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Estimating BrAC from Transdermal Alcohol Concentration Data Using the BrAC Estimator Software Program

Susan E. Luczak, Ph.D. and

Department of Psychology, University of Southern California

I. Gary Rosen, Ph.D.

Department of Mathematics, University of Southern California

Abstract

Background—Transdermal alcohol sensor (TAS) devices have the potential to allow researchers and clinicians to unobtrusively collect naturalistic drinking data for weeks at a time, but the transdermal alcohol concentration (TAC) data these devices produce do not consistently correspond with breath alcohol concentration (BrAC) data. We present and test the BrAC Estimator software, a program designed to produce individualized estimates of BrAC from TAC data by fitting mathematical models to a specific person wearing a specific TAS device.

Methods—Two TAS devices were worn simultaneously by one participant for 18 days. The trial began with a laboratory alcohol session to calibrate the model and was followed by a field trial with 10 drinking episodes. Model parameter estimates and fit indices were compared across drinking episodes to examine the calibration phase of the software. Software-generated estimates of Peak BrAC, time of peak BrAC, area under the BrAC curve were compared with breath analyzer data to examine the estimation phase of the software.

Results—In this single-subject design with breath analyzer peak BrAC scores ranging from .013 to .057, the software created consistent models for the two TAS devices, despite differences in raw TAC data, and was able to compensate for the attenuation of peak BrAC and latency of the time of peak BrAC that are typically observed in TAC data.

Conclusions—This software program represents an important initial step for making it possible for non-mathematician researchers and clinicians to obtain estimates of BrAC from TAC data in naturalistic drinking environments. Future research with more participants and greater variation in alcohol consumption levels and patterns, as well as examination of gain scheduling calibration procedures and nonlinear models of diffusion, will help to determine how precise these software models can become.

Keywords

transdermal alcohol sensor; transdermal alcohol concentration; real-time assessment; ecological momentary assessment; BrAC estimation

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Researchers and clinicians who wish to capture real-time levels of alcohol consumption currently have limited data collection method options. The use of a breath analyzer or a drinking diary during drinking episodes requires continuous active participation that increases participant burden and decreases the naturalism of the drinking environment. In addition, these methods are not appropriate for monitoring individuals who may not be motivated to give accurate accounts of their drinking. Even in motivated participants, such methods have the potential to produce inaccurate results, with breath analyzer readings being too high due to mouth alcohol, being too low due to not taking deep lung breaths, and failing to capture peak BrAC due to the time between measurements. Drinking diary inaccuracies are likely in those who are drinking in a manner where they cannot gauge the amount of alcohol they have consumed (e.g., mixed drinks, sharing pitchers, playing drinking games).

Transdermal alcohol sensor (TAS) devices, including the WrisTAS™ (Giner, Inc., Newton, MA), TAC® (BI, Inc., Boulder, CO), and SCRAM® (Alcohol Monitoring Systems, Inc., Denver, CO), offer a promising method for unobtrusively collecting continuous alcohol levels in naturalistic settings over long periods of time. Until now, however, these TAS devices have been used almost exclusively as abstinence monitors (see Marques and McKnight, 2009; Sakai et al., 2006). This is primarily for two reasons: first, the alcohol community, which has traditionally relied upon blood alcohol concentration (BAC) and breath alcohol concentration (BrAC) as the standard quantitative indices of intoxication, has no experience in, or benchmarks for, interpreting or analyzing the transdermal alcohol concentration (TAC) data that TAS devices produce; and second, evidence has shown that, unlike the breath analyzer, there is significant variation from individual to individual and device to device when correlating TAC with BAC or BrAC (Dumett et al., 2008).

If BAC or BrAC estimates could be reliably derived from TAC data, researchers and clinicians would be able to passively and unobtrusively obtain weeks of easily interpreted, detailed data on an individual's naturalistic alcohol consumption (see Dougherty et al., 2012). Fundamental information on the time-varying patterns of consumption could prove useful in studies of differences between social and problem drinkers, cognition and behavior while intoxicated, symptomatology (e.g., sensitization, tolerance, withdrawal, craving, relapse), and clinical intervention and prevention efforts.

The purpose of this study is to present and test a software program, the BrAC Estimator, that uses a comprehensive mathematical data analysis system to produce estimates of BrAC from TAC data. (Note that from here on we refer to BrAC only, but that either BAC or BrAC estimates can be produced from the software depending upon which type of data are input into the calibration models; see Hustad and Carey, 2005, for differences between BAC and BrAC.) Packaging these mathematical advancements in a software program intended for non-mathematicians makes these models readily available for use by researchers, clinicians,

and medical professionals. The anticipated result of this software is the capability to analyze BrAC levels at the required resolution and finesse for a great variety of experimental and analytic studies of alcohol-related phenomena.

Mathematical Models of the BrAC Estimator Software Program

The BrAC Estimator software program is based upon a mathematically sophisticated first principles forward model for the transport of alcohol from the blood through the skin to the TAS sensor and its oxidation by the TAS sensor (see Dumett et al., 2008; Rosen et al., 2013; in press, for details on the mathematical models). Unlike a breath analyzer, which relies on a relatively simple model from elementary chemistry (i.e. Henry's Law) for the exchange of gases between circulating pulmonary blood and alveolar air that has been observed to be reasonably robust across people, the transport and filtering of alcohol by the skin is more appropriately modeled (to be consistent with human physiology and physics) as a diffusion equation (i.e. the standard linear Fick's law of diffusion; see Okubo, 1980). The parameters for modeling and measuring this diffusion process vary based on a number of factors (e.g., skin layer thicknesses, TAS device anomalies) and thus need to be individually determined for each person wearing each device in order to convert TAC output into more interpretable BrAC values. Four parameters are needed to model this system, which can be obtained during an alcohol administration session where the individual wears a particular device and is monitored for both TAC (via the TAS device) and BrAC (via a breath analyzer device) throughout the course of the session. Once this calibration session is conducted and the parameters are determined for this individual and device, the participant can then wear the device in the field and the individualized model parameters can be used to convert the TAC data into estimates of BrAC for all subsequent drinking episodes (without requiring any additional BrAC readings beyond those obtained during the initial calibration session).

The first two of the four model parameters are q_1 , which describes the rate at which alcohol diffuses through the various layers of the skin, and q_2 , which describes the effective net rate at which alcohol enters and leaves the skin and is processed by the transdermal sensor. The software program uses the data TAC and BrAC data from the alcohol calibration session to optimally choose values for the two parameters (denoted by q_1^* and q_2^*) and to produce a model of TAC that closely approximates the TAC data generated by the TAS device. As a result of filtering effects in this forward process model, however, the estimated BrAC signal can exhibit excessive magnitude and/or oscillations that are non-physical. To remedy this, two additional parameters (i.e. penalty terms) are required to *regularize* the problem and make the resulting solutions more physically reasonable (Banks and Kunish, 1989; Bertsekas, 1999; Bradley et al., 1977). These penalty, or regularization, parameters are r_1 and r_2 . The software program uses the laboratory calibration data to optimally choose r_1 and r_2 (denoted by r_1^* and r_2^*) so that the inversion or *deconvolution* process provides an optimal estimate of BrAC. All four parameters are combined in an impulse response function (a curve that represent the individualized output response of the entire skin-TAC-TAS system to an input consisting of an impulse of instantaneous duration with BrAC of .001% alcohol), which represents the model used to correctly transform the TAC data obtained from the TAS device into meaningful BrAC data (accurate in terms of both magnitude and time) for that person wearing that device.

It is important to note that, because this system models alcohol from the blood through the skin and TAS device (using BrAC and TAC data) back only to BrAC (not back to ingestion or metabolism through the stomach, gut, or liver), that individual characteristics (e.g., gender, age, height, weight) and drinking episode characteristics (e.g., rate of consumption, stomach contents) that affect BrAC levels (see Watson et al., 1980; 1981) do not change the parameters. This means that only the one set of individualized model parameters is needed per person-device pair to model all subsequent drinking episodes.

User Interface of the BrAC Estimator Software Program

The BrAC Estimator software is run in Matlab on either Mac or PC computers. It uses the Excel output file of TAC data from the TAS device software, adding the BrAC data obtained by the breath analyzer during the calibration session into this file in a new column. The BrAC Estimator software can be run in either “auto” or “interactive” mode. Auto mode, which would most likely be used by a non-mathematician, only requires the user to input time ranges for the start and stop of the baseline signal (the low-level noise signal that is recorded by the TAS device when worn), alcohol calibration session, and each drinking episode.

The program output produces a BrAC estimate for every TAC data point (depending on the TAS device, ranging from every 10 seconds to every 30 minutes) and writes these estimates into the original Excel file as a new column of data. The software also computes the peak BrAC (% alcohol), time of peak BrAC (hours), and area under the estimated BrAC curve (% alcohol x hours) for each drinking episode, and plots the estimated BrACs and TACs as predicted by the model; the raw BrAC from the breath analyzer and raw TAC from the TAS device are also included in these plots to allow for visual comparison.

Current Study

In this study, we examine the accuracy of the models created in both the calibration and estimation phases of the BrAC Estimator software. First, we test the accuracy of the calibration phase by using different drinking episodes from a single subject wearing two TAS devices to calibrate the models. If the models were fully accurate, the four model parameters (q_1^* , q_2^* , r_1^* , r_2^*) together would yield equivalent impulse response curves, regardless of which drinking episode was used to calibrate the model. Additionally, the differences between the raw (TAS device) and software-estimated TAC data and between the raw (breath analyzer) and software-estimated BrAC data as assessed by the indices of relative error and by BrAC summary scores (i.e. peak BrAC, time of peak BrAC, and area under the BrAC curve) would be small. Second, we test the accuracy of the estimation phase by comparing the program's output of BrAC summary scores with those calculated from breath analyzer data.

Materials and Methods

Procedure

All data were collected by one participant, the first author, which was not considered human subjects research by the University of Southern California Institutional Review Board. For 18 days, the participant wore two WrisTAS™ 7 devices that were set to record TAC measurements at 5-minute intervals and collected BrAC measurements every 15 to 30 minutes during drinking episodes with the Alco-Sensor IV (Intoximeters, Inc., St. Louis, MO).

In the laboratory calibration session (see Luczak et al., 2002), the participant consumed an alcoholic beverage evenly over 15 minutes to reach a peak BrAC of approximately .050 mg % as determined by body water weight (Watson et al., 1980; 1981). BrAC was recorded every 15 minutes from the start of the session until returning to .000.

The participant continued to wear the TAS devices for the next 17 days in the field trial. During each drinking episode, the participant took BrAC readings every 30 minutes until the level returned to .000 or in one episode until she went to sleep; in another episode where alcohol quantity was low, she took BrAC readings every 15 minutes.

The breath analyzer is considered valid ($\pm .005$) with deep lung breaths taken after 15 minutes of not drinking alcohol, due to mouth alcohol affecting BrAC readings. To reduce this time period in the field, the participant rinsed her mouth twice and refrained from consuming alcohol for at least 5 minutes before taking each BrAC reading. In two instances where the BrAC reading appeared to be too high, she rinsed her mouth again, waited an additional 5 minutes, and re-tested her BrAC; the initial BrAC value was then omitted. Note that BrAC measurements would not be required for typical study participants during the field trial (just during the laboratory calibration session where they would be obtained by trained research staff), but to test the accuracy of the software program output, BrAC data were required for all drinking episodes in this study.

Data Analysis

At the end of the 18 days, the TAC data from the two devices were downloaded into two Excel data files. BrAC data from the breath analyzer were added to these files. The researcher (second author) ran the software in auto mode.

We used two indices of model fit: 1) the relative L_2 error, which is the square root of the sum of squares of the difference between the two signals being compared, and 2) the relative L_∞ error, which is the maximum absolute value of the difference between the two signals being compared. The L_2 error is a measure of the *area* between the two curves whereas the L_∞ error provides a uniform or upper bound for the *distance* between the two curves. If the L_∞ error is small, then the L_2 error must be small as well. However, the converse is not necessarily true; it is possible for two signals to be close in an L_2 sense (i.e. they are close on average over that time interval) and still be far apart in the L_∞ sense (i.e. the distance is far between the predicted and actual curve at a specific time or times in that interval).

We also evaluated the performance of the BrAC Estimator software using the three BrAC summary scores. We compared these scores from the BrAC software (which we denote as the “Est BrAC” method) with the TAC data (“Raw TAC”), BrAC from a breath analyzer (“Raw BrAC”), and Raw BrAC fit to a smooth piecewise polynomial curve (“Spline BrAC”; Schultz, 1973).

Results

Table 1 summarizes the 11 drinking episodes recorded over the 18 days. Figure 1 shows the two sets of TAC data from each TAS device along with the contemporaneous BrAC data from the breath analyzer (Datasets 1 and 2). From visual inspection of these two graphs, the general pattern of TAC measurements is similar across the two TAS devices, although the TAC peak for the calibration episode is lower in Dataset 2 than in Dataset 1.

Calibration Phase

Tables 2a and 2b present tabular calibration results for Datasets 1 and 2, respectively, using each of the 11 drinking episodes as the calibration session. The results of the calibration phase using Episode 1 as the calibration session are displayed graphically in Figure 2 and are representative of the calibration results for each of the 11 drinking episodes (all plots available upon request). From Figure 2, it can be seen that the estimated TAC closely approximates the Raw TAC throughout the drinking episode and the estimated BrAC approximates the Raw BrAC closely for much of the drinking episode.

Model Parameters Across Devices and Episodes—The values of the four optimal model parameters in the two datasets (shown in the top four rows of Tables 2a and 2b) indicate the calibration results were consistent across the two TAS devices, despite the devices producing different TAC values. The relative L_2 and L_∞ error fit indices (shown in the middle four rows of Tables 2a and 2b) were also similar across the two datasets using any of the 11 drinking episodes.

The models estimating TAC had an average relative L_2 error ($RE_{TAC,2}$) of 14–15% ($SD = 9\%$) and an average relative L_∞ error ($RE_{TAC,\infty}$) of 18–20% ($SD = 7\%$). The models estimating BrAC had an average relative L_2 error ($RE_{BrAC,2}$) of 27% ($SD = 9\text{--}11\%$) and an average relative L_∞ error in BrAC ($RE_{BrAC,\infty}$) of 33–39% ($SD = 12\text{--}19\%$). It is clear, however, that there is variance among the calibration models when created using TAC data from the 11 different drinking episodes. This is illustrated in Figure 3, which shows the variability of the impulse response functions when using each of the 11 drinking episodes to calibrate the model.

Model Estimates of BrAC—The bottom half of Table 2 shows the Est BrAC scores compared with those obtained from Raw BrAC and Spline BrAC. Plots of all 11 episodes indicated Est BrAC matched well to the Raw BrAC. On average, peak of Est BrAC ($Peak_{Est}$), was within .004 (12%) of $Peak_{Spline}$ in both datasets. $Peak_{Est}$ only differed from $Peak_{Spline}$ by more than .005 in Episodes 2 and 11. Note that Episode 11 was one of the longer drinking sessions with three drinks consumed over 2 hours. For time of peak BrAC, $Time_{Est}$ differed from $Time_{Spline}$ on average by 18 minutes (33–34%) in both datasets.

Time_{Est} differed by less than 15 minutes from Time_{Spline} for five episodes in each dataset, and by less than 30 minutes for all episodes except for Episode 4 (40 minutes). In Episode 4, Peak_{Est} only differed by .001 in Dataset 1 and by .002 in Dataset 2 from Peak_{Spline}, with the Raw BrACs being .054, .057, and .055 over the hour that contained both Time_{Est} and Time_{Spline}, indicating little BrAC variation over this time. For the area under the BrAC curve, AUC_{Est} was within .010 of AUC_{Spline} for all episodes except for Episode 5, which differed by .021 in both datasets. Episode 5 was the longest drinking episode, with three drinks consumed over 5 hours with intervals between drinks and multiple BrAC peaks and declines. In summary, Est BrAC summary scores were similar to the Spline BrAC summary scores across episodes. The episodes that had the largest discrepancy between the Est BrAC and Spline BrAC scores were different for each of the BrAC summary variables, but were logical when examining both the drinking patterns and the output differences.

Estimation Phase

We then used the model calibrated with Episode 1 to deconvolve the BrAC signal from the TAC signal for each of the subsequent 10 drinking episodes in each dataset (as would be done in the usual protocol). The results are tabulated in Tables 3a and 3b, with the last two columns showing the mean absolute difference and standard deviation of Est BrAC compared with the Spline BrAC models. Figure 4 provides graphic displays of some of the data summarized in Table 3. In Figure 4a, we show the estimated BrAC curves for Episode 7 from Dataset 2 where the BrAC Estimator software performed relatively well. In Figure 4b, we show the results of Episode 5 from Dataset 1 where the method performed less well.

Peak BrAC—For all 10 episodes, Peak_{Est} had a mean difference from Peak_{Spline} of .011 ($\pm .011$) in Dataset 1 and .006 ($\pm .006$) in Dataset 2. The misfit for Episode 5 using the Est BrAC was larger in Dataset 1 (.038) than in Dataset 2 (.022), which contributed to the difference in average peak differences across datasets. Peak values were within .005 of Peak_{Spline} for half of the episodes and only above .020 for Episode 5. Raw TAC provided similar estimates of peak BrAC in both datasets, with Peak_{TAC} differing from Peak_{Spline} on average by .007 ($\pm .007$) in Dataset 1 and .006 ($\pm .006$) in Dataset 2.

Time of Peak BrAC—Time_{Est} differed on average from Time_{Spline} by 30 (± 20) minutes, the typical interval between Raw BrAC readings. When examined for each episode, Time_{Est} was within 15 minutes of Time_{Spline} for 9 (41%) episodes and within 30 minutes for all episodes except Episode 4 (65 minutes), which was the second longest drinking episode at 150 minutes of drinking with the steady BrAC level (within .003) for over an hour. Time_{TAC} was on average over an hour (70 ± 29 minutes) later than Time_{Spline}, being over an hour later in 17 (77%) episodes and not within 15 minutes of Time_{Spline} for any episode.

Area Under BrAC Curve—AUC_{Est} differed from AUC_{Spline} on average .024 for Dataset 1 and .014 for Dataset 2. AUC_{Est} was within .010 for 11 (50%) episodes, but above .025 for 5 (23%) episodes. The variability across datasets is likely due in part to the software program selecting slightly different start and stop points for the drinking episode given the baseline level of noise of the individual sensors. AUC_{TAC} differed on average from AUC_{Spline} by .024 in Dataset 1 and .028 in Dataset 2 and was within .010 for 12 (55%)

episodes, but above .025 for 7 (31%) episodes. Thus, the AUC_{Est} and AUC_{TAC} were similar.

Discussion

Calibration Phase

The BrAC Estimator software was able to fit each individual drinking episode well (based on fit indices, BrAC summary scores, and visual comparison of TAC and BrAC plots), suggesting that diffusion as modeled by four parameters is an appropriate paradigm to describe the transdermal transport of alcohol from the blood through the skin to the TAS device. Our results also indicate that there was variance in the values of the optimal model parameters across the two TAS devices, highlighting the need to calibrate the model not just to the individual, but also to the device. Despite the differences in the raw TACs across devices, the BrAC Estimator software created consistent models for the two TAS devices that yielded similar BrAC estimates.

We also found variation in BrAC Estimator software models when the calibration was conducted using different drinking episodes. There are a number of mathematical approaches that might improve the performance of the BrAC Estimator method. One such technique is a frequency domain analysis of the different drinking episodes, which could potentially help us to identify drinking patterns that could then be correlated with the different values of the parameters. It is possible that the values of the parameters themselves may serve to characterize different drinking patterns or profiles. To explore this, we recalibrated the model using Episodes 3 and 8 from Dataset 2, which produced similar parameter values, and then inverted the other episode. With the model calibrated using Episode 3 instead of Episode 1, BrAC software estimates for Episode 8 improved for peak BrAC from .043 to .039 (peak Raw BrAC was .036), relative L_2 error improved from .017 to .009, and relative L_∞ error improved from .015 to .008 (see Figure 5). With the model calibrated using Episode 8 instead of Episode 1, software estimates for Episode 3 improved for peak BrAC from .019 to .017 (peak Raw BrAC was .017), relative L_2 error improved from .004 to .003, and relative L_∞ error improved from .008 to .005 (see Figure 6). Thus, a more intricate alcohol calibration protocol yielding a richer calibration data set and a procedure involving gain scheduling may improve the accuracy of the model estimates.

Another mathematical approach that might improve the performance of the BrAC Estimator software would be to replace the linear diffusion model with a more sophisticated nonlinear paradigm. This technique would allow the diffusivity constant q_1 to depend on the alcohol concentration and/or the gradient of ethanol concentration at that depth in the skin. Such a modification would add a significant level of complexity to both the mathematical analyses and computations that may improve model fit.

Estimation Phase

In the estimation phase, the BrAC Estimator software models were able to compensate for the attenuation of peak BrAC and the latency of the time of peak BrAC typically observed in TAC data, as well as the variation in TAC data across devices, to produce consistent

measures of BrAC. The software modeling did not appear to be affected by eating (e.g., empty stomach in Episode 6, eating while drinking in Episode 10, and drinking after eating in Episode 4), which was expected given the mathematical models in the software use BrAC data, an indicator of alcohol in the bloodstream (alcohol that has already passed through the gut). The BrAC Estimator software was better (in terms of BrAC summary scores) at estimating drinking episodes that had clear ascending and descending limbs (e.g., Episodes 2 and 7). The software models performed less well for drinking sessions when alcohol was consumed sporadically over a longer periods of time, resulting in relatively even levels of BrAC for long time periods or multiple ups and downs in BrAC levels (e.g., Episodes 5 and 11). In addition, less distinct start and stop time points for these drinking episodes also likely contributed to the relatively poorer estimate of the area under the curve. The plots of BrAC modeled by the software for the more plateaued drinking episode curves, however, still mapped onto the raw TAC and raw BrAC values relatively well. Thus, it appears the fit of the BrAC Estimator modeling may be more affected by the shape of the drinking curve and discernable start and stop points than by level of peak BrAC or stomach content, although additional modeling of the shape of the curve using signal processing tools and frequency domain analysis are needed to mathematically support these observations.

The software estimates of peak BrAC measure were within the $\pm .005$ reported error range of the breath analyzer for all but two drinking episodes, and was within .020 (the equivalent of approximately one standard drink) for all episodes. The raw TAC peak estimates, however, had similar accuracy levels as the software models, as did the area under the curve for most episodes. The most noteworthy improvement produced by the BrAC Estimator software compared with the raw TAC data was for time of peak BrAC. These estimates were improved by over 30 minutes on average, being within 20–30 minutes of the breath analyzer peak (obtained at 30-minute intervals) as compared with being on average over an hour delayed for the raw TAC data. The raw TAC technique is attractive in that it requires no active participation by the subject in collecting the data with the exception of having to properly wear the TAS sensor. The BrAC Estimator software method requires a laboratory calibration session prior to the field trial, but no active participation by the subject during naturalistic drinking episodes. Thus, if it is appropriate to administer alcohol to an individual in the laboratory, the BrAC Estimator software can improve accuracy of BrAC estimates in the field, particularly the time displacement, without incurring real-time subject burden.

Limitations and Future Directions

Our findings should be viewed within the limitations of this study. First, this data set only contained 11 drinking episodes over 18 days, although it did include 93 BrAC readings taken over 35 hours (10 hours of drinking) with very few missing data points and data from two TAS devices; thus, it was relatively comprehensive for each drinking episode. Second, how our findings from a single subject fit with different types of subjects and higher alcohol quantities needs to be determined. The model, however, was able to fit all 22 episodes in the two data sets. Furthermore, we do not expect differences in model fit based on individual characteristics that affect BrAC levels (e.g., age, gender, BMI), given the BrAC scores already account for these, or that affect model parameters (e.g., skin thickness), given the model is calibrated to the individual and device. Finally, we used the breath analyzer data to

compare with software results, but recognize that raw BrAC data are also subject to error and are only recorded at 30-minute intervals. Thus, the raw BrAC peak levels and times likely missed higher BrAC levels that occurred between data collection time points, which could underestimate the accuracy of the software BrAC summary scores.

These limitations can be addressed in future research that tests the BrAC Estimator modeling program across a variety of consumption patterns and a range of peak BrACs in both the calibration session and field trial and with additional participants. More varied alcohol administration protocols for the calibration session(s), together with gain scheduling and nonlinear models, may also improve model fit.

In conclusion, this research provides information for understanding how the TAS device, while currently in relatively early stages of development, may be used to generate quantitative measures of BrAC in real-time drinking episodes. With the development the BrAC Estimator software program to calculate these models for non-mathematicians, the TAS technology becomes a more informative tool for alcohol researchers and clinicians.

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Figure 1.

TAC (crosses) and BrAC (dots) data for a) Dataset 1 (top panel) and b) Dataset 2 (bottom panel). These two datasets were collected by the same participant over the same 18 days using two TAS devices and a breath analyzer.

Figure 2.

TAC and BrAC calibration results for Drinking Episode 1 for a) Dataset 1 (top panels) and b) Dataset 2 (bottom panels). The upper panel shows the Raw TAC (crosses) along with the Est TAC (solid line). The lower panel shows the Raw BrAC (dots) along with the Est BrAC (solid line) obtained by using the optimal values of the model (q_1^* , q_2^*) and regularization (r_1^* , r_2^*) parameters to deconvolve the TAC data shown in the upper panel.

Figure 3.

Calibrated impulse response functions for all 11 drinking episodes for a) Dataset 1 (top panel) and b) Dataset 2 (bottom panel). Each line labeled Event No. 1–11 represents the impulse response functions determined by drinking episodes 1–11, respectively. These functions indicate the BrAC Estimator software calibration results were consistent across the two datasets, but that there is a substantial variance among the models created using the 11 different drinking episodes.

Figure 4.

Drinking episode results: a) Episode 7 in Dataset 2 on which the method performed well (upper panel), and b) Episode 5 in Dataset 1 on which the method performed less well (lower panel). These panels show results of calculating estimated BrAC with the software (Est BrAC; dashed line) compared with a breath analyzer (Raw BrAC, crosses) and a TAS device (Raw TAC; dots).

Figure 5.

Model results for Episode 8 in Dataset 2 when calibrated by Episode 1 (top panel) and Episode 3 (bottom panel). These graphs indicate improvement in model fit when calibrating the model with a drinking episode that more closely matches the episode being inverted.

Figure 6.

Model results for Episode 3 in Dataset 2 when calibrated by Episode 1 (top panel) and Episode 8 (bottom panel). These graphs indicate improvement in model fit when calibrating the model with a drinking episode that more closely matched the episode being inverted.

Table 1

Summary Data for the 11 Drinking Episodes

Drinking episode	BrAC interval (minutes)	Alcohol type	Total drinks	Minutes of drinking	Number of BrAC readings	Minutes of BrAC readings	Comments
1	15	95% EtOH in 1:4 mixer	2	15	15	225	BrAC omitted at 90 minutes
2	15	Bottle of beer	1	45	7	90	None
3	30	Bottles of beer	2	75	8	150	None
4	30	Pitchers of beer	3.5	150	9	225	Went to sleep at 225 minutes when BrAC was .036
5	30	Margaritas, bottle of beer, wine	3	300	14	420	BrAC omitted at 310 minutes
6	30	Margarita	1	30	5	120	None
7	30	Wine	1.5	90	6	150	Redid 2 BrACs that were high
8	30	Bottle of beer	1	30	5	105	BrAC omitted at 30 minutes
9	30	Bottle of beer, wine	2.5	120	9	250	TAS off from 235-245 minutes
10	30	Wine	1	60	5	120	None
11	30	Margaritas, wine	3	120	10	270	None

Table 2
Calibration Results Using Each of the 11 Drinking Episodes as the Calibration Session for a) Dataset 1 and b) Dataset 2

	Drinking episode											<i>M</i>	<i>SD</i>
	1	2	3	4	5	6	7	8	9	10	11		
Parameter													
<i>q</i> ₁ [*]	.93	.47	1.55	.29	2.35	.46	.82	.53	1.11	2.27	.63	1.04	.721
<i>q</i> ₂ [*]	1.24	1.17	1.77	1.20	1.47	1.04	.83	.20	1.53	1.76	.97	1.20	.452
<i>r</i> ₁ [*]	.10	.10	.10	.21	.16	.11	.11	.10	.19	.14	.10	.13	.040
<i>r</i> ₂ [*]	.10	.10	.11	.90	.37	.25	.20	.10	1.08	.28	.11	.33	.342
Relative Error													
RE _{TAC,2}	.06	.21	.05	.18	.06	.33	.27	.10	.17	.15	.10	15%	9%
RE _{TAC,∞}	.17	.22	.20	.18	.13	.26	.29	.12	.32	.20	.11	20%	7%
RE _{BrAC,2}	.24	.38	.20	.18	.19	.37	.17	.35	.19	.17	.49	27%	11%
RE _{BrAC,∞}	.77	.45	.54	.29	.19	.49	.17	.39	.21	.24	.61	39%	19%
Peak BrAC													
Peak _{raw}	.052	.023	.036	.057	.052	.023	.018	.017	.026	.013	.048	-	-
Peak _{spline}	.052	.023	.036	.057	.052	.023	.018	.019	.026	.013	.050	-	-
Peak _{Est}	.049	.017	.032	.058	.055	.020	.018	.014	.024	.014	.068	12%	12%
Time of peak													
Time _{raw}	.75	.50	1.50	2.00	3.00	.58	1.58	.83	2.08	1.08	.92	-	-
Time _{spline}	.75	.50	1.50	1.83	2.92	.67	1.50	.58	2.08	.92	1.17	-	-
Time _{Est}	.67	.83	1.00	2.50	2.50	1.08	1.50	.67	2.25	1.00	1.67	33%	30%
Area under curve													
AUC _{spline}	.110	.016	.077	.168	.201	.029	.027	.020	.055	.018	.120	-	-
AUC _{Est}	.110	.016	.087	.167	.222	.026	.026	.017	.057	.017	.111	6%	5%

Table 2b

	Drinking episode											M	SD
	1	2	3	4	5	6	7	8	9	10	11		
Parameter													
q_1^*	1.30	.318	.518	.316	1.53	0.44	0.53	.539	0.63	1.24	0.87	0.75	0.424
q_2^*	1.63	2.32	2.19	1.15	1.56	1.21	1.29	2.13	1.56	2.07	0.87	1.64	0.484
r_1^*	0.10	0.12	0.10	0.19	0.15	0.12	0.16	0.11	0.21	0.11	0.10	0.23	0.039
r_2^*	0.10	.08	0.11	1.08	0.48	0.29	0.37	0.09	0.90	0.20	0.11	0.35	0.346
Relative error													
RE _{TAC,2}	.07	.15	.04	.19	.06	.34	.24	.10	.17	.12	.07	14%	9%
RE _{TAC,∞}	.16	.24	.07	.18	.17	.27	.23	.13	.31	.16	.09	18%	7%
RE _{BrAC,2}	.23	.41	.23	.18	.19	.38	.21	.35	.18	.16	.41	26%	9%
RE _{BrAC,∞}	.41	.44	.27	.27	.20	.49	.23	.44	.20	.21	.49	33%	12%
Peak													
Peak _{Raw}	.052	.023	.036	.057	.052	.023	.018	.017	.026	.013	.048	-	-
Peak _{Spline}	.052	.023	.036	.057	.052	.023	.018	.019	.026	.013	.050	-	-
Peak _{Est}	.057	.015	.037	.059	.057	.021	.018	.014	.025	.014	.063	11%	11%
Time of peak													
Time _{Raw}	0.75	0.50	1.50	2.00	3.00	0.58	1.58	0.83	2.00	1.08	0.92	-	-
Time _{Spline}	0.75	0.50	1.50	1.83	2.92	0.67	1.50	0.58	2.08	0.92	1.17	-	-
Time _{Est}	0.83	0.83	1.00	2.42	2.50	1.17	1.50	0.75	2.17	0.83	1.67	34%	33%
Area under curve													
AUC _{Spline}	.106	.016	.077	.168	.201	.029	.027	.020	.055	.018	.120	-	-
AUC _{Est}	.109	.016	.081	.166	.222	.026	.026	.016	.054	.018	.111	6%	6%

Note. q_1^* and q_2^* = optimal parameter estimates, r_1^* and r_2^* = optimal regularization parameter estimates, E = error, RE = relative error, TAC = transdermal alcohol concentration, 2 = L2 error, ∞ = L_∞ error, Peak = peak BrAC score (% alcohol), Time = time of peak BrAC (hours), AUC = area under the BrAC curve (% alcohol × hours), Raw = breath analyzer BrAC, Spline = spline curve fit to the breath analyzer BrAC, Est = BrAC Estimator software.

Table 3

Inversion Results for the 11 Drinking Episodes with Model Calibrated on Drinking Episode 1 for a) Dataset 1 and b) Dataset 2

	Drinking episode											M diff	SD
	1	2	3	4	5	6	7	8	9	10	11		
Peak													
Peak _{Raw}	.052	.023	.036	.057	.052	.023	.018	.017	.026	.013	.048	-	-
Peak _{Spline}	.052	.023	.036	.057	.052	.024	.018	.017	.026	.014	.049	-	-
Peak _{TAC}	.035	.017	.050	.057	.074	.022	.018	.017	.036	.020	.044	.0074	.00747
Peak _{Est}	.050	.022	.056	.066	.090	.029	.019	.024	.041	.030	.057	.0114	.01094
Time of peak													
Time _{Raw}	0.75	75.00	95.75	123.25	144.00	166.08	192.08	217.17	240.67	265.08	335.75	-	-
Time _{Spline}	0.75	75.00	95.75	123.08	143.92	166.25	192.00	217.17	240.75	264.83	336.00	-	-
Time _{TAC}	1.17	76.17	96.25	125.17	145.50	167.42	193.25	217.67	242.33	265.67	337.17	1.108	0.5221
Time _{Est}	0.67	75.50	95.17	124.17	143.25	166.83	192.25	217.17	241.25	264.75	336.50	0.492	0.3185
Area													
AUC _{Spline}	.106	.016	.076	.156	.200	.027	.027	.016	.056	.018	.119		
AUC _{TAC}	.092	.014	.131	.094	.329	.026	.028	.017	.087	.027	.123	.0282	.04011
AUC _{Est}	.101	.022	.128	.134	.292	.039	.036	.027	.088	.038	.120	.0241	.02691

Table 3b

	Drinking episode											M diff	SD
	1	2	3	4	5	6	7	8	9	10	11		
Peak													
Peak _{Raw}	.052	.023	.036	.057	.052	.023	.018	.017	.026	.013	.048	-	-
Peak _{Spline}	.052	.023	.036	.057	.052	.024	.018	.017	.026	.014	.049	-	-
Peak _{TAC}	.052	.017	.052	.061	.072	.022	.017	.014	.033	.017	.040	.0064	.00634
Peak _{Est}	.057	.018	.043	.051	.074	.023	.017	.016	.030	.020	.037	.0063	.00610
Time of peak													
Time _{Raw}	0.75	75.00	95.75	123.25	144.00	166.08	192.08	217.17	240.67	265.08	335.75	-	-

Table 3b												
	Drinking episode										M diff	SD
	1	2	3	4	5	6	7	8	9	10	11	
Time _{Spline}	0.75	75.00	95.75	123.08	143.92	166.25	192.00	217.17	240.75	264.83	336.00	-
Time _{TAC}	1.25	76.25	97.17	125.17	144.92	167.67	193.42	217.83	242.17	265.85	337.49	0.43640
Time _{Est}	0.83	75.6	95.58	124.17	143.42	166.92	192.25	217.25	241.33	264.85	336.65	0.33329
Area												
AUC _{Spline}	.106	.016	.076	.156	.200	.027	.027	.016	.056	.018	.119	-
AUC _{TAC}	.123	.012	.115	.105	.322	.019	.019	.009	.072	.020	.111	.0236
AUC _{Est}	.101	.016	.097	.108	.222	.027	.025	.017	.058	.025	.078	.02725

Note. Diff = difference, Peak = peak BrAC score (% alcohol), Time = time of peak BrAC (hours), AUC = area under the BrAC curve (% alcohol × hours), Raw = breath analyzer BrAC, Spline = spline curve fit to the breath analyzer BrAC, TAC = transdermal alcohol concentration, Est = BrAC Estimator software.