4. DATA REDUCTION AND EVALUATION PROCEDURES

William Mirsky

University of Michigan
Ann Arbor, Michigan

Work at the University of Michigan has primarily been concerned with the computational procedures that are involved in exhaust emissions data reduction and the use of these computational procedures for determining the quality of the data that is obtained from exhaust measurements. We focused on four problem areas. The first was the various methods for performing the carbon balance. As has already been mentioned, Federal regulations specify that a ±5-percent tolerance on the carbon balance should be met. There are at least four techniques that can be used to perform this carbon balance. Each technique gives a different error for the carbon balance. The second problem area was the method for calculating water correction factors. In the various exhaust measurement instruments that are used, some of the water is condensed from the exhaust sample and the concentration must be converted to either a totally wet or totally dry measurement. Because of the involvement of the water correction factor in the data reduction computations, part of our effort was to examine the methods used for determining this water correction factor. The third problem area was how to calculate the exhaust molecular weight. The fourth problem area was assessing the quality of the data. Is there a way of determining the quality of the data immediately from an analysis of the results or does one make comparisons with trends established over a series of runs?

Our accomplishments are as follows:

1. Review of the literature for methods of performing the carbon balance
    - (a) Spindt (Gulf Research) (ref. 1)
    - (b) Stivender (General Motors Research) (ref. 2)
    - (c) Eltinge (Ethyl Research and Development Laboratories) (ref. 3)

2. Fundamental approach to performing the carbon balance
   - (a) Find X equations for the X unknowns
   - (b) Methods:
     - 1.1 Spindt (K), 4 equations in 4 unknowns
     - 1.2 Expanded Spindt (K), 15 equations in 15 unknowns
     - 2.1 XTC, 15 equations in 15 unknowns
     - 3.1 K and XTC, 16 equations in 16 unknowns
     - 3.2 Modified Stivender, 12 equations in 12 unknowns
   - (c) Features of the University of Michigan methods:
     - (1) Model the combustion process more accurately
     - (2) Clearly identify assumptions and simplifications
     - (3) Eliminate need for water correction
     - (4) Give concentrations of 10 (11) major exhaust components
     - (5) Compute exhaust molecular weight
     - (6) Provide means for data assessment
     - (7) Agree well with Eltinge's method

First, we reviewed the literature dealing with the methods for performing the carbon balance. We found three important works in this area. One method by Spindt at Gulf Research (ref. 1) seems to be very commonly used not only in the automotive industry but in many combustion studies. The second method was developed by Stivender at General Motors Research (ref. 2), and the third is a graphical method developed by Eltinge at the Ethyl Research and Development Laboratories (ref. 3).

In examining these computational procedures we found that the carbon balance could be performed in a more fundamental manner. This fundamental method consists of finding a sufficient number of equations to be able to solve for the unknowns that appear in the combustion equation model. By following this approach we were able to use an expanded and more accurate combustion equation that gave us more accurate information about the combustion model and about the emissions measurements. Based on this fundamental approach, we developed the following five methods: The first method (1.1) is equivalent to the Spindt method in that four equations are used for four unknowns. It is a fairly simple model. The combustion equation is expanded by using a more accurate air composition that includes argon, water vapor, and variable carbon dioxide (CO_2) levels in the intake air and by taking into consideration 10 or 11 products in the exhaust (method 1.2). Methods 1.1 and 1.2 both use the equilibrium constant equation for the water gas reaction as one of the equations. Method 2.1 substitutes an equation that involves the sum of the mole factions in place of the equilibrium constant equation. Method 3.2 involves both the equilibrium constant and the sum of the more factions. Method 3.2 involves a modified Stivender system, which does not require an oxygen measurement. Note that we have gone from four equations involving four unknowns to 16 equations and 16 unknowns.

This approach gives us a computational method with the following features: first, we have a more accurate combustion equation involving more of the stable combustion products. Second, the assumptions and simplifications are clearly identified. Third, we eliminate the need for a water correction factor since there is no separate computation that involves the water correction factor. Measurements in either the dry, dried, or wet states can be used. If no water is condensed out of the sample, the measurement is wet. If water is condensed in the water trap, the measurement is somewhat dried but there is still some water vapor present. The sample must be passed through a drier to eliminate all the water. These are the three different types of measurements that can be handled in our computational procedure. These methods give the concentrations of 10 or 11 major exhaust components as well as the fuel-air ratio, whereas a procedure such as the Spindt method gives only the fuel-air ratio. From the concentrations of the 10 or 11 major exhaust components, we can then compute the exhaust molecular weight. This value is more reliable than one based on equilibrium computations as is commonly done.

Our method has also been of value in assessing the quality of the data. The method for assessing data quality was as follows: We started with a run that showed agreement for all the four computational methods. We then performed, on the computer, a calculation whereby we incremented the concentration of an exhaust species such as CO_2 while holding all other measurements constant. The effect would be similar to making an error in the CO_2 measurement. The results show the fuel-air ratio error obtained for each of the four computational methods. As shown in figure 4-1(a), if method 2.1 gives a +5-percent error, method 3.2 would give a +2-percent error, method 1.2 would give a -1-percent error, and method 3.1 would give approximately a -5-percent error. This illustrates the fact that the percentage of error in the carbon balance is a function of the method being used. A useful factor that comes out of this is the sensitivity factor that we call specific error. For example, the CO_2 specific error is the increase in fuel-air ratio error due to a 1-percent increase in CO_2. Each computational method shows a different specific error. Our analysis shows that the specific error varies with the concentration as shown in figure 4-1(b). Similar studies were made using many other variables, such as carbon monoxide (CO), hydrocarbons (HC), oxygen (O_2), and ambient humidity. This information can be applied in assessing the exhaust emissions data in the following manner: An error in the CO_2 measurement such that the CO_2 measured is higher than the true CO_2 concentration would cause, depending on the concentration, an increase or decrease of the error as is shown in table 4-1. The magnitudes and signs of the errors from the four different methods show which measurement is primarily responsible for the difference between the measured and the calculated fuel-air ratios.

Tables 4-2 and 4-3 are two examples in which errors in the calculated fuel-air ratio based on four different calculation procedures are compared with measured test results. Table 4-2 (example 1) shows that all four methods gave fuel-air ratio errors of about 6 percent. On the basis of the +5-percent carbon balance criterion, this run would not be considered an acceptable run. Normally, all four methods would not give essentially the same result. The chances of having compensating errors so as to end up with the same results are very small, and one would have to presume that the calculated results are good. On the basis of these results, we would conclude either that there is an error in the fuel measurement value or the air measurement value or that there was an air leak in the system. In fact, in this particular case an air leak was discovered in the induction system.

In table 4-3 (example 2), the +5-percent error was not exceeded. The expanded Spindt method (method 1.2) gave an error of about 3 percent. Normally, this would be considered to be a good run. However, when the data were reduced by the three other methods, we got errors of 24, -10, and 10 percent. What we do now is to find out which of the measurements is the most probable cause for this error. Examining the fuel-air ratio errors shows that a correction of +10 percent is required for method 3.1, while method 3.2 would require a -10-percent correction. The specific errors for CO_2 of -1.4 and +0.5 percent for methods 3.1 and 3.2 in table 4-4 shows that these changes will not result from corrections in the CO_2 concentrations. However, it appears that CO might be in error here because the two CO specific errors of -0.9 and +0.8 percent are about equal and of opposite signs, indicating that the two fuel-air ratio errors of methods 3.1 and 3.2 could be reduced to approximately zero by a change in CO concentration. This would not be accomplished by an O_2 correction or by a hydrocarbon correction. This analysis therefore points to CO as the measurement causing the bad data point.

Next, we determine the necessary correction of CO, by using specific sensitivities, required to reduce all four fuel-air ratio errors to zero. Method 1.2 would require a -15-percent change in CO (table 4-4). Method 2.1 would require a -12-percent change. When the CO concentration was reduced by 11.8 percent, a value arrived at after two tries, the fuel-air ratio errors for all four methods were reduced to less than 1 percent, as shown. This procedure allows us to assess the quality of data from a single run and to pinpoint the source of error when the error is due primarily to one bad measurement. The analysis becomes more complicated when more than one measurement is in error. Also note that a Spindt error which is less than 5 percent does not necessarily mean a good data run. The other computational methods are as acceptable as the Spindt method and often show much higher fuel-air errors as illustrated in example 2.

Our analysis has been applied to over 500 runs and has proved to be a reliable means for quickly assessing emissions data. This study is being continued to further refine the procedure for assessing data quality.

REFERENCES

1. Spindt, R. S.: Air-Fuel Ratios from Exhaust Gas Analysis. SAE Paper No. 650507, 1965.

2. Stivender, D. L.: Development of a Fuel-Based Mass Emission Measurement Procedure. SAE Paper No. 710604, 1971.

3. Eltinge, L.: Fuel-Air Ratio and Distribution from Exhaust Gas Composition. Ethyl Corporation Report 68-1, Jan. 1968.

TABLE 4-1. - SPECIFIC ERROR SUMMARY

	Method			
	1.2	2.1	3.1	3.2
CO_2	↑↓	↑	↓	↑
CO	↑	↑	↓	↑
O_2	↓	↑	↓	–
HCC	↑	↑	↑	↑

TABLE 4-2. - COMPARISON OF ERRORS IN THE CALCULATED FUEL-AIR RATIO BASED ON FOUR DIFFERENT CALCULATION PROCEDURES - EXAMPLE 1

Method	XTC	FACAL	FAM	F/A percent error
1.2	1.005	0.07565	0.07140	5.96
2.1	-----	.07576	↓	6.11
3.1	-----	.07557		5.84
3.2	-----	.07569		6.01

Spindt error >5 percent.
Other methods give same result.
Found air leak from induction system.

TABLE 4-3. - COMPARISON OF ERRORS IN THE CALCULATED FUEL-AIR RATIO BASED ON FOUR DIFFERENT CALCULATION PROCEDURES - EXAMPLE 2

Method	XTC	FACAL	FAM	F/A percent error
1.2	1.0578	0.10752	0.10436	3.030
2.1	------	.13017	↓	24.733
3.1	------	.09386		-10.053
3.2	------	.11529		10.477

Spindt error <5 percent.
Other methods give high errors.
Implies measurement error(s).

TABLE 4-4. - ERROR ANALYSIS - SPECIFIC ERRORS OF EXAMPLE 2

Method	CO_2 (67022)	CO (129820)	O_2 (4310)	HCC (15688)
1.2	0.0	+0.2	-0.05	+0.13
2.1	+1.1	+2.0	+0.05	+0.18
3.1	-1.4	-0.9	-0.10	+0.07
3.2	+0.5	+0.8	0.0	+0.15

From: $$\text{Specific error} = \frac{\text{Required change F/A error}}{\text{Percent increase in concentration}}$$

Get: $$\text{Percent increase concentration} = \frac{\text{Required change F/A error}}{\text{Specific error}}$$

Method	
1.2	-3.03/+0.2 = -15.15 percent change CO
2.1	-24.73/+2.0 = -12.37
3.1	+10.05/-0.9 = -11.17
3.2	-10.48/+0.8 = -13.10

After -11.8 percent change in CO, result is

Method	XTC	FACAL	FAM	F/A percent error
1.2	1.001	0.10502	0.10436	0.632
2.1	-----	.10525	↓	.850
3.1	-----	.10486		.483
3.2	-----	.10511		.717

DISCUSSION

COMMENT - W. Westfield: I'd like to add one thing that Dr. Mirsky didn't add. We supplied him with approximately 400 data points, many of which we knew were questionable. In the analysis of the work that he did for us he came up with a grouping of data points that appeared to be outside acceptable ranges. In going back and looking at the unacceptable data points I think the vast majority of those points were "idle mode" data points. We feel this is further support for getting rid of the procedure and computational process that really drives us up a tree when we try to come up with a cycle factor.

Q - T. Souza: Aren't there two ways of calculating emissions? One is based on exhaust volume where the concentrations in the exhaust are measured. The exhaust volume is then calculated and the pollutants are based on the ratio of the concentrations of the different gases. The second way is to simply assume that all the carbon in the fuel coming into the engine appears as carbon in some constituents in the exhaust.

A - W. Mirsky: Yes, there are two methods. What you're doing in performing the carbon balance is accounting for the carbon; but you also have to account for all the other atoms that come in with the fuel and air based on measurements in the exhaust. In the simple combustion equation you don't take into account all of the moles of the products so that the value that you substitute in the mathematical model is not quite the right value. What the four methods start out with are unknown quantities of air and fuel and you have to solve these. You first set a carbon balance and an oxygen balance. Then you introduce another unknown. In the Spindt method it turns out to be hydrogen and water so you have to have two more equations; that's how you get four equations and four unknowns in a modified Spindt method. The combustion model is not complete since the argon and some of the other species in the exhaust have been ignored. What you are trying to do is decide whether or not the value that you calculate does, in fact, agree with what you measure. If you have an error in CO_2 then you get different errors between the measured and calculated value depending on what method you use. The sensitivity curve shows that for a 1-percent change in CO_2 there can be four different answers for the errors between the calculated and the measured fuel-air ratio. This whole approach was to look at the problem comprehensively and understand what really went into the Spindt method, the Stivender method, and the Eltinge method. One of the problems is to decide whether the measured fuel-air ratio and calculated fuel-air ratio agree. The second problem is to come up with a computation for the molecular weight of the exhaust. Many people use the equilibrium concentrations in order to come up with the molecular weight of the exhaust. In our calculations we find that at a particular fuel-air ratio you can get a variety of molecular weights depending on how complete the combustion process is. If the combustion process is complete, you tend to approach the molecular weight as given by the equilibrium calculations. If the combustion process is not complete, as you would get from a very poor quality mixture, the molecular weight is then considerably lower.

Q - R. Tucker: In example 2 with the expanded Spindt method you show the sum of the exhaust products mole fraction to be approximately 1.06. We've encountered the same problem of the sum of the mole fractions exceeding 1. Do you have any explanation for this?

A - W. Mirsky: The reason the sum of the mole fractions exceeds 1.0 or is less than 1.0 is that the measurements are not good. With a consistent set of measurements that satisfy the four different methods XTC will approach a value of 1.0, thereby providing a very nice parameter by which you can tell whether or not the measurements are good. In the first example, the XTC value is very close to 1.0. As a result, all of the calculated values come out to be the same. When your measurements are self-consistent, your XTC becomes equal to 1.0. If your measurements are not self-consistent, in other words, if they don't satisfy these equations properly, then the deviate from 1.0 and you can get either higher or lower values than 1.0.

Q - G. Kittredge: I'd like to ask Dr. Mirsky about his investigation of exhaust analyses and ways of complying with the carbon balance of our standards. I just reread that part of our standards in which we talk about carbon balance. It is an extremely tersely worded sentence. Are you making a recommendation that we make a change in the standards to be more compatible with the analysis that you have made?

A - W. Mirsky: My comment would be that you have to be more specific when you say that ±5 percent of tolerance on carbon balance will have to be met. Depending on which method I use, I can be outside that tolerance or within the tolerance. What I'm saying is that the method of computation will have to be specified. With our extensive work, we've examined this question very thoroughly and have written a report for the FAA that should be published soon. I would say at this time that the XTC value, or the sum of the mole fractions, is a more important parameter to meet than the fuel-air ratio. It tells you whether or not your instruments are self-consistent. We tend to recommend, although this has to be looked into further, a ±5 percent tolerance on the expanded Spindt method plus a ±5 percent tolerance on the XTC. We examined well over 500 runs and plotted the XTC and fuel-air ratio error. When you have good runs the points tend to congregate around the origin of those axes. For the high power runs, the group of points tends to go around the origin. In the taxi modes, there is a departure from the origin and a good percentage of the points start to fall outside the acceptable limits. In the idle mode, almost all of the runs tend to be outside the acceptable ranges. I would say that you have to specify the method of computation.

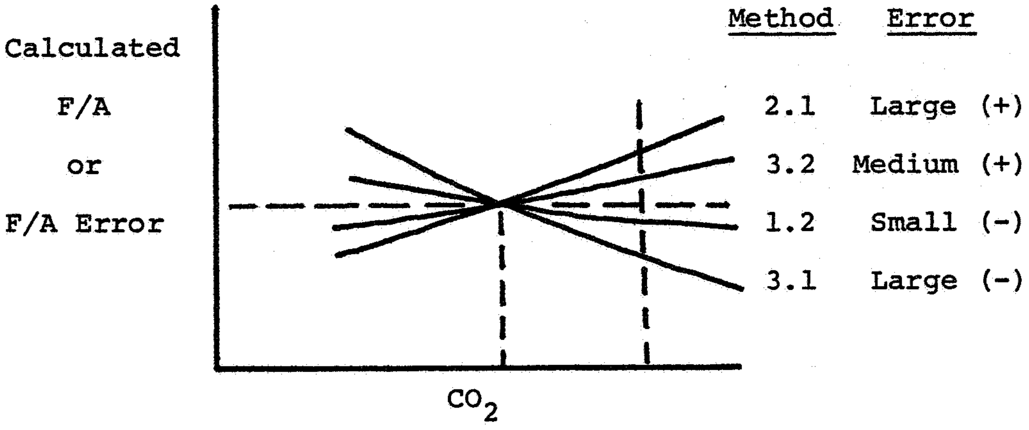
COMMENT - B. Rezy: We've heard a lot of comments on test procedures and different methods of calculation. I would like to propose that we finalize this and come up with one method so that everyone uses the same standard system. There are three ways of going about this: we could have the government set up the procedure; we could have a committee set up to determine these standards; or we could have GAMA set the standards. I would like to propose that we have a committee get together and determine what standards we should be going by.

Q - G. Kittredge: I thought the ground work was laid after an earlier meeting to ask the SAE aircraft exhaust emissions measurement committee E31 to evaluate and make recommendations concerning the light aircraft powerplant measurement procedures. I don't know whether that's actually been implemented. Does anybody else know?

A - W. Westfield: Since I am vice chairman of the committee, I'd have to say no. Nobody has started the work yet.

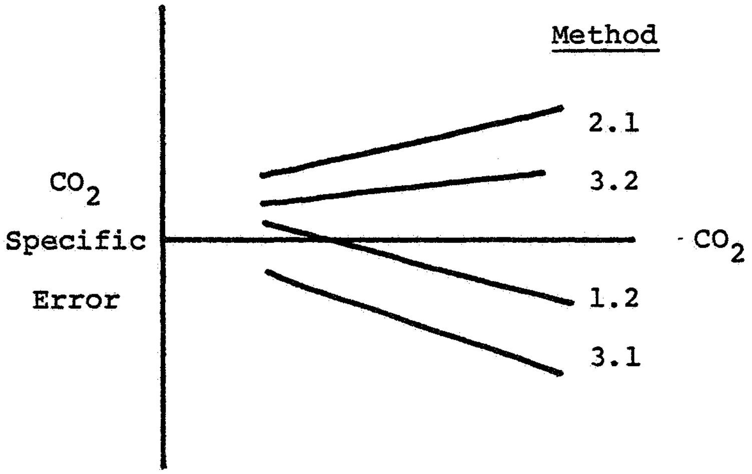
COMMENT - E. Kempke: Dr. Mirsky's techniques are interesting and I agree with Bernie Rezy of TCM that there does need to be further discussion and exploration of which techniques should be used. I feel that probably that's about the extent of what can be accomplished in this meeting. The subject is a very specialized one and it does need, as a minimum, a special meeting of those that are most intimately involved to discuss and try to get some more clarification of what's been proposed. I know in talking with others that there may exist some different ideas about what should be explored as well. We agree that the Spindt technique may have some deficiencies at the lower power conditions and, therefore, other alternatives should be looked at.

COMMENT - L. Helms: Speaking for the technical policy committee, I was not familiar with the effort of SAE that George Kittredge mentioned. However, we cannot stand the luxury of another 6 months or a year's delay. We are literally running out of lead time. I would like to reinforce the recommendation that a joint committee be formed between our GAMA people and the ones here and get on with it. I don't know how long the SAE panel has been debating or been delaying but we cannot stand additional delays.



$$\text{SPECIFIC ERROR} = \text{SLOPE} = \frac{\text{CHANGE IN \% ERROR}}{\text{1\% INCREASE}}$$

a) SENSITIVITY PLOT, SPECIFIC ERROR



b) SPECIFIC ERROR CURVES

Figure 4-1