238	93.89137	0.221

TABLE 22A: MIRAN CALIBRATION CURVE DATA - TOLUENE

Miran Reading Absorbance (A)	Concentration in MIRAN in ppm:	Corrected Miran Reading A-Ao
0.0266	0	0
0.03	5.420165	0.0034
0.041	16.25077	0.0144
0.054	27.06198	0.0274
0.065	37.85381	0.0384
0.076	48.62630	0.0494
0.087	59.37948	0.0604

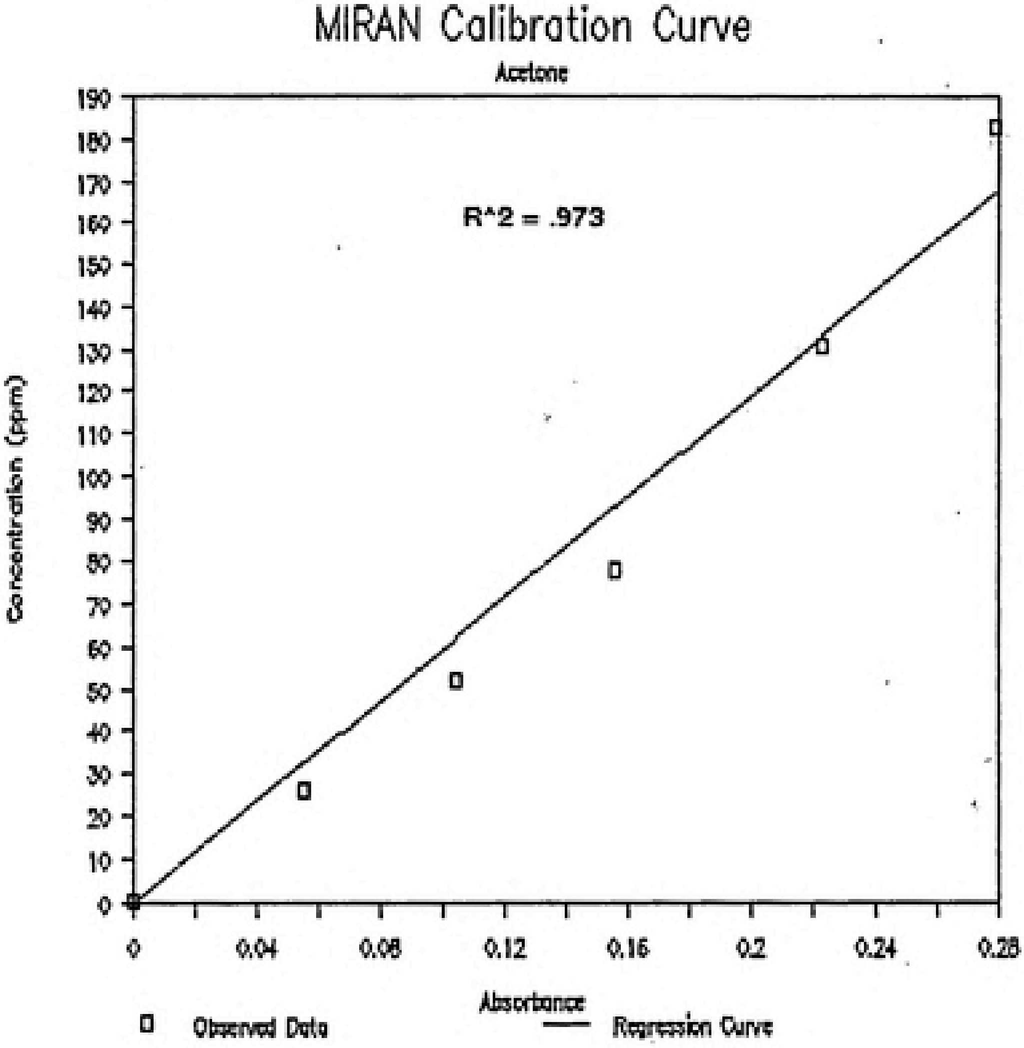

Figure 8A. MIRAN calibration and regression curves.

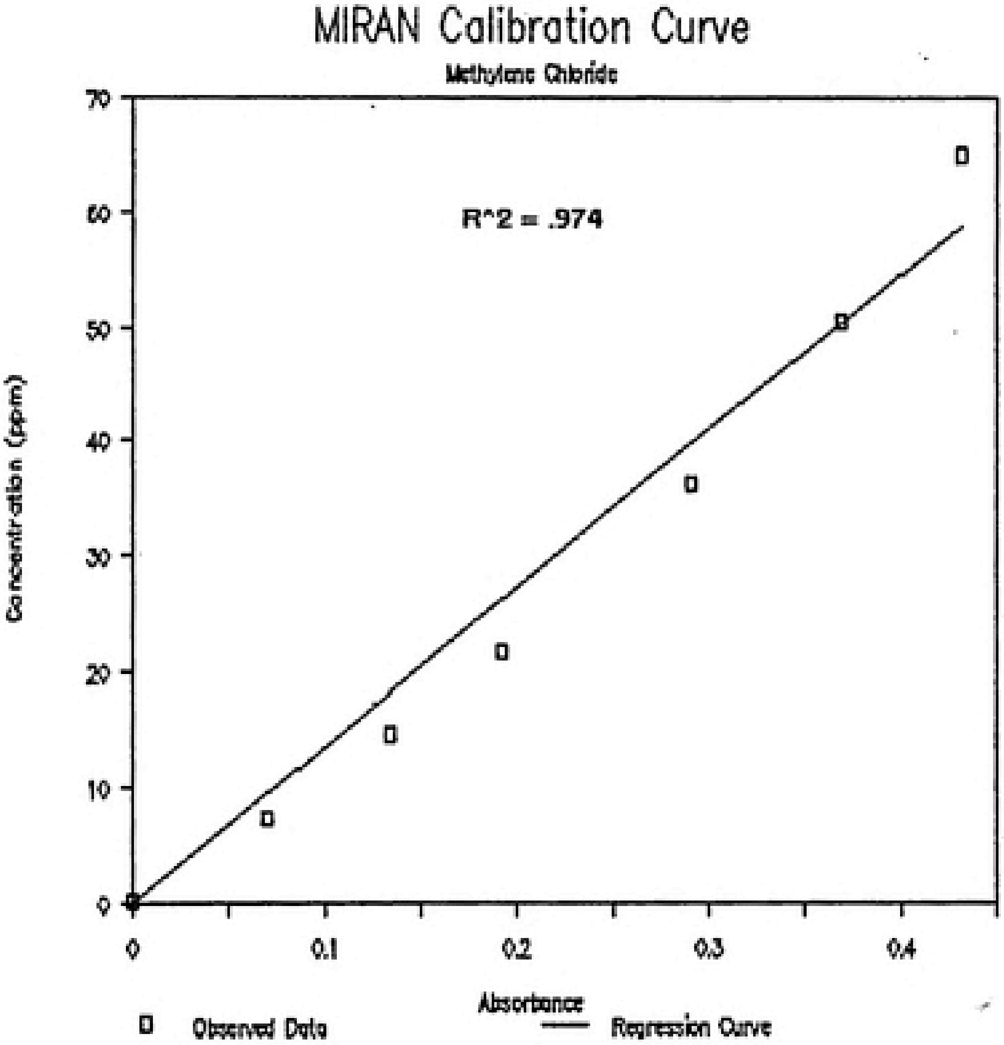

Figure 9A. MIRAN calibration and regression curves.

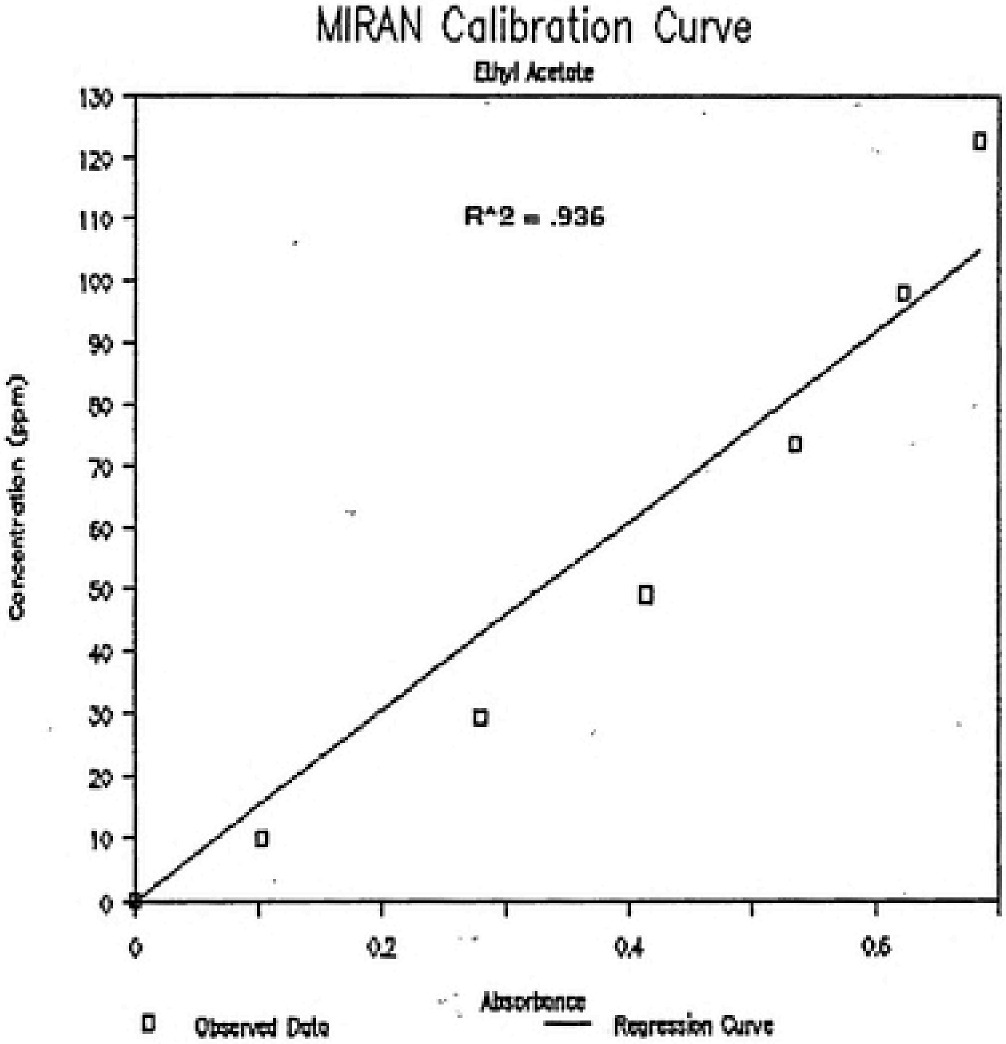

Figure 10A. MIRAN calibration and regression curves.

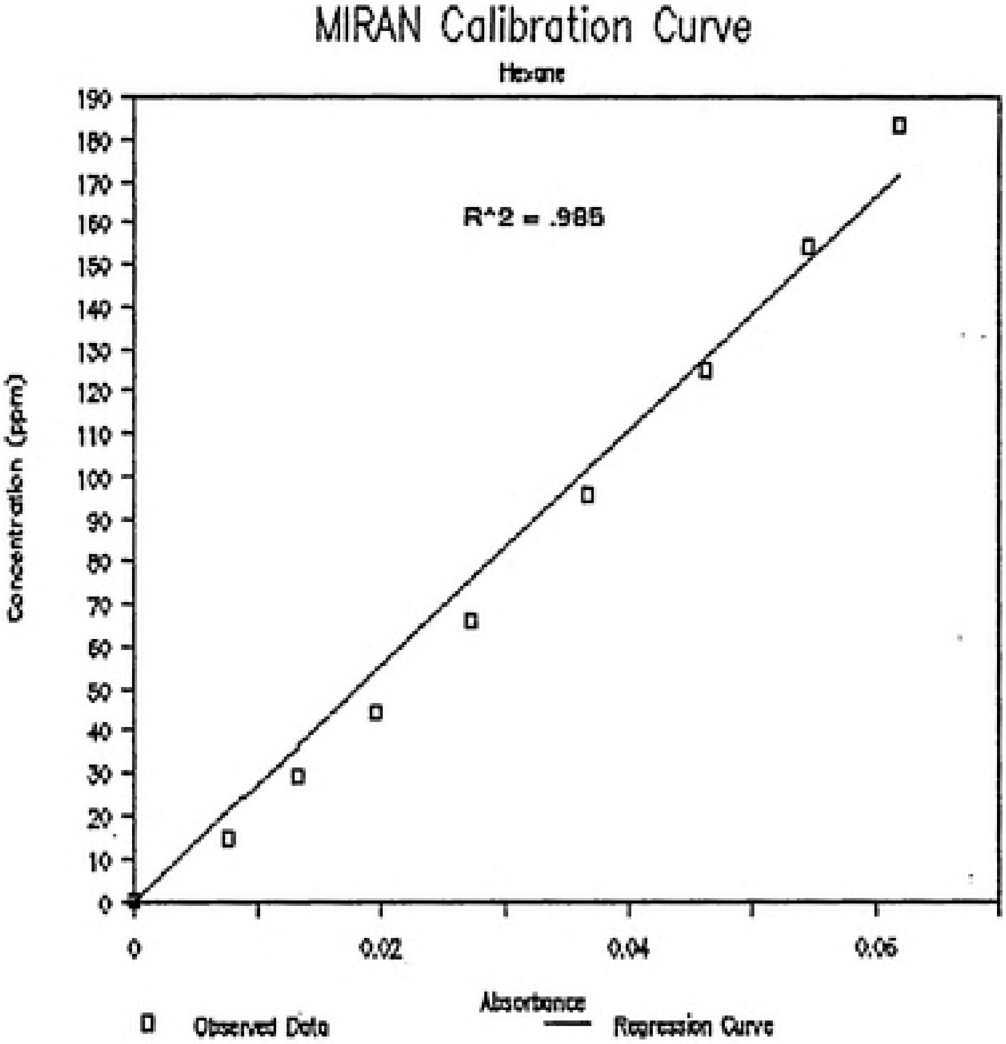

Figure 11A. MIRAN calibration and regression curves.

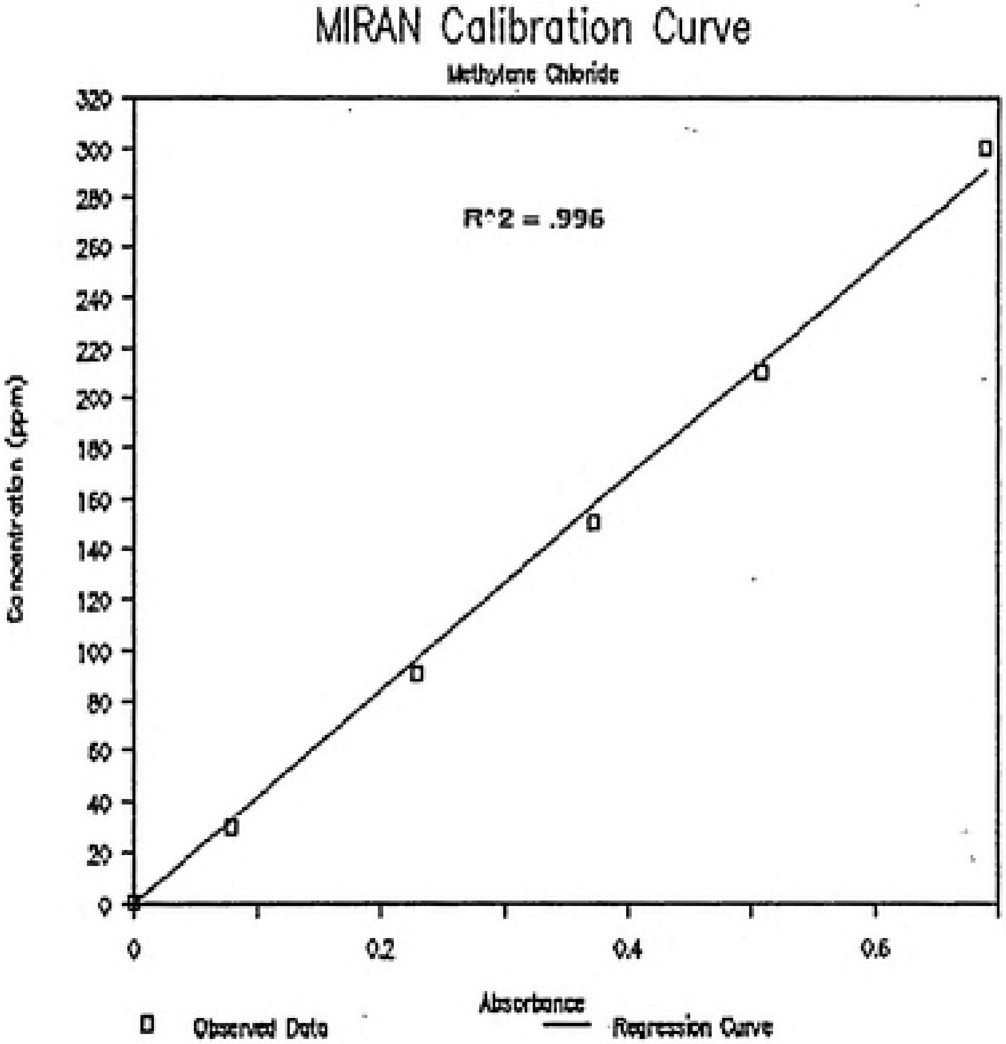

Figure 12A. MIRAN calibration and regression curves.

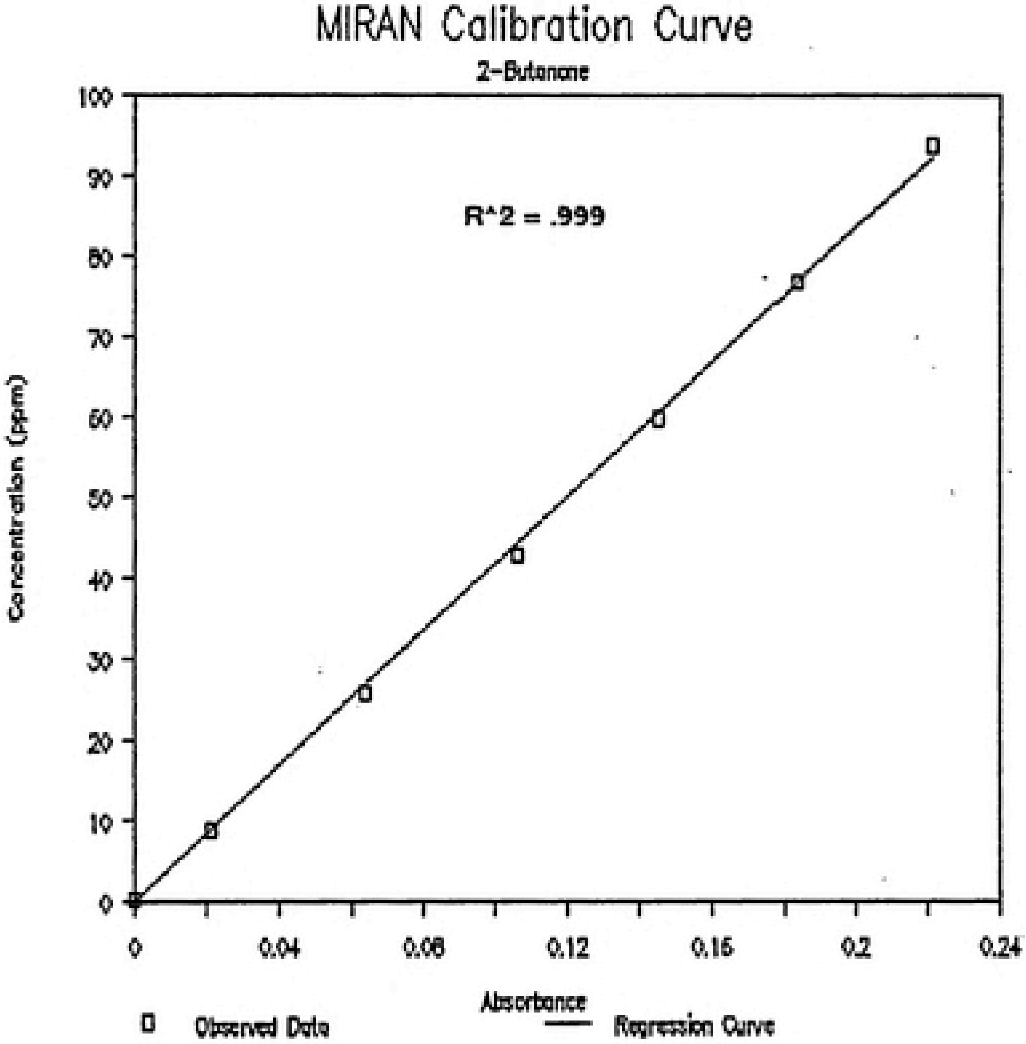

Figure 13A. MIRAN calibration and regression curves.

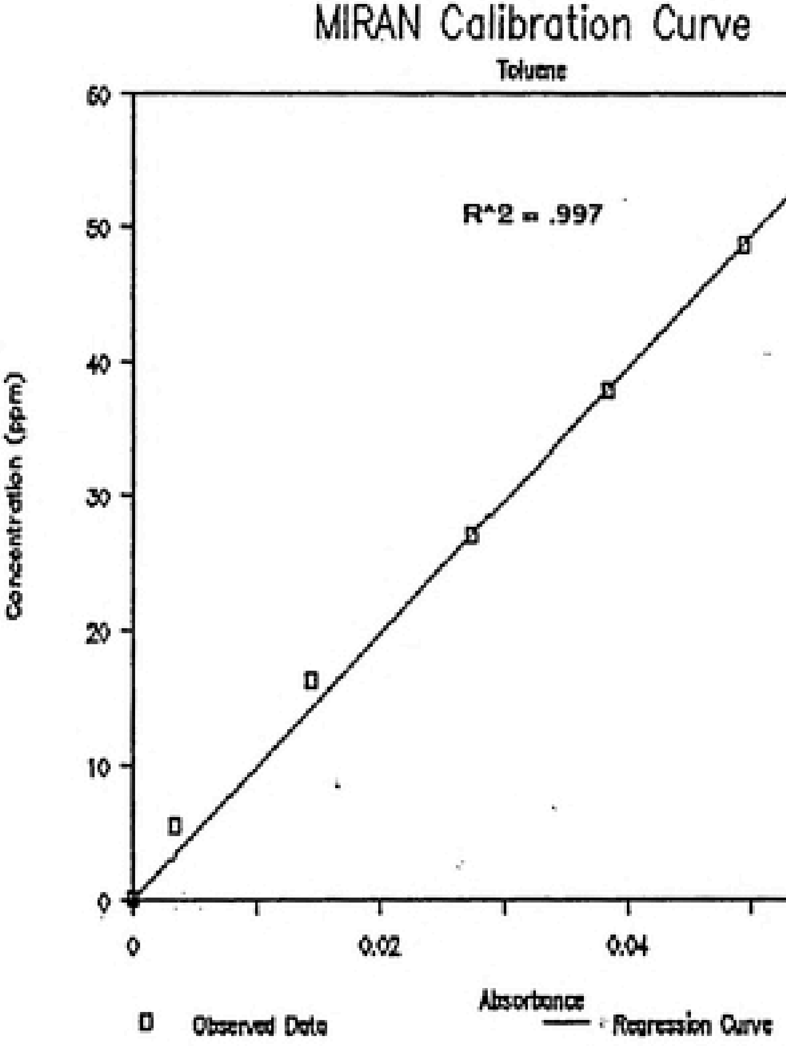

Figure 14A. MIRAN calibration and regression curves.

TABLE 23A: DATA FOR MIRAN CALIBRATION – BUTYL ACETATE – EXAMPLE WITH FORMULAS AND SYMBOLS DISPLAYED

Wavelength (um):	8.1	
Pathlength (m):	12.6	
Slit Width (mm):	2	
Molecular Weight (g/mole):	116.16	MW
Density (g/ml):	0.882	p
Molar Volume (l/mole):	24.09025	Molar Vol = 22.4*(T+273)/273
Volume of Flask (l):	2.23	Vf
Temperature (C):	20.6	T
Vapor Pressure at given temperature (psia):	0.170048	log VP = (A-(B/C+T)/760*14.7
Maximum Concentration at Equilibrium (ppm):	11567.91	VP/14.7*10^6
Lower Explosive Limit (ppm):	17000	LEL
MIRAN Volume (l):	5.64	Vm

PPM CALCULATIONS FOR FLASK:

Amount of Liquid injected into flask (ml):		Concentration of Vapor in flask (ppm):	
0.1	Vi	8202.543	Vi*p*R*T*10^6/(MW*Vf*P)

CONCENTRATION CALCULATIONS:

Amount of gas extracted & injected into MIRAN (l): W		New concentration (C) in flask in ppm:	Concentration in MIRAN (Cm) in ppm:
0	ml	8202.543	0
0.005	5	8184.172	7.271758
0.005	5	8165.843	7.255472
0.005	5	8147.554	7.239222
0.01	10	8111.100	14.44601
0.01	10	8074.809	14.38138
0.01	10	8038.680	14.31703
		C = Co*EXP(-W/Vf)	Cm = W*Co/Vm

CHAMBER CONCENTRATION CALCULATIONS:

Chamber Volume (Ft^3):	830.36	
Chamber Volume (l):	23516.28	Vc
Flow through chamber with door closed (cfm):	713	
Amount of liquid required to give chamber concentration of 1/2 LEL if complete evaporation occurs (ml):	1092.783	(LEL/2)*MW*Vc/(p*Molar Vol*10^6)

TABLE 24A: MIRAN CALIBRATION CALCULATIONS & PHYSICAL DATA – ACETONE

Wavelength (um):	8.2
Pathlength (m):	6
Slit Width (mm):	2
Molecular Weight (g/mole):	58.08
Density (g/ml):	0.791
Molar Volume (l/mole):	24.13948
Volume of Flask (l):	2.23
Temperature (C):	21.2
Vapor Pressure at given temperature (psia):	3.783914
Maximum Concentration at Equilibrium (ppm):	257409.1
Lower Explosive Limit (ppm):	26000
MIRAN Volume (l):	5.64

PPM CALCULATIONS FOR FLASK:

Amount of Liquid injected into flask (ml):	Concentration of Vapor in flask (ppm):
1	147425.6

CONCENTRATION CALCULATIONS:

Amount of gas extracted & injected into MIRAN (l):		New concentration in flask in ppm:	Concentration in MIRAN in ppm:
0	ml	147425.6	0
0.001	1	147359.5	26.13929
0.001	1	147293.4	52.26688
0.001	1	147227.4	78.38274
0.002	2	147095.4	130.5910
0.002	2	146963.6	182.7525
0.003	3	146766.0	260.9247
0.003	3	146568.7	338.9917
0.004	4	146306.0	442.9411
0.005	5	145978.3	572.6451
0.005	5	145651.4	702.0585

CHAMBER CONCENTRATION CALCULATIONS:

Chamber Volume (Ft^3):	830.36
Chamber Volume (l):	[illegible]
Flow through chamber with [illegible]:	[illegible]
Amount of liquid required to give chamber concentration of 1/2 LEL if complete evaporation occurs (ml):	929.8954

TABLE 25A: MIRAN CALIBRATION CALCULATIONS & PHYSICAL DATA
BUTYL ACETATE

Wavelength (um):	8.1
Pathlength (m):	12.6
Slit Width (mm):	2
Molecular Weight (g/mole):	116.16
Density (g/ml):	0.882
Molar Volume (l/mole):	24.09025
Volume of Flask (l):	2.23
Temperature (C):	20.6
Vapor Pressure at given temperature (psia):	0.170048
Maximum Concentration at Equilibrium (ppm):	11567.91
Lower Explosive Limit (ppm):	17000
MIRAN Volume (l):	5.64

PPM CALCULATIONS FOR FLASK:

Amount of Liquid injected into flask (ml):	Concentration of Vapor in flask (ppm):
0.1	8202.543

CONCENTRATION CALCULATIONS:

Amount of gas extracted & injected into MIRAN (l):		New concentration in flask in ppm:	Concentration in MIRAN in ppm:
0	ml	8202.543	0
0.005	5	8184.172	7.271758
0.005	5	8165.843	14.52723
0.005	5	8147.554	21.76645
0.01	10	8111.100	36.21247
0.01	10	8074.809	50.59385
0.01	10	8038.680	64.91089

CHAMBER CONCENTRATION CALCULATIONS:

Chamber Volume (Ft^3):	830.36
Chamber Volume (l):	23516.28
Flow through chamber with door closed (cfm):	713
Amount of liquid required to give chamber concentration of 1/2 LEL if complete evaporation occurs (ml):	1092.783

TABLE 26A: MIRAN CALIBRATION CALCULATIONS & PHYSICAL DATA
ETHYL ACETATE

Wavelength (um):	8
Pathlength (m):	12.6
Slit Width (mm):	2
Molecular Weight (g/mole):	88.11
Density (g/ml):	0.902
Molar Volume (l/mole):	24.24615
Volume of Flask (l):	2.23
Temperature (C):	22.5
Vapor Pressure at given temperature (psia):	1.618833
Maximum Concentration at Equilibrium (ppm):	110124.7
Lower Explosive Limit (ppm):	22000
MIRAN Volume (l):	5.64

PPM CALCULATIONS FOR FLASK:

Amount of Liquid injected into flask (ml):	Concentration of Vapor in flask (ppm):
0.25	27826.54

CONCENTRATION CALCULATIONS:

Amount of gas extracted & injected into MIRAN (l):		New concentration in flask in ppm:	Concentration in MIRAN in ppm:
0	ml	27826.54	0
0.002	2	27801.60	9.867570
0.004	4	27751.77	29.58501
0.004	4	27702.04	49.26713
0.005	5	27640.00	73.82568
0.005	5	27578.09	98.32923
0.005	5	27516.33	122.7778

CHAMBER CONCENTRATION CALCULATIONS:

Chamber Volume (Ft^3):	830.36
Chamber Volume (l):	23516.28
Flow through chamber with door closed (cfm):	713
Amount of liquid required to give chamber concentration of 1/2 LEL if complete evaporation occurs (ml):	1042.166

TABLE 27A: MIRAN CALIBRATION CALCULATIONS & PHYSICAL DATA
HEXANE

Wavelength (um)	3.4
Pathlength (m)	0.75
Slit Width (mm)	2
Molecular Weight (g/mole):	86.18
Density (g/ml):	0.661
Molar Volume (l/mole):	24.20512
Volume of Flask (l):	2.23
Temperature (C):	22
Vapor Pressure at given temperature (psia):	2.567920
Maximum Concentration at Equilibrium (ppm):	174688.4
Lower Explosive Limit (ppm):	11000
MIRAN Volume (l):	5.64

PPM CALCULATIONS FOR FLASK:

Amount of Liquid injected into flask (ml):	Concentration of Vapor in flask (ppm):
0.5	41626.27

CONCENTRATION CALCULATIONS:

Amount of gas extracted & injected into MIRAN (l):		New concentration in flask in ppm:	Concentration in MIRAN in ppm:
0	ml	41626.27	0
0.002	2	41588.95	14.76108
0.002	2	41551.67	29.50894
0.002	2	41514.42	44.24357
0.003	3	41458.61	66.32571
0.004	4	41384.31	95.72898
0.004	4	41310.14	125.0795
0.004	4	41236.11	154.3775
0.004	4	41162.21	183.6230

CHAMBER CONCENTRATION CALCULATIONS:

Chamber Volume (Ft^3):	838.7
Chamber Volume (l):	23752.47
Flow through chamber with door closed (cfm):	713
Amount of liquid required to give chamber concentration of 1/2 LEL if complete evaporation occurs (ml):	703.6703

TABLE 28A: MIRAN CALIBRATION CALCULATIONS & PHYSICAL DATA
METHYLENE CHLORIDE

Wavelength (um):	13.3
Pathlength (m):	5.25
Slit Width (mm):	2
Molecular Weight (g/mole):	84.93
Density (g/ml):	1.325
Molar Volume (l/mole):	24.28717
Volume of Flask (l):	2.23
Temperature (C):	23
Vapor Pressure at given temperature (psia):	7.669125
Maximum Concentration at Equilibrium (ppm):	521709.2
Lower Explosive Limit (ppm):	120000
MIRAN Volume (l):	5.64

PPM CALCULATIONS FOR FLASK:

Amount of Liquid injected into flask (ml):	Concentration of Vapor in flask (ppm):
1	169913.1

CONCENTRATION CALCULATIONS:

Amount of gas extracted & injected into MIRAN (l):		New concentration in flask in ppm:	Concentration in MIRAN in ppm:
0	ml	169913.1	0
0.001	1	169836.9	30.12644
0.002	2	169684.7	90.35231
0.002	2	169532.5	150.5242
0.002	2	169380.6	210.6421
0.003	3	169152.9	300.7382
0.002	2	169001.2	360.7215

CHAMBER CONCENTRATION CALCULATIONS:

Chamber Volume (Ft^3):	830.36
Chamber Volume (l):	23516.28
Flow through chamber with door closed (cfm):	713
Amount of liquid required to give chamber concentration of 1/2 LEL if complete evaporation occurs (ml):	3723.815

TABLE 29A: MIRAN CALIBRATION CALCULATIONS & PHYSICAL DAT
MEK

Wavelength (um):	8.5
Pathlength (m):	18.75
Slit Width (mm):	2
Molecular Weight (g/mole):	72.11
Density (g/ml):	0.805
Molar Volume (l/mole):	24.09025
Volume of Flask (l):	2.23
Temperature (C):	20.6
Vapor Pressure at given temperature (psia):	1.413066
Maximum Concentration at Equilibrium (ppm):	96126.99
Lower Explosive Limit (ppm):	20000
MIRAN Volume (l):	5.64

PPM CALCULATIONS FOR FLASK:

Amount of Liquid injected into flask (ml):	Concentration of Vapor in flask (ppm):
0.4	48238.84

CONCENTRATION CALCULATIONS:

Amount of gas extracted & injected into MIRAN (l):		New concentration in flask in ppm:	Concentration in MIRAN in ppm:
0	ml	48238.84	0
0.001	1	48217.22	8.552987
0.002	2	48173.99	25.65129
0.002	2	48130.81	42.73427
0.002	2	48087.66	59.80193
0.002	2	48044.55	76.85429
0.002	2	48001.48	93.89137

CHAMBER CONCENTRATION CALCULATIONS:

Chamber Volume (Ft^3):	830.36
Chamber Volume (l):	23516.28
Flow through chamber with door closed (cfm):	713
Amount of liquid required to give chamber concentration of 1/2 LEL if complete evaporation occurs (ml):	874.4337

TABLE 30A: MIRAN CALIBRATION CALCULATIONS & PHYSICAL DATA
TOLUENE

Wavelength (um):	13.7
Pathlength (m):	11.25
Slit Width (mm):	2
Molecular Weight (g/mole):	92.14
Density (g/ml):	0.865
Molar Volume (l/mole):	24.20512
Volume of Flask (l):	2.23
Temperature (C):	22
Vapor Pressure at given temperature (psia):	0.470059
Maximum Concentration at Equilibrium (ppm):	31976.81
Lower Explosive Limit (ppm):	13000
MIRAN Volume (l):	5.64

PPM CALCULATIONS FOR FLASK:

Amount of Liquid injected into flask (ml):	Concentration of Vapor in flask (ppm):
0.15	15284.86

CONCENTRATION CALCULATIONS:

Amount of gas extracted & injected into MIRAN (l):		New concentration in flask in ppm:	Concentration in MIRAN in ppm:
0	ml	15284.86	0
0.002	2	15271.16	5.420165
0.004	4	15243.79	16.25077
0.004	4	15216.47	27.06198
0.004	4	15189.20	37.85381
0.004	4	15161.98	48.62630
0.004	4	15134.81	59.37948

CHAMBER CONCENTRATION CALCULATIONS:

Chamber Volume (Ft^3):	830.36
Chamber Volume (l):	23516.28
Flow through chamber with door closed (cfm):	713
Amount of liquid required to give chamber concentration of 1/2 LEL if complete evaporation occurs (ml):	672.6773

TABLE 31A: DATA USED TO CALCULATE VAPOR PRESSURES (FROM REFERENCE 5)

Formula Used: $\log P = A - (B/(T + C))$

Where: T = Ambient temperature in degrees Centigrade

P = Vapor pressure in mm Hg

The following constants were used:

ical Name	A	B	C
Acetone	7.11714	1210.595	229.664
Butyl Acetate	7.12712	1430.418	210.745
Ethyl Acetate	7.10179	1244.95	217.88
Hexane	6.87601	1171.17	224.41
Methylene Chloride	7.4092	1325.9	252.6
Toluene	6.95464	1344.8	219.48
MEK	7.06356	1261.34	221.97

TABLE 32A: VENTILATION SURVEY OF CHAMBER

CHAMBER DIMENSIONS

Width (in):	120
Length (in):	116.5
Height (in):	103.5

AIR VENT DIMENSIONS

Width (in):	4.125
Length (in):	14.125
Height (in):	103.5

CHAMBER AREA MINUS AIR VENT AREA (in^2)
13863.46

CHAMBER VOLUME (in^3)
1434869.

CHAMBER AREA (ft^2)
96.27408

CHAMBER VOLUME (ft^3)
830.3640

SURVEY DATA

Survey Point	Left Vent Velocity (fpm)	Right Vent Velocity (fpm)
1	750	800
2	650	700
3	650	650
4	700	700
5	560	600
6	480	500
7	450	500
8	550	500
9	400	500
10	200	380
11	400	340
12	450	350
13	250	400
14	180	320
15	250	240
16	350	200
17	300	400
18	250	320
19	300	150
20	300	150
Average Velocity (fpm):	421	435
Vent Area (ft^2):	0.833333	0.833333
Flow thru each vent (cfm):	350.8333	362.5
Total flow thru room (cfm):	713.3333	

TABLE 33A: ACETONE CHAMBER TEST DATA

Raw chamber data:

Time (min)	Absorbance Run 1	Temp	Absorbance Run 2	Temp
0	0.035	22.5	0.0335	22.4
1	0.0962	22.4	0.1033	22.4
2	0.1591	22.4	0.1948	22.4
3	0.1839	22.4	0.234	22.4
4	0.2011	22.4	0.2542	22.4
5	0.1917	22.4	0.2521	22.4
6	0.1947	22.4	0.2491	22.4
7	0.1964	22.4	0.2455	22.4
8	0.1818	22.4	0.243	22.4
9	0.1424	22.4	0.2417	22.4
10	0.0913	22.4	0.1673	22.4
11	0.06	22.4	0.1011	22.4
12	0.0433	22.4	0.0646	22.4
13	0.0355	22.4	0.0454	22.4
14	0.0319	22.4	0.0369	22.4
15	0.0303	22.4	0.0325	22.4
16			0.0302	22.4

Corrected Chamber Data and Resultant Concentrations Using MIRAN Calibration Curve:

Time (min)	Absorbance Run 1	Concentration in ppm:	Absorbance Run 2	Conc in ppm:
0	0.0065	3.8909	0.005	2.9930
1	0.0677	40.525	0.0748	44.776
2	0.1306	78.178	0.1663	99.548
3	0.1554	93.024	0.2055	123.01
4	0.1726	103.32	0.2257	135.10
5	0.1632	97.693	0.2236	133.84
6	0.1662	99.489	0.2206	132.05
7	0.1679	100.50	0.217	129.89
8	0.1533	91.766	0.2145	128.40
9	0.1139	68.181	0.2132	127.62
10	0.0628	37.592	0.1388	83.087
11	0.0315	18.856	0.0726	43.459
12	0.0148	8.8594	0.0361	21.609
13	0.007	4.1902	0.0169	10.116
14	0.0034	2.0352	0.0084	5.0283
15	0.0018	1.0774	0.004	2.3944
16			0.0017	1.0176

TABLE 34A: CHAMBER TEST DATA - BUTYL ACETATE

Raw chamber data:

Time (min)	Absorbance Run 1	Temp (C)	Absorbance Run 2	Temp (C)
0	0.0141	20.6	0.0161	20.4
1	0.021	20.5	0.0597	20.4
2	0.0671	20.6	0.0977	20.4
3	0.1013	20.5	0.1144	20.4
4	0.1081	20.5	0.1225	20.4
5	0.1161	20.6	0.1372	20.4
6	0.1196	20.5	0.1418	20.6
7	0.1192	20.5	0.142	20.5
8	0.1216	20.5	0.1401	20.4
9	0.1235	20.5	0.1427	20.5
10	0.123	20.5	0.1386	20.4
11	0.12	20.6	0.1127	20.4
12	0.1003	20.5	0.07	20.4
13	0.064	20.4	0.0429	20.4
14	0.037	20.4	0.0271	20.3
15	0.0243	20.4	0.0189	20.4
16	0.0186	20.4	0.0151	20.5
17	0.0155	20.4		
18	0.0144	20.4		

Time (min)	Corrected Raw Data: Run 1	Concentration in ppm:	Corrected Raw Data: Run 2	Concentration in ppm:
0	0	0	0.0019	0.2599
1	0.0068	0.9304	0.0455	6.2258
2	0.0529	7.2383	0.0835	11.425
3	0.0871	11.918	0.1002	13.710
4	0.0939	12.848	0.1083	14.818
5	0.1019	13.943	0.123	16.830
6	0.1054	14.422	0.1276	17.459
7	0.105	14.367	0.1278	17.487
8	0.1074	14.695	0.1259	17.227
9	0.1093	14.955	0.1285	17.582
10	0.1088	14.887	0.1244	17.021
11	0.1058	14.476	0.0985	13.477
12	0.0861	11.781	0.0558	7.6351
13	0.0498	6.8141	0.0287	3.9270
14	0.0228	3.1197	0.0129	1.7651
15	0.0101	1.3819	0.0047	0.6431
16	0.0044	0.6020	0.0009	0.1231
17	0.0013	0.1778		
18	0.0002	0.0273		

TABLE 35A: CHAMBER TEST DATA – ETHYL ACETATE

Raw chamber data:

Time (min)	% Absorbance Run 1	Temp (C)	% Absorbance Run 2	Temp (C)
0	0.0314	22.5	0.0327	22.4
1	0.1281	22.4	0.262	22.4
2	0.3784	22.4	0.5209	22.4
3	0.4809	22.4	0.6092	22.4
4	0.5076	22.5	0.6521	22.4
5	0.5157	22.5	0.6562	22.4
6	0.5328	22.4	0.6519	22.4
7	0.568	22.4	0.6509	22.4
8	0.5412	22.4	0.6461	22.4
9	0.5347	22.4	0.6308	22.4
10	0.5148	22.4	0.6359	22.4
11	0.4051	22.4	0.5419	22.4
12	0.2563	22.4	0.3556	22.4
13	0.1443	22.4	0.2022	22.4
14	0.0893	22.5	0.12	22.4
15	0.0599	22.4	0.0772	22.4
16	0.0446	22.4	0.0542	22.4
17	0.0374	22.5	0.0427	22.4
18	0.0338	22.5	0.0374	22.4
19	0.0327	22.6	0.0347	22.4
20			0.0332	22.4
21			0.0324	22.4

Time (min)	Corrected Raw Data: Run 1	Concentration in ppm:	Corrected Raw Data: Run 2	Concentration in ppm:
0	0	0	0.0013	0.1988
1	0.0967	14.789	0.2306	35.267
2	0.347	53.070	0.4895	74.863
3	0.4495	68.746	0.5778	88.368
4	0.4762	72.829	0.6207	94.929
5	0.4843	74.068	0.6248	95.556
6	0.5014	76.683	0.6205	94.899
7	0.5366	82.067	0.6195	94.746
8	0.5098	77.968	0.6147	94.012
9	0.5033	76.974	0.5994	91.672
10	0.4834	73.931	0.6045	92.452
11	0.3737	57.153	0.5105	78.075
12	0.2249	34.396	0.3242	49.583
13	0.1129	17.266	0.1708	26.122
14	0.0579	8.8552	0.0886	13.550
15	0.0285	4.3587	0.0458	7.0046
16	0.0132	2.0188	0.0228	3.4870
17	0.006	0.9176	0.0113	1.7282
18	0.0024	0.3670	0.006	0.9176
19	0.0013	0.1988	0.0033	0.5047
20			0.0018	0.2752
21			0.001	0.1529

TABLE 36A: CHAMBER TEST DATA – HEXANE

Raw chamber data:

Time (min)	Absorbance Run 1	Temp (C)	Absorbance Run 2	Temp (C)
0	0.0114	22	0.0162	22.1
1	0.012	22	0.0265	22
2	0.0243	22	0.0423	22.1
3	0.0414	21.9	0.0524	22.1
4	0.0544	22	0.0581	22.1
5	0.0549	22	0.059	22.1
6	0.0565	22	0.0592	22.1
7	0.0565	22	0.0583	22.1
8	0.0569	22	0.0549	22.1
9	0.0557	22	0.0395	22.1
10	0.035	22	0.0258	22.1
11	0.0231	22	0.0179	22.1
12	0.0172	22.1	0.0143	22.1
13	0.0141	22.1	0.0127	22.1
14	0.0127	22	0.0121	22.1
15	0.012	22.1		

Time (min)	Corrected Raw Data: Run 1	Concentration in ppm:	Corrected Raw Data: Run 2	Concentration in ppm:
0	0	0	0.0048	13.291
1	0.0006	1.6614	0.0151	41.812
2	0.0129	35.720	0.0309	85.563
3	0.03	83.071	0.041	113.53
4	0.043	119.06	0.0467	129.31
5	0.0435	120.45	0.0476	131.80
6	0.0451	124.88	0.0478	132.36
7	0.0451	124.88	0.0469	129.86
8	0.0455	125.99	0.0435	120.45
9	0.0443	122.66	0.0281	77.810
10	0.0236	65.349	0.0144	39.874
11	0.0117	32.397	0.0065	17.998
12	0.0058	16.060	0.0029	8.0302
13	0.0027	7.4764	0.0013	3.5997
14	0.0013	3.5997	0.0007	1.9383
15	0.0006	1.6614		

TABLE 37A: CHAMBER TEST DATA - METHYLENE CHLORIDE

Raw chamber data:

Time (min)	Absorbance Run 1	Temp (C)	Absorbance Run 2	Temp (C)
0	0.0228	20.1	0.0233	19.9
1	0.1242	20.1	0.1989	20.1
2	0.2527	20.1	0.4141	20.3
3	0.3055	20	0.5157	20.3
4	0.3381	20	0.5989	20.5
5	0.3577	20	0.615	20.6
6	0.35	20	0.6224	20.7
7	0.368	20	0.6356	20.8
8	0.3753	20.1	0.6449	20.8
9	0.3755	20.1	0.6368	20.9
10	0.3194	20	0.5594	20.9
11	0.1819	20	0.3374	20.9
12	0.1037	19.9	0.1771	20.9
13	0.0563	20.1	0.0979	21
14	0.0345	20	0.057	21
15	0.0242	20	0.0353	21
16	0.019	20.1	0.0246	21.1
17	0.0174	20.1	0.0191	21.2
18			0.0165	21.3

Time (min)	Corrected Raw Data: Run 1	Concentration in ppm:	Corrected Raw Data: Run 2	Concentration in ppm:
0	0.0068	2.8741	0.0073	3.0854
1	0.1082	45.732	0.1829	77.306
2	0.2367	100.04	0.3981	168.26
3	0.2895	122.36	0.4997	211.20
4	0.3221	136.14	0.5829	246.37
5	0.3417	144.42	0.599	253.17
6	0.334	141.17	0.6064	256.30
7	0.352	148.77	0.6196	261.88
8	0.3593	151.86	0.6289	265.81
9	0.3595	151.94	0.6208	262.39
10	0.3034	128.23	0.5434	229.67
11	0.1659	70.120	0.3214	135.84
12	0.0877	37.068	0.1611	68.092
13	0.0403	17.033	0.0819	34.616
14	0.0185	7.8193	0.041	17.329
15	0.0082	3.4658	0.0193	8.1575
16	0.003	1.2680	0.0086	3.6349
17	0.0014	0.5917	0.0031	1.3102
18			0.0005	0.2113

TABLE 38A: CHAMBER TEST DATA – MEK

	Raw chamber data:			
Time (min)	Absorbance Run 1	Temp (C)	Absorbance Run 2	Temp (C)
0	0.0176	20.4	0.0305	20.6
1	0.0793	20.4	0.1243	20.5
2	0.1472	20.4	0.1961	20.4
3	0.1811	20.4	0.2287	20.6
4	0.196	20.4	0.251	20.7
5	0.1897	20.4	0.2504	20.8
6	0.1887	20.4	0.2589	20.8
7	0.1944	20.4	0.2582	20.8
8	0.1955	20.3	0.2514	20.9
9	0.154	20.3	0.1945	20.8
10	0.0914	20.4	0.1173	20.9
11	0.0537	20.4	0.0678	20.9
12	0.0355	20.3	0.0414	21
13	0.0269	20.4	0.0298	21
14	0.0224	20.4	0.0238	21.1
15	0.0203	20.4	0.0207	21.3
16			0.0192	21.2

Time (min)	Corrected Raw Data: Run 1	Concentration in ppm:	Corrected Raw Data: Run 2	Concentration in ppm:
0	0.0006	0.2506	0.0135	5.6390
1	0.0623	26.022	0.1073	44.819
2	0.1302	54.385	0.1791	74.810
3	0.1641	68.545	0.2117	88.428
4	0.179	74.769	0.234	97.742
5	0.1727	72.137	0.2334	97.492
6	0.1717	71.719	0.2419	101.04
7	0.1774	74.100	0.2412	100.75
8	0.1785	74.560	0.2344	97.909
9	0.137	57.225	0.1775	74.142
10	0.0744	31.077	0.1003	41.895
11	0.0367	15.329	0.0508	21.219
12	0.0185	7.7275	0.0244	10.191
13	0.0099	4.1352	0.0128	5.3466
14	0.0054	2.2556	0.0068	2.8403
15	0.0033	1.3784	0.0037	1.5455
16			0.0022	0.9189

TABLE 39A: CHAMBER TEST DATA – TOLUENE

Raw chamber data:

Time (min)	Absorbance Run 1	Temp (C)	Absorbance Run 2	Temp (C)
0	0.034	22.1	0.0292	22.3
1	0.0628	22.2	0.0422	22.3
2	0.0814	22.2	0.0627	22.4
3	0.0837	22.2	0.0765	22.4
4	0.0832	22.2	0.081	22.3
5	0.0802	22.2	0.0842	22.3
6	0.0783	22.2	0.0873	22.3
7	0.0771	22.2	0.0878	22.4
8	0.0603	22.2	0.0888	22.4
9	0.0437	22.3	0.0824	22.4
10	0.0347	22.3	0.0586	22.4
11	0.0302	22.3	0.0413	22.4
12	0.0282	22.3	0.0332	22.4
13	0.0273	22.3	0.0294	22.4
14			0.0276	22.4

Time (min)	Corrected Raw Data: Run 1	Concentration in ppm:	Corrected Raw Data: Run 2	Concentration in ppm:
0	0.0074	7.3162	0.0026	2.5705
1	0.0362	35.790	0.0156	15.423
2	0.0548	54.179	0.0361	35.691
3	0.0571	56.453	0.0499	49.335
4	0.0566	55.959	0.0544	53.784
5	0.0536	52.993	0.0576	56.948
6	0.0517	51.114	0.0607	60.012
7	0.0505	49.928	0.0612	60.507
8	0.0337	33.318	0.0622	61.496
9	0.0171	16.906	0.0558	55.168
10	0.0081	8.0083	0.032	31.637
11	0.0036	3.5592	0.0147	14.533
12	0.0016	1.5818	0.0066	6.5253
13	0.0007	0.6920	0.0028	2.7683
14			0.001	0.9886

TABLE 40A: Predicted Evaporation Rate Data Using the Kawamura-Mackay Model

Velocity (fpm)	Acetone	Butyl Acetate	Ethyl Acetate	Hexane	Methylene Chloride	MEK	Toluene
65	0.002417	0.000562	0.002166	0.002929	0.005104	0.001686	0.000961
110	0.003237	0.000804	0.002960	0.003938	0.006724	0.002297	0.001355
220	0.004876	0.001303	0.004526	0.006014	0.010032	0.003539	0.002151
300	0.005931	0.001631	0.005553	0.007326	0.012163	0.004346	0.002668
425	0.007469	0.002103	0.007018	0.009236	0.015262	0.005496	0.003392

Acetone Regression Output:		Butyl Acetate Regression Output:	
Constant	0.001659	Constant	0.000325
Std Err of Y Est	0.000150	Std Err of Y Est	0.000041
R Squared	0.995888	R Squared	0.996612
No. of Observations	5	No. of Observations	5
Degrees of Freedom	3	Degrees of Freedom	3
X Coefficient(s)	0.000013	X Coefficient(s)	0.000004
Std Err of Coef.	0.000000	Std Err of Coef.	0.000000

Hexane Regression Output:		Ethyl Acetate Regression Output:	
Constant	0.001979	Constant	0.001441
Std Err of Y Est	0.000192	Std Err of Y Est	0.000146
R Squared	0.995685	R Squared	0.995771
No. of Observations	5	No. of Observations	5
Degrees of Freedom	3	Degrees of Freedom	3
X Coefficient(s)	0.000017	X Coefficient(s)	0.000013
Std Err of Coef.	0.000000	Std Err of Coef.	0.000000

Toluene Regression Output:		Meth Chloride Regression Output:	
Constant	0.000597	Constant	0.003562
Std Err of Y Est	0.000077	Std Err of Y Est	0.000292
R Squared	0.995298	R Squared	0.996164
No. of Observations	5	No. of Observations	5
Degrees of Freedom	3	Degrees of Freedom	3
X Coefficient(s)	0.000006	X Coefficient(s)	0.000028
Std Err of Coef.	0.000000	Std Err of Coef.	0.000001

MEK Regression Output:	
Constant	0.001111
Std Err of Y Est	0.000113
R Squared	0.995878
No. of Observations	5
Degrees of Freedom	3
X Coefficient(s)	0.000010
Std Err of Coef.	0.000000