TECHNICAL NOTE

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The Elimination Rate of Mouth Alcohol: Mathematical Modeling and Implications in Breath Alcohol Analysis

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ABSTRACT: Mouth alcohol, if present in high enough concentrations, can falsely bias the accurate measurement of end-expiratory breath alcohol. Mouth alcohol will be eliminated over time, however, and can be modeled with a single term decaying exponential of the form: $B_0e^{-kt} + C$. It is important, however, to determine the model and its parameters when alcohol is already present within the biologic system. Using three individuals as their own controls, mouth alcohol was administered both before and after alcohol consumption followed by breath alcohol analysis performed at approximately 0.5 min intervals. The results showed that both model parameters (B_0 and k) are effected and that the asymptotic value (C) is reached much sooner when alcohol already exists in the end-expiratory breath. Considering only three individuals were involved, the forensic-science importance appears to be that, as the end-expiratory breath alcohol concentration increases, the time necessary for the mouth alcohol to decrease to unbiased levels is decreased. Fifteen min of observation time prior to breath alcohol analysis appears to be more than adequate at forensically relevant concentrations.

KEYWORDS: toxicology, alcohol, breath-alcohol analysis, mathematical modeling

Accuracy and precision are fundamental to the forensic-science as well as clinical and research applications of breath alcohol analysis. One factor that can bias the accurate measurement of end-expiratory breath alcohol concentration (BrAC) is the presence of "mouth alcohol" or residual unabsorbed alcohol within the oropharynx cavity. Mouth alcohol can arise from a variety of sources such as recent ingestion, regurgitation, foreign matter, etc. [*1*]. Most jurisdictions incorporate observation and time deprivation protocol to guard against this condition.

This issue of "mouth alcohol" has been investigated by others but typically with subjects having no alcohol in their systems [*2,3*]. It needs to be understood that only those alcohol concentrations within the oral cavity that exceed that of the true end-expiratory BrAC are of concern. Only in this condition could it falsely increase the true end-expiratory result and be of forensic concern. Concentrations below that of the end-expiratory value are of little forensic concern because a mixing, not additive, effect occurs.

The elimination of mouth alcohol over time follows a fairly predictable first-order single term exponential model. This was previously shown by Dubowski following logarithmic transformation of the data [*4*]. Accurate determination of model parameters,

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however, should employ nonlinear regression. Once accurate parameters can be determined, the influence of biological and procedural factors on model performance can be assessed.

The model parameters vary significantly depending on whether alcohol exists in the biological system and a true end-expiratory BrAC can be established. Using individuals as their own controls and providing mouth alcohol both prior to and following alcohol consumption reveals model differences. The purpose of this study was to describe the model obtained from both conditions and discuss their forensic significance. It is important that mouth alcohol be evaluated with alcohol already present in the biological system since this best reflects the actual law enforcement and forensic context. It is demonstrated that as the true end-expiratory BrAC increases, the time necessary for mouth alcohol to be eliminated to a insignificant concentration decreases.

Methods

Three male volunteers were the subjects for the study. Prior to consuming an alcoholic beverage, each subject was instructed to rinse the mouth with approximately 5 mL of an 80 proof alcoholic beverage. They did so for approximately 10 s and then expelled the beverage. The time of expelling became the reference ($t = 0$) for subsequent measurement and modeling purposes since the intent was to evaluate the rate at which alcohol clears itself from within the oral cavity. (The value $t = 0$ in Fig. 2 refers to the time of expelling the rinsed beverage.)

The subjects then began to provide breath samples into a BAC Verifier Datamaster infrared breath alcohol instrument (National Patent Analytical Systems, Inc., Mansfield, Ohio). The times between expelling the sample and the first measurement varied between and within subjects but were recorded in each case. The subjects were instructed to simply provide a short exhalation of only 2 to 3 s since the purpose was to obtain that initial maximum BrAC produced within the oral cavity and provided early in the exhalation profile that could potentially bias a BrAC measurement. Although this did not accurately reflect the forensic breath alcohol measurement context where full end-expiratory samples are requested, it was selected to obtain the maximum concentrations that could potentially bias the results. The other reason for providing a short sample was to prevent the instrument's sampling parameters (one of which is 5 s minimum exhalation) from being met and have it accept the sample. This would cause the instrument to proceed to its purge phase and prevent the continuous sampling rate of exhalations every 0.5 min.

The measurements from the BAC Verifier Datamaster were collected and recorded by means of a data acquisition system consisting of a Commodore 64 computer with associated hardware and software. The computer was connected to the instrument by means of a data acquisition board consisting of an analog-to-digital converter [5]. The analog signal from the instrument consisted of a final processed voltage (0 to 2 VDC) taken from its detector board. None of the measurements, therefore, were processed through the instrument's analog-to-digital conversion or mathematical algorithms. The data acquisition computer contained an algorithm analogous to that in the instrument and sampled the data at approximately 4 Hz, the same as the instrument performs. In this way each subject's breath alcohol profile was retained on a disk for subsequent analysis.

Figure 1 shows a short exhalation profile from one of the subjects which contained mouth alcohol. The peak value in each of the profiles was used for modeling purposes since this best approximated the maximum BrAC that could be obtained due to the presence of mouth alcohol. When the maximum value existed near the end of the data stream, this value was rejected since by this time the subject was no longer exhaling and simply noise was present. The peak value was obtained from that first 2 to 3 s when the subject was presumably exhaling.

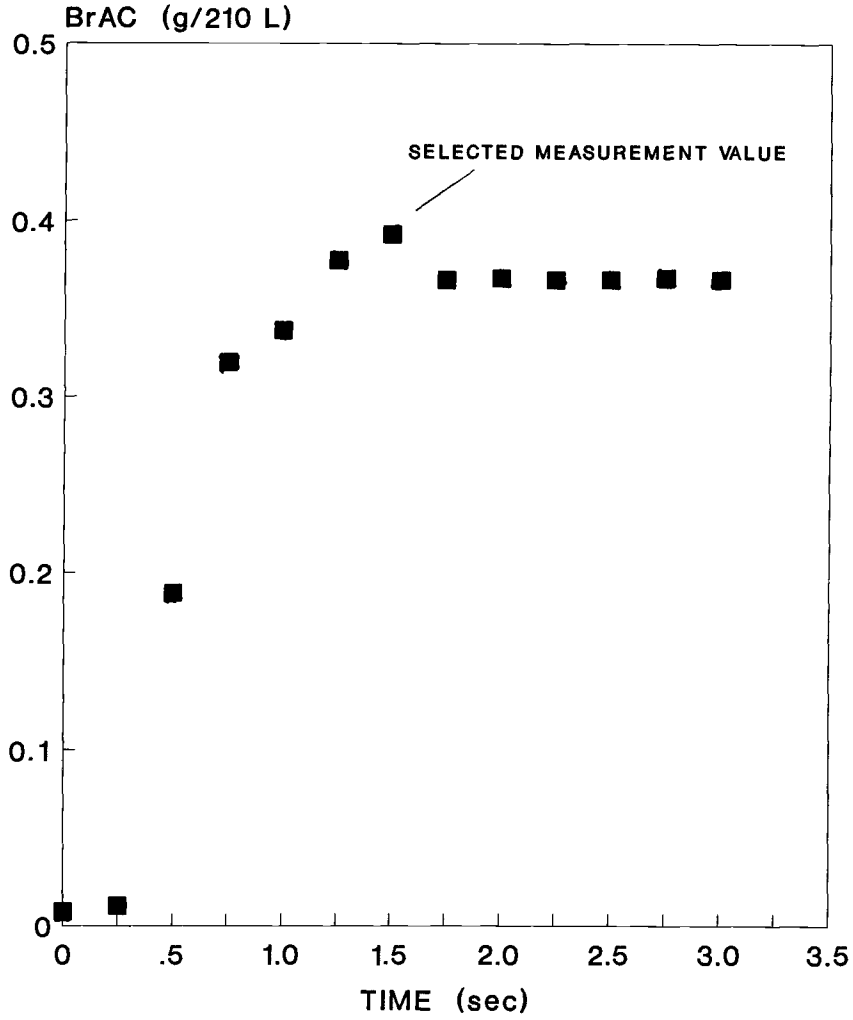

FIG. 1—*Example of a short breath alcohol exhalation profile showing the maximum measurement retained for modeling purposes.*

Following the expelling of the alcoholic beverage the subjects provided the short breath samples approximately every 30 s for nearly 14 min for subject 1 and nearly 10 min for subjects 2 and 3. Between the subject's sequential samples, the instrument's sample chamber was cleared with the alcohol-free breath of the individual collecting the data and operating the instrument and computer. During the entire time of approximately 10 to 14 min the data acquisition system collected data at the 4 Hz rate. This provided approximately 28 measurements for subject 1 and 20 measurements for subjects 2 and 3 saved to a disk for subsequent analysis. All measurements were truncated to three decimal places and reported as g/210 L of breath.

After providing the initial set of mouth alcohol measurements the subjects began to consume alcoholic beverages. After consuming the beverages the subjects provided ten end-expiratory breath samples beginning not less than 50 min after the last drink. These ten samples were also collected through the data acquisition system to allow for comparison with the mouth alcohol measurements and ranged from 12 to 15 min between the three subjects to complete. Not all of the ten samples provided by each subject met

the instrument's sampling criteria but were manually accepted by means of a "NOVOL" device, which causes the instrument to immediately accept the sample. The "NOVOL" switch causes the instrument to override its sampling parameter requirements of minimum exhalation time, flow rate, and mathematical slope requirements. Each of these samples were being collected by the data acquisition system as well and were therefore used in the analysis since they approximated end-expiratory samples and in every case equalled or exceeded 6.5 s of continuous exhalation. The mean and standard deviation of these ten measurements were then computed for the purpose of determining the individual's actual BrAC at that time.

Each subject was again given approximately 5 mL of 80 proof alcoholic beverage to rinse in the mouth and expel. Again they began to provide short breath samples approximately 30 s apart in the same manner as previously described. This continued again for approximately 14 min and 10 min for the three subjects with the data being retained on disk for subsequent analysis.

Due to the reference voltage in the computer's analog-to-digital conversion circuit the maximum BrAC that could be computed was approximately 0.42 to 0.45 g/210 L. This meant that these first data values employed in subsequent modeling may have had significant error associated with them. Only the first data value in each curve would have been affected since only one was retained. Thereafter, the BrAC was below the conversion scale maximum.

It was assumed that the values decreased over time in accordance with a single-term exponential decay model of the general form:

$$BrAC = B_0 e^{-kt} \tag{1}$$

where

B_0 = Extrapolated intercept value at $t = 0$
k = First order elimination rate constant (min^{-1})

Equation 1 describes the model prior to alcohol consumption. Following alcohol consumption the model was assumed to have the general form:

$$BrAC = B_0 e^{-kt} + C \tag{2}$$

where

C = Mean of ten BrAC measurements

From Eqs 1 and 2 the linear semilog plots were determined with B_0 and k being estimated from the intercept and slope respectively. These initial estimates of B_0 and k were then used in a nonlinear regression program (SPSS/PC+ Advanced Statistics, SPSS, Inc., Chicago) employing the Levenberg-Marquardt Algorithm [*6,7*]. From the nonlinear regression method, implying nonlinear in the parameters [*8*], the final model parameters were determined for each subject's mouth alcohol elimination curve.

Results

Figure 2 shows the mouth alcohol elimination profiles both prior to and following alcohol consumption for each of the three subjects. Figure 2 also shows the exponential functions that best describe the data following the non-linear regression procedure.

The two horizontal lines observed in the graphs on the right side of Fig. 2 represent the mean ± 3 SD for the ten consecutive breath samples provided after alcohol consumption. The mean is the constant term in their respective exponential functions and represents the asymptote toward which the model approaches. Data values that fell below

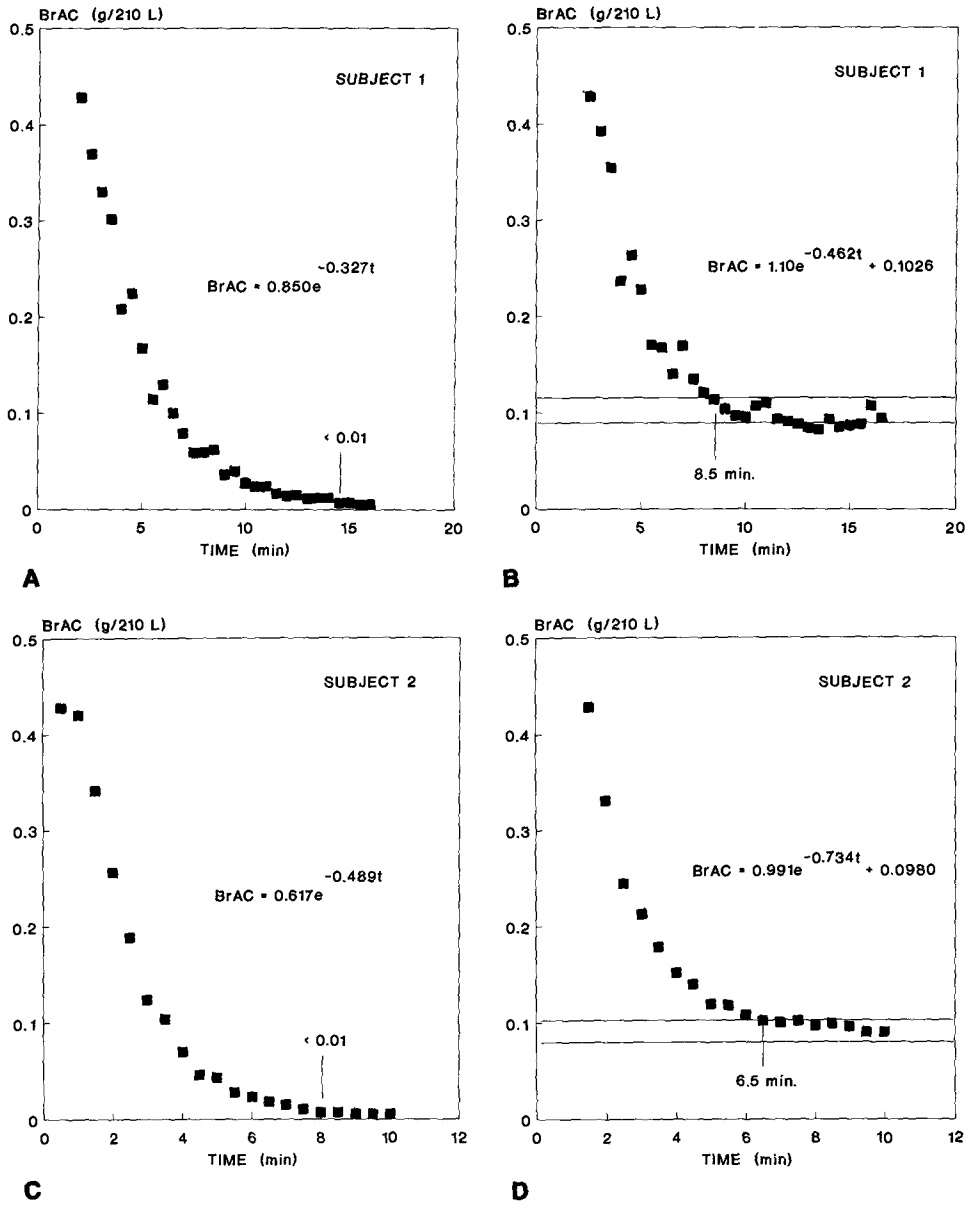

FIG. 2—*The mouth alcohol elimination curves for each subject prior to alcohol consumption* (left) *and following alcohol consumption* (right).

the mean or constant term and beyond were not used since this would result in taking the natural log of some negative values (impossible mathematically) upon transformation. The data on the left side of Fig. 2 approach the asymptotic value of zero and therefore all points were used in estimating the model since, of course, none fell below zero.

Figure 3 shows the logarithmic transformation and plot for subject 1 under both experimental conditions. It was the slope and intercept values of these curves that provided the initial estimates for nonlinear regression and eventual parameter determination. The differences in the curves due to the different experimental conditions are apparent.

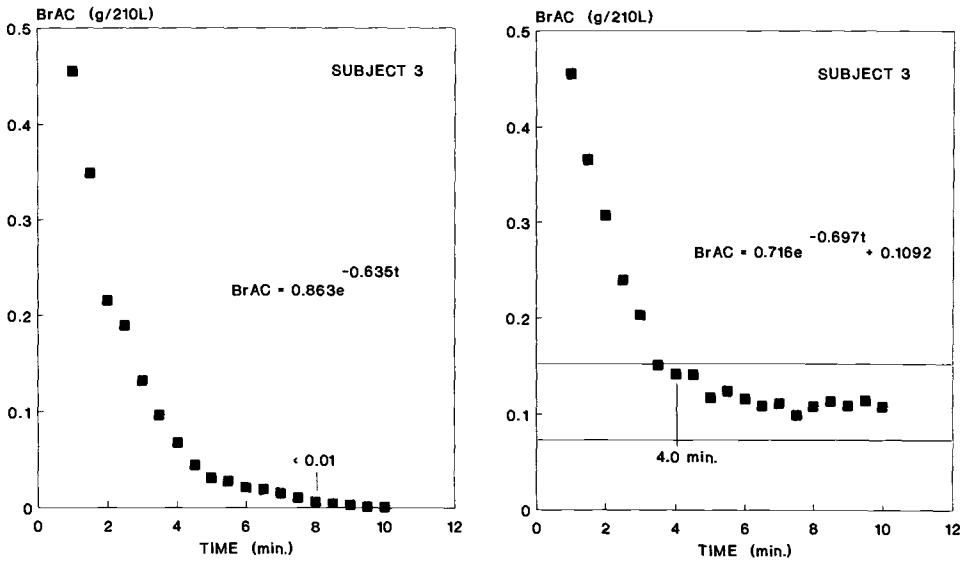

FIG. 2—*Continued*

Table 1 shows the parameter estimates for the two models from each of the three subjects. The initial estimates from log transformation are shown along with the fitted estimates from nonlinear regression. It is observed that the coefficients B_0 and k for all subjects following alcohol consumption are not necessarily similar but are in all cases larger than the coefficients preceding alcohol consumption. The estimated and fitted parameters provide a basis for comparing the two methods of estimation. In addition, Table 1 shows the coefficient of determination (R^2), which is an estimate of the degree to which the data fits the model [*9*]. R^2 can be computed in a variety of ways, although SPSS/PC+ appears to use one of the preferred algorithms [*10,11*]. All models show very good fit to the data, although it is recognized that the same data was used to both estimate the parameters and determine their degree of fit.

Table 2 shows the times at which nonbiasing results were obtained under both experimental conditions. The absolute as well as percent differences are shown.

Discussion

Mathematical Modeling

Although the method of log transformation and linear estimation is easy to perform it is generally less accurate than a nonlinear regression method for parameter estimation and should be approached with caution [*8*]. Natural log transformation produces a linear relationship which, when applying simple linear regression, assumes an equal and normal [*12*] error distribution around the fitted line throughout the range. Transforming data does not transform the error distribution in the same way and introduces bias in the analysis [*12*]. Nonlinear regression, which fits the data to an assumed model, uses a least-squares method and leaves the data in their original scale. Data transformation methods provide good initial estimates for nonlinear methods and where only one exponential term is involved the required accuracy of initial estimates is reduced [*13*].

Frequent data sampling during rapidly changing portions of the curve are usually necessary for adequate modeling and parameter estimation [*4*]. In order to compare the effect of 1 min sampling intervals, the data from subject 1 was reduced to approximately 1 min intervals beginning with the same initial value (0.428 g/210 L) for both the before drinking and after drinking conditions. The resulting exponential models were:

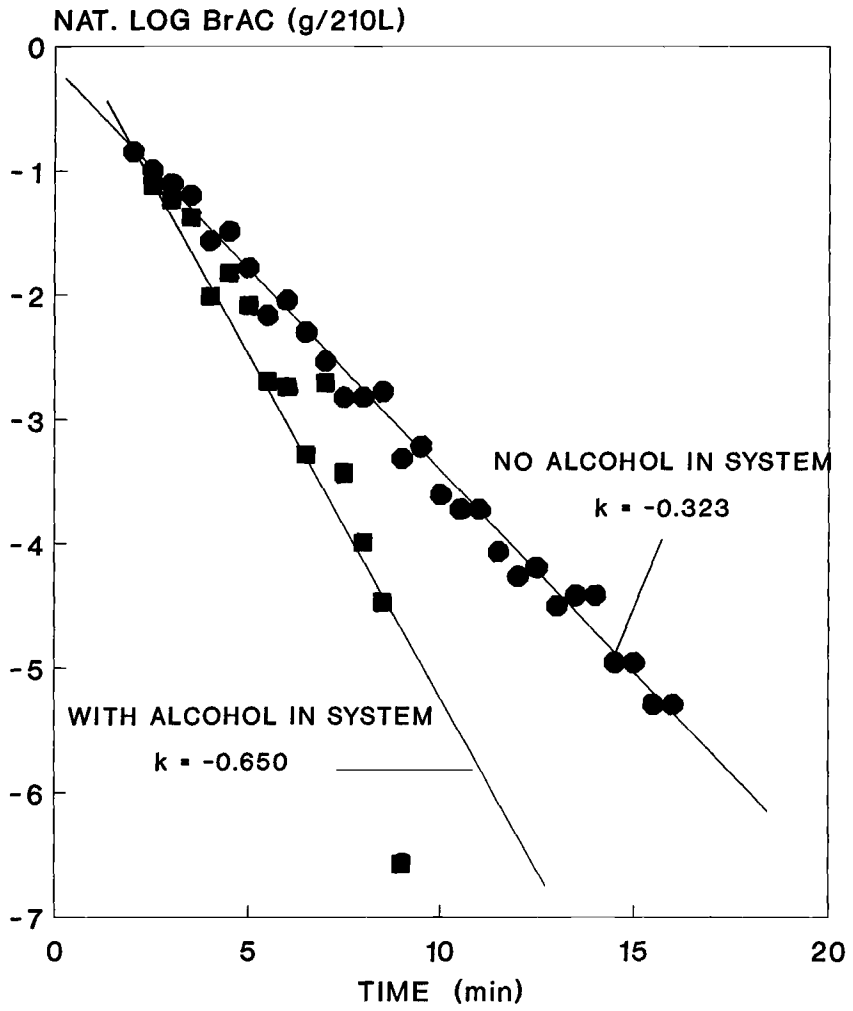

FIG. 3—*The logarithmic transformation and plot of both curves for subject 1 used to determine initial parameter estimates.*

Before drinking (1 minute interval): $0.838e^{-0.329t}$ ($R^2 = 0.996$)

Before drinking (0.5 minute interval): $0.850e^{-0.327t}$ ($R^2 = 0.991$)

After drinking (1 minute interval): $1.06e^{-0.449t} + 0.1026$ ($R^2 = 0.969$)

After drinking (0.5 minute interval): $1.10e^{-0.462t} + 0.1026$ ($R^2 = 0.961$)

It is observed that the values for B_0 and k change very little when sampling occurs at one instead of 0.5 min intervals and appear adequately approximated. In some modeling circumstances it has been shown that increasing the number of data points do not necessarily improve the parameter estimate [*15*]. It is recommended, however, that where possible, 0.5 min sampling intervals occur with mouth alcohol elimination data when the objective is accurate model estimation.

Some kinetic models follow sums of decaying exponentials including two or three terms. Figure 3 reveals a fairly linear relationship throughout all of the data suggesting a single-term exponential best describes the relationship. A combination of linear and curvilinear

TABLE 1—*Summary of model parameters for all subjects prior to and following alcohol consumption.*

	Subject 1		Subject 2		Subject 3	
	Without Alcohol	With Alcohol	Without Alcohol	With Alcohol	Without Alcohol	With Alcohol
Estimated B_0	0.810	2.49	0.621	0.374	0.949	0.889
Fitted B_0	0.850	1.10	0.617	0.991	0.863	0.716
Estimated k	−0.323	−0.650	−0.529	−0.831	−0.653	−0.812
Fitted k	−0.327	−0.462	−0.489	−0.734	−0.635	−0.697
R^2	0.991	0.961	0.976	0.998	0.996	0.990
n	29	14	20	13	19	11
Ten Tests:						
Mean		0.1026		0.0980		0.1092
SD		0.0050		0.0029		0.0127

NOTE: The estimated parameters are derived from simple natural log transformation.
The fitted parameters are derived from nonlinear regression estimation.
R^2—The coefficient of determination.

TABLE 2—*Times for mouth alcohol to eliminate to nonbiasing concentrations under the two testing conditions.*

Subject	Without Alcohol (Min)	With Alcohol (Min)	Difference (Min)	Difference (Percent)
1	14.5	8.5	6.0	41.4
2	8.0	6.5	1.5	18.8
3	8.0	4.0	4.0	50.0

portions to the logarithmic transformation in Fig. 3 would suggest more than one exponential term in the model [*16*].

Exponential models, as opposed to polynomial ones, have mathematical advantage and wide physiologic applications with the parameters usually of biologic importance [*17*]. With only three subjects it is difficult to assess the intersubject variability of the parameters and further work needs to be done here. B_0 is the parameter representing the maximum BrAC, due to the presence of mouth alcohol, that can occur at $t = 0$. B_0 would be most accurately determined if the instrument were capable of measuring near 1.0 g/210 L and the individual began exhaling immediately after expelling the alcoholic beverage. It is difficult to say whether inter or intrasubject biological variability contributes to differences in B_0. The parameter k reflects the rate at which the measurements approach their asymptotic value with the shorter times being reflected by larger absolute values. It is clearly apparent that when alcohol exists in the end expiratory breath, k is significantly affected. Some factors that may influence B_0 and k are surface area of the oral cavity, whether breathing occurs through the mouth or nasal passages, respiratory rate, type of alcoholic beverage, and the true end expiratory BrAC. Each of these factors requires further work and consideration.

Further parameters of interest in this type of analysis may be the time constant τ $\left(\tau = \frac{1}{k}\right)$ and the half lives $\left(t_{1/2} = \frac{\ln 2}{k}\right)$ of elimination. Time constants and half lives are both seen to decrease when alcohol exists in the end-expiratory breath. The large between-subject variability in the parameter k would appear to preclude the use of time constants or half-lives in distinguishing whether alcohol existed in the system. Different experimental design may reduce this between-subject variability.

Forensic-Science Considerations

The result of greatest forensic significance is the reduced time required to reach the asymptotic concentration when alcohol exists in the biologic system (Table 2). This is the condition of most individuals arrested for driving while intoxicated (DWI) offenses. In all subjects, the time required to reach the asymptote plus 3 SD was greatly reduced when end-expiratory BrAC existed (Table 2). It should be noted that this time is also influenced by the variability of the ten breath measurement and the resulting ± 3 SD interval. An observation period of 15 min appears to be more than adequate to ensure mouth alcohol will not bias the result when a true end-expiratory BrAC near 0.10 g/210 L exists.

When a breath alcohol measurement falls below 3 SD above the asymptote (or C in Eq. 2) then it cannot be statistically distinguished from the individual's true population of BrAC values. This does not imply that there is no mouth alcohol present at this time but simply that it will not bias the true end-expiratory measurements. The forensic concern is not that all mouth alcohol is eliminated but simply that the true end expiratory BrAC is not falsely biased with large systemic error. For subject 1 the measured value of 0.114 g/210 L in Fig. 2 was the first value to fall below C + 3 SD and occurred at approximately 8.5 min after expelling. For the same subject in Fig. 2, prior to consuming alcohol, the same measurement occurred at approximately 5.5 min after expelling. This suggests that significant concentrations of mouth alcohol can exist at these times, yet be of no consequence if the true end expiratory BrAC is at or above these levels. This hypothesis, of course, needs to be further verified with a larger set of individuals.

It is further hypothesized, although not presently confirmed, that at higher end-expiratory breath alcohol concentrations the parameter k will be of a higher absolute value and the asymptotic value will be reached even sooner. As a result, the higher the true BrAC the less time is necessary to wait for the mouth alcohol to be eliminated to where it does not bias the end-expiratory result.

The mechanism involved appears to be a mixing and not additive effect between deep lung and mouth alcohol concentrations. A 0.10 g/210 L concentration in the oral cavity does not add to but in fact mixes with that coming from the distal portions of the respiratory tract. The oral cavity could simply be considered an extension of the respiratory tract which may also have a 0.10 g/210 L concentration and simply mix with that coming from other portions of the lungs. Multiple alveoli, each assumed to have 0.10 g/210 L of alcohol, do not add but mix as the breath exhalation is provided. The mixing of respiratory gases is known in other areas of respiratory physiology as well [*18–21*].

Finally, the exponential model supports the value of duplicate analyses in detecting the presence of biasing mouth alcohol. Duplicate breath samples administered approximately three minutes apart can detect significant differences during the rapidly changing portion of the elimination curve. Jurisdictions are encouraged to employ the quality control measures of both a 15 min observation period and duplicate analyses to best ensure that mouth alcohol does not bias the true end-expiratory BrAC in a forensic context.

Conclusions

The model describing the elimination rate of mouth alcohol is of forensic importance. The models are importantly different when alcohol exists in the biological system and a true underlying BrAC exists. The concern with mouth alcohol is that it may bias the true BrAC with the significant factors being time and end-expiratory value. As the true end expiratory BrAC increases, the time necessary to wait for mouth alcohol elimination appears to decrease as shown in the present study with only three subjects. Certainly further work needs to be done in this area including more subjects with different end-expiratory BrAC values. A 15 min observation period appears to be more than adequate

to prevent a biased measurement from mouth alcohol at forensically important levels. However, the forensic-science context of breath alcohol measurement demands that both an observation period and duplicate analyses be present to provide confidence in unbiased results.

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