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The Algorithmic Structure of the Air/Fuel Ratio Calculation

(There is really only one A/F ratio equation)

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Feature Articles

The Algorithmic Structure of the Air/Fuel Ratio Calculation

(There is really only one A/F ratio equation.)

William M. Silvis*

<Abstract>
A confusing number of equations have been developed and published for calculating the air/fuel ratio of an operating engine from the composition of its exhaust gasses These equations make varying use of the information available from the gas concentration measurements, but all are based on the same physics and chemistry of combustion The MEXA 9000 line of motor exhaust analyzers had been required to support 72 different equations of this type It can be shown that the combustion chemistry has a structure that can be used to design a single algorithm that duplicates the results of these many equations The new MEXA 7000 series uses this algorithm to simplify the measurement of this important parameter and provide the user with greater flexibility

1. Introduction

There seems to be an uncountable number of different equations for calculating the air to fuel ratio of an engine's combustion process from its exhaust emissions As an example, in our company, the control computer for the MEXA motor exhaust analysis system had been required to support 72 such equations Many authors have published papers that are referenced as sources for them

However, there is only one mother nature All of these equations are based on the same chemistry and physics of the same combustion phenomena This paper presents a unified method, an algorithm, that produces the same results as any of them Elements of the calculation that describe the fuel and air properties are

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空燃比計算のためのアルゴリズムの構造

(空燃比計算式は，実際には一種類しかない)

1 はじめに

排気ガスから空燃比を求める計算式について多くの論文が発表されている．当社の自動車排気ガス測定装置では72種類の計算式が用意されていた．しかし，燃焼に関する自然の法則は一つしかなく，計算式は同じ物理化学に基づいている．

本稿では，これらの計算式と同じ結果が得られるアルゴリズムについて紹介する．燃料や空気の性状などを，パラメータを求める計算方法として表し計算を単純化している．また，測定の非理想状態に対する補正も多くを取り入れた．

2 空燃比計算式の簡単な歴史

D'Alleva1)が最初に論文を発表し，排気ガス成分と空燃比との関係を説明した．排気ガス濃度から空燃比を読み取る図を発表し，1936年当時広く必要とされた．

included as parameters Different utilization of the available information, which has resulted in very different looking equations, are presented simply as alternative methods for calculating the same parameter: the amount of water in the exhaust Also, a number of small corrections for non-idealities of the measurement process, which are usually overlooked, are included

2. A Brief History of the Development of A/F Equations

D'Alleva1) wrote the earliest paper regularly cited in the literature He described the relationship between the exhaust gas composition and the air fuel ratio He published charts that could be used to read the A/F ratio based on exhaust concentrations, according to the fuel h/c ratio This was in 1936, when charts were a common and necessary engineering practice

Spindt2) published the next step forward He published an actual formula using CO, CO_2, HC and O_2 It did not require an assumption of complete combustion

In 1973, William Holl3) at AC Spark plug published formulae that did not require a measurement for oxygen Since the formulae are algebraically complex, he developed simplified equations by using power series approximations and ignoring the higher order terms

In 1974 Simons4) from the German TUEV recognized that the extra degree of freedom provided by an O_2 measurement could be used to calculate the equilibrium constant K This improved the agreement of his formula to measured test data It showed that K could vary, and that it was generally lower than the 3 5 that was commonly assumed

In 1979 Brettschneider5) added terms to Spindt's equation to account for both water in the ambient air and to incorporate a measured NOx into the equation He also included terms for oxygenated fuels

Thus the published methods fall into three classes, - those represented by Spindt/Brettschneider, by Holl, and by Simons Each class distinguishes itself from the others in the manner in which the water from combustion is estimated To see this, we look at some of the details of the algorithm

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Spindt2)は，さらに進んで，CO, CO_2, HCおよびO_2を用いて，完全燃焼を仮定する必要がない計算式を発表した．

1973年，William Holl3)は酸素の測定が不要な計算式を発表した．式は複雑であったが，べき級数近似による簡略式を開発した．

1974年，Simons4)は，O_2の測定により平衡定数(K)が計算できることに気づき，計算値と実測値との一致度が改善された．Kは変動し，通常仮定される3 5より低いことを示した．

1979年，Brettschneider5)は大気中の水分とNOx測定値を考慮した項を，Spindtの計算式に追加した　また，含酸素燃料に対する項も加えた．

以上，発表された方法は，Spindt/Brettschneiderに代表されるもの，Hollに代表されるもの，Simonsに代表されるもの，三つのグループに大別される．各グループの違いは，燃焼による水分を推定する方法にある．

3. Building an Algorithm to Calculate A/F

First, consider the chemical equation for ideal complete combustion This is the basis for computing the stoichiometric amount of oxygen (or air) that is used to burn a given fuel This quantity is used to calculate the normalized air fuel ratio, lambda (or phi, the inverse of lambda), and this equation is a good start toward a practical chemical equation to describe actual combustion:

$$C_x H_y O_z + \left(x + \frac{y}{4} - \frac{z}{2}\right) O_2 \rightarrow xCO_2 + \frac{y}{2} H_2O \qquad \cdots\cdots\cdots(1)$$

So we see that when the combustion is complete, and the mixture of reactants is stoichiometric, the moles of oxygen required are:

$$n_{stoich} = x + \frac{y}{4} - \frac{z}{2} \qquad \cdots\cdots\cdots(2)$$

For the more general case, there may be more or less moles of oxygen (air) than the stoichiometric amount In this case, the factor lambda, the excess oxygen factor or normalized air fuel ratio, is used to describe the combustion chemistry It is the ratio of the moles of oxygen actually used to the stoichiometric amount

$$\lambda = \frac{n}{n_{stoich}} = \frac{n}{\left(x + \frac{y}{4} - \frac{z}{2}\right)} \qquad \cdots\cdots\cdots(3)$$

It is clear then, that to calculate air fuel ratios from actual, measured exhaust gas concentrations, we need to calculate *n*, the amount of oxygen actually used in the combustion To do this, we need a more practical chemical equation for the combustion, one that also accounts for the non-ideal conditions, such as incomplete combustion and the moisture and CO_2 already in the ambient air An unbalanced chemical equation for this combustion that includes terms for these factors is:

$$\begin{aligned} &C_x H_y O_z + n\,(O_2 + A\ \ N_2 + B\ \ CO_2 + C\ \ H_{abs}\ \ H_2O) \rightarrow \\ &\quad aCO_2 + bCO + cH_2 + dH_2O + eO_2 + fN_2 + gNO_x + hC_{x'}H_{y'}O_{z'} \end{aligned} \qquad \cdots\cdots\cdots(4)$$

To be able to calculate *n*, we obtain a set of equations for the unknown mole quantities by balancing this equation We write 5 equations; the 4 atomic balances (C, H, O, N) and the total mole balance

Carbon balance : $x + n\ \ B = a + b + x'\ \ h$ ·········(5)

Hydrogen balance : $2\ \ n\ \ C\ \ H_{abs} + y = 2\ \ c + 2\ \ d + y'\ \ h$ ·········(6)

Oxygen balance: $z + 2n + 2n\ \ B + n\ \ C\ \ H_{abs} = 2a + b + d + 2e + g + z'\ \ h$ ··(7)

Nitrogen balance : $2\ \ n\ \ A = 2f + g$ ·········(8)

Total moles(dry) balance : $n_{tot} = a + b + c + e + f + g + h$ ·········(9)

3　空燃比計算のためのアルゴリズムの構築

理想的な完全燃焼の場合，化学反応は式(1)で表される　この式は，燃焼に必要な酸素(または空気)の理論量を求める基本である．理論混合気が完全燃焼する時，必要な酸素のモル数(n_{stoich})は式(2)で表される．

通常は理論量より多いか少ない酸素が存在する．この場合，空気過剰率(λ)が燃焼反応を記述するために使われる．λは使用された酸素のモル数(n)と理論量(n_{stoich})との比である．実際の空燃比を求めるには，不完全燃焼や大気中の水分とCO_2などを含む燃焼反応式が必要であり，これを式(4)に示す．ここで，C, H, O, Nの平衡と全体のモル数から式(5)～(9)を得る．

通常，水分を除去したHC, CO, CO_2およびNOxの濃度が測定される．濃度とモル数とは式(10)の関係となる．式(10)は，既知のパラメータと濃度を測定するCO_2, CO, HCのモル数を含んでいるから，全モル数(n_{tot})は式(11)から求めることができる．次に，酸素の平衡から，nを求める式(12)が得られる．

ここで，nを解きλを計算するには，水のモル数dに対する式をまとめればよ

We normally measure the concentrations of HC, CO, CO_2 and NOx Concentrations are mole fractions They are usually measured on a dry basis, that is, after most water has been removed from the sample They can be related to the mole quantities by the following equation, ($n_{H_2Ocooler}$ is the moles of water left in the sample after it exits the cooler)

$$[X] = \frac{n_X}{n_{tot} + n_{H_2O_{cooler}}} \qquad \cdots\cdots\cdots(10)$$

Since the first equation above includes only known parameters and mole quantities whose concentrations are always measured, CO_2, CO, and HC, it can be used to calculate n_{tot} :

$$n_{tot} = \frac{x + B \quad n}{[CO_2] + [CO] + [HC]} \ (1\text{–}[H_2O]_{cooler}) \qquad \cdots\cdots\cdots(11)$$

There are now the four unknowns, *n*, *c*, *d*, and *f*, and the remaining 4 equations The oxygen balance provides a convenient solution for *n*:

$$n = \frac{2a + b + d + 2e + g + z'h - z}{2 + 2 \quad B + C \quad H_{abs}} \qquad \cdots\cdots\cdots(12)$$

At this point, we only need to develop an expression for *d*, the moles of water, in order to solve for *n* and therefore lambda It is also at this point that the methods of Spindt and Brettschneider differ from the methods of Simons The differences in these approaches can be viewed simply as a difference in the technique used to calculate *d* Brettschneider and Spindt use another chemical reaction, the water/gas reaction, and Simons uses the remaining two equations, the nitrogen balance and the total moles balance

3 1 Brettschneider/Spindt Method

At the high temperature and pressures in the exhaust cylinder during the combustion of a rich mixture of air and fuel, the CO_2 and H_2O in the mixture dissociate, creating some H_2 and some CO. This is described by the following chemical equation for the water/gas reaction These species reach an equilibrium described by the equilibrium constant for this reaction, K The equilibrium depends on the combustion temperature and is influenced by catalytic converters

$$CO_2 + H_2 \rightarrow CO + H_2O \qquad \cdots\cdots\cdots(13)$$

The equilibrium is described by:

$$K = \frac{b \quad d}{a \cdot c} \qquad \cdots\cdots\cdots(14)$$

い．この点こそが，Spindt/Brettschneiderの方法がSimonsの方法と異なる点である Brettschneider/Spindtは，水性ガス反応平衡を利用しているのに対し，Simonsは窒素および全体のモル数の平衡を利用している．

3 1 Brettschneider/Spindtの方法

高い温度と圧力において過濃混合気が燃焼する時，CO_2およびH_2Oは解離し，H_2とCOが生成される．反応平衡定数Kは式(14)で示される．水素の平衡から水素のモル数cの式が得られ，式(14)に代入して水のモル数dが式(15)から得られる．

3 2 Simonsの方法

Simonsは，窒素および全体のモル数の平衡を利用してdを求めている．窒素，酸素および水素の平衡からf，nおよびcの式を求め全体のモル数の平衡，式(9)に代入すると，式(16)が得られる．

3 3 O_2の測定値がないときの方法

水性ガス反応平衡からdが既知のとき，式(17)によって酸素のモル数eを求めることができる．これが3番目の方法，すなわち酸素の測定値がないときの発想である．

Next, from the hydrogen balance we can get an expression for the hydrogen moles, *c*, and substituting this into the equilibrium condition, we get the following expression for the moles of water:

$$d = \frac{y + 2\ \ n\ \ C\ \ H_{abs} - y'h}{2\left(\frac{b}{a\ \ K} + 1\right)} \qquad \cdots\cdots\cdots(15)$$

3 2 Simons Method

Simons described another approach His method uses the nitrogen and mole balance to find *d* We can obtain expressions for f, n and c from the nitrogen balance, the oxygen balance and the hydrogen balance Substituting those into the total mole balance, we get the following algebraic simplification:

$$d = \frac{\left(n_{tot} - a - b - \left(\frac{y - y'h}{2} + n\ \ C\ \ H_{abs}\right) - e - \frac{g}{2} - h\right)\ \frac{2+2\ \ B+C\ \ H_{abs}}{A} - 2a - b - 2e - g - z'h + z}{1 - \frac{2+2\ \ B+C\ \ H_{abs}}{A}} \qquad \cdots(16)$$

3 3 Method when no O_2 measurement is available

Note that if *d* is known from the water gas equilibrium, similar steps can be used to calculate *e*, the oxygen This is useful for cases when the oxygen concentration is not measured This is the idea behind the third type of A/F calculation, the "no O_2" type

$$e = \frac{n_{abs} - a - b - c - \frac{A}{(2+2B+C\ \ H_{abs})}\ \ (2a + b + d + 2e + g + z'h - z) + \frac{g}{2} - g - h}{1 + \frac{2A}{2+2B+C\ \ H_{abs}}} \qquad \cdots(17)$$

3 4 Fixed Point Iteration

At this point it is important to note that the equations above are circular The calculation for *n* depends on *d*, which in turn depends on *n* The circularity arises when some of the second order effects that are usually ignored are included Of course, this could be resolved by a great deal of algebra and a very complicated closed form equation for *n* could be written However, this is not necessary It is convenient to use a fixed point iteration We assume an initial value for *n*, use it to calculate *d* and subsequently another *n* This is repeated until the new values for *n* are no longer significantly different This happens after just a few iterations

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3 4 不動点反復法

上記の式が循環的なことが重要な点である．nの計算はdに依存し，dの計算はnに依存する．代数的に処理すると非常に複雑な式を解かなければならないが，不動点反復法によればその必要はない．nの初期値を仮定し，これを用いてdを計算し，続いて次のnを計算する．nの新しい値に有意差がなくなるまで繰り返す．

4 アルゴリズム

本提案のアルゴリズムは次のように要約される．

(1) nの初期値を1 0，dの初期値を1 0とする．
(2) 式(11)によってHC, CO, CO_2濃度からn_{tot}を計算する．
(3) 式(10)によって各濃度からモル数を計算する．
(4) 水のモル数dを次のいずれかから計算する．
  BrettschneiderのK，つまり式(9)
  酸素を測定しない場合は，式(17)によってdを使ってeを計算する．
  または，式(16)からdを計算する．

4. Algorithm

The following steps summarize the algorithm:

(1) Assume an initial value of 1 0 for n, and an initial value of 1 0 for d

(2) Calculate n_{tot} from HC, CO, and CO_2 concentrations according to equation 11

(3) Calculate the mole fractions from the concentrations and n_{tot} according to equation10

(4) Calculate the water moles, d, from one of:
the Brettschneider K formula, equation 15
If an oxygen measurement is not available, use this d and calculate e by equation 17
Or calculate d from equation16

(5) Calculate n from the total oxygen moles equation 12

(6) Compare this to the old value for n If the difference is small, go to the next step
Otherwise, go back and repeat, starting with the n_{tot} calculation, step 2

(7) Once n is calculated, calculate lambda from n/n_{Stoich} , equation 3

5. Example

As an example, we can compare the A/F ratio calculated from this algorithm to that from the equation published by Brettschneider The following table shows a comparison using data he included in his paper The algorithm and the Brettschneider equation give identical results

Parameters

Fuel $C_xH_yO_z$	
x	1
y	1 817
z	0

Exhaust $C_xH_yO_z$	
x'	1
y'	1 817
z'	0

Air	
Habs	4 85
$[O_2]_{amb}$	20 99%
$[N_2]_{amb}$	79 01%
$[CO_2]_{amb}$	0 000%
GMW_{air}	28 97

Bench	
Cooler 'C	na
K	3 5

No	CO_2 %	CO ppm	THC ppm	NOx ppm	O_2 %	λ Algorithm	λ B-calc	Diff
1	10 06055	77675 8	3975 0	360 0	0 17496	**0 7811**	0 78109	0 00%
3	11 49805	54423 8	3481 0	737 5	0 21246	**0 8432**	0 84322	0 00%
5	12 99805	29121 1	2856 0	1473 8	0 30621	**0 9172**	0 91719	0 00%
7	14 06055	10498 0	1715 5	2131 0	0 42493	**0 9822**	0 98224	0 00%
9	14 39844	3843 4	887 5	2318 5	0 58118	**1 0149**	1 01489	0 00%
11	13 43555	1187 3	315 7	1938 8	2 04980	**1 1025**	1 10249	0 00%
13	11 89844	937 3	137 5	356 3	4 09277	**1 2309**	1 23085	0 00%
15	10.94727	1093.6	278.2	87.5	5.28613	**1.3213**	1.32135	0.00%

An appropriate choice of parameters for this algorithm has been shown to duplicate nearly all of the 72 various equations that previously had been supported by individually programmed computer subroutines

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(5) 式(12)からnを計算する．

(6) 計算したnの値と前のnの値を比較する．差が小さければ次のステップへ，そうでなければステップ2に戻ってn_{tot}の計算から繰り返す．

(7) nの計算ができれば，式(3)からλを計算する．

5 計算例

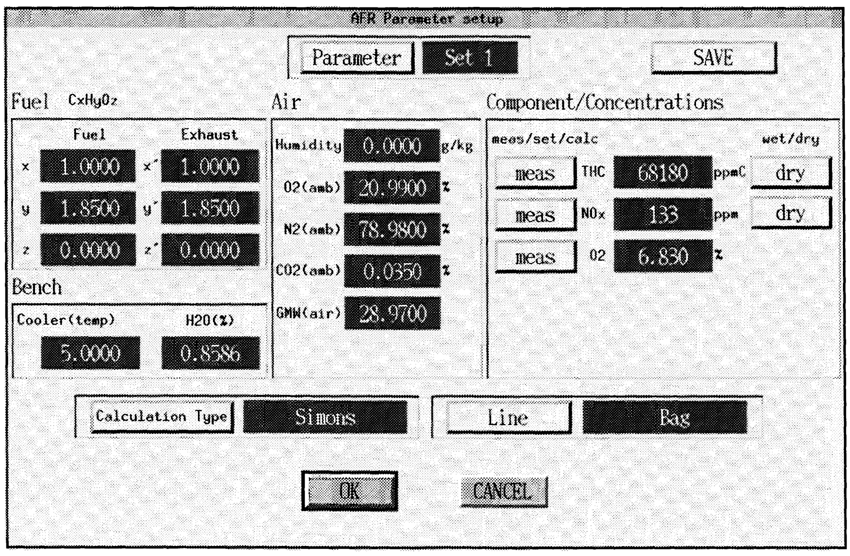
一例として本アルゴリズムとBrettschneiderによる結果の比較を次の表に示す．また，本アルゴリズムのパラメータを適切に選択することで，個別にプログラムされていた72種類の空燃比計算式のほとんどと同じ結果が得られた．

6 MEXA-7000 A/Fパラメータ画面

MEXA-7000にはタッチパネル式スクリーン(図)が組み込まれ，ユーザがパラメータを設定し易くしている．画面左側に燃料の性状を炭素，水素，酸素の原子数比x, y, zとして設定する．排気ガス中の未燃焼成分の原子数比は別に設定できる．中央に空気の性状を，右側に濃度測定値の詳細を設定する 計算方法は中央の

6. MEXA 7000 A/F Parameter Screen

In order to make it convenient for the user to specify the parameters that define this algorithm, a convenient touch panel screen, illustrated in the following figure, has been built into the Main Control Unit of the MEXA 7000 series emissions bench



Parameter Set 1

Fuel CxHyOz
Fuel: x 1.0000, y 1.8500, z 0.0000
Exhaust: x' 1.0000, y' 1.8500, z' 0.0000

Bench
Cooler(temp) 5.0000
H2O(%) 0.8586

Air
Humidity 0.0000 g/kg
O2(amb) 20.9900 %
N2(amb) 78.9800 %
CO2(amb) 0.0350 %
GMW(air) 28.9700

Component/Concentrations
meas/set/calc — wet/dry
meas THC 68180 ppmC dry
meas NOx 133 ppm dry
meas O2 6.830 %

Calculation Type Simons
Line Bag

In the upper left area are the fields for the properties of the fuel These are expressed in the usual x, y, z notation for the molecular ratios of the hydrogen, carbon and oxygen The ratios found unburned in the exhaust gas can be specified separately The fields in the middle area can be used to specify the properties of the combustion air, in case it is useful to alter these to match the values used in a particular equation On the right side one can specify details about the concentration measurements such as wet or dry basis or if an assumed value should be used The method for the calculation is selected by a drop down list in the center.

As an important added convenience, sets of these parameters can be saved under a user definable name for quick recall This makes it a simple matter to switch the calculation for different fuels or sampling points

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ドロップダウンリストから選択する．さらに，一連のパラメータは保存･呼出しができ，燃料やサンプル採取点が変わっても計算方法を簡単に切り替えることができる．

7 結論

従来の空燃比計算式の多くを，一つの手順に置き換えるアルゴリズムを示した．簡単な反復法により，複雑な代数式を導入することなく，非理想状態に対する補正をすることができる．MEXA-7000のセットアップ画面とパラメータの設定で，測定成分やサンプル採取点の違い，ユーザの好みにフレキシブルに対応できる．

(抄訳　エンジン計測開発部　浅野一朗)

7. Conclusion

An algorithm has been demonstrated that can replace the myriad of available air fuel ratio equations with a single procedure A simple iterative technique accommodates terms to correct for non-ideal effects without introducing badly complicated algebraic forms Parameters to the procedure and a convenient setup screen on the MEXA 7000 provide the flexibility to adapt to different available measurements, sample points, and user preferences

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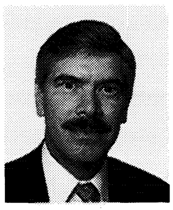

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