

# Rapid Calculation of Solid Fat Index Values from Dilatometer Readings

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## ABSTRACT

Equations are presented for the reduction of dilatometer readings to AOCS solid fat index (SFI) values. The equations include corrections for expansion of the confining fluid. The corrections were derived from fundamental equations describing the thermal expansion of water. These equations permit machine calculation of SFI values without the use of tables of corrections, resulting in a significant reduction in computational time.

## INTRODUCTION

The AOCS dilatometric solid fat index (SFI) procedure (1) is widely used in the determination of the plastic range of many products. Unfortunately, the conversion of dilatometer readings to SFI values can be a tedious task involving much computation. The need to interpolate volume corrections for thermal expansion of the confining fluid from a table does not make this task any easier. Furthermore, the occasional need to use reference temperatures other than 60 C introduces additional complications as correction tables for other reference temperatures do not accompany the method and must either be constructed or obtained from other sources.

These problems can all be overcome by calculating SFI values with a programmable calculator or a computer. Machine calculation results in a great reduction in computational time and eliminates the need for tables of volume corrections as the corrections can be rapidly calculated from first principles. The following paragraphs detail the appropriate equations which are presented in a general form. They can be reorganized to allow a number of approaches to machine calculation depending on the needs and constraints of a specific laboratory, computer, or calculator.

## MATHEMATICAL DESCRIPTION OF COMPUTATIONS

The SFI of a fat at any temperature  $t$  can be thought of as the specific melting dilation (total dilation minus thermal expansion) between  $t$  and some reference temperature  $T$  at which the sample is completely liquid. The equation expressing this quantity is:

$$SFI = \frac{R(T) - R(t) - Vc(t)}{W} - \frac{R(T) - R(T') - Vc(T')}{W} \times \frac{T - t}{T - T'} \quad (1)$$

- where
- $T$  = a reference temperature, usually 60 C, at which the sample is completely liquid.
  - $T'$  = a second, lower, reference temperature, usually 37.8 C, at which the sample is completely liquid.
  - $t$  = any temperature  $\leq T$ .
  - $R(t)$  = dilatometer reading at  $t$  in microliters.
  - $Vc(t)$  = volume correction for the thermal expansion of glass and water between  $t$  and  $T$  in microliters.
  - $W$  = the sample weight, g.

Unlike the expression in the official method, the above equation is general with respect to temperature. This expression assumes the coefficients of thermal expansion for both solid and liquid fat to be identical and independent of temperature over the temperature range of interest. All other terms being measurable, let us direct our attention to the calculation of the required values of  $Vc(t)$ .

A number of assumptions and approximations are made in arriving at the volume corrections tabulated in the AOCS SFI procedure. These corrections are necessary because a certain amount of variability is allowed in the initial reading at the upper reference temperature. As a result, the volume of confining fluid immersed at any given temperature for a given sample may vary somewhat from laboratory to laboratory. While this laboratory-to-laboratory bias is compensated for by the tabulated volume corrections, it is particularly important to realize that these values do not correct for all of the variability in the volume of the confining fluid. Thus, no correction is made for the fact that the temperature of the confining fluid which is *not* immersed will vary from laboratory to laboratory and even from bath to bath within a laboratory. Nor is any adjustment made in the tabulated corrections for that variation in the immersed volume of confining fluid which results from changes in sample volume when going from one temperature to another. Of these two effects, the former is less significant and corrected for only with great difficulty. The second effect will, to a good approximation, be constant from one laboratory to the next for a particular sample.

Recognizing that we wish to correct for lab-to-lab variability in the initial reading at the upper reference temperature, we can proceed in developing the required equations. The expression for water expansion between  $t$  and  $T$  may be derived from the general expression for thermal expansion of water. Thus, for temperature  $t$

$$V_t = V_0(1 + \alpha t + \beta t^2 + \gamma t^3 + \delta t^4). \quad (II)$$

The values of the coefficients can be obtained from the literature, various reference works, or handbooks. The values used here are:

$$\begin{aligned} \alpha &= -6.581 \times 10^{-5} \\ \beta &= 8.507 \times 10^{-6} \\ \gamma &= -6.769 \times 10^{-8} \\ \delta &= 3.75 \times 10^{-10} \end{aligned}$$

An expression similar to (II) can be written for temperature  $T$ , namely:

$$V_T = V_0(1 + \alpha T + \beta T^2 + \gamma T^3 + \delta T^4). \quad (III)$$

Defining a function  $f(t) = \alpha t + \beta t^2 + \gamma t^3 + \delta t^4$  and combining (II) and (III) we obtain an expression for the expansion of water between  $t$  and  $T$ , namely:

$$V_T - V_t = V_0 [ f(T) - f(t) ] \quad (IV)$$

It now remains for us to define  $V_0$ . Strictly speaking, it is the volume of water under consideration measured at 0 C. Within the limits of temperature being considered here, no significant errors ( $<0.5\%$ ) are introduced by neglecting temperature effects. Thus, in the official method, 2 ml of water are used as the confining fluid, and the dilatometer is immersed to the 0.300 ml mark. The amount of water, in microliters, contained in that portion of the dilatometer which is immersed is, therefore, given by the following

TABLE I  
Comparison of Volume Corrections for 60 C

| Bath temp. | 60 C Reading (microliters) |                   |      |      |      |      |      |      |      |      |
|------------|----------------------------|-------------------|------|------|------|------|------|------|------|------|
|            | 1000                       | 1100              | 1200 | 1300 | 1400 | 1500 | 1600 | 1700 | 1800 | 1900 |
| 0 C        | 22.0 <sup>a</sup>          | 22.0 <sup>b</sup> | 20.3 | 20.3 | 18.6 | 18.6 | 16.9 | 16.9 | 15.2 | 15.2 |
| 5          | 22.2                       | 22.2              | 20.4 | 20.5 | 18.7 | 18.7 | 17.0 | 17.0 | 15.3 | 15.3 |
| 10         | 21.8                       | 21.8              | 20.1 | 20.1 | 18.5 | 18.4 | 16.8 | 16.7 | 15.1 | 15.1 |
| 15         | 21.1                       | 21.0              | 19.4 | 19.5 | 17.8 | 17.8 | 16.2 | 16.2 | 14.6 | 14.6 |
| 20         | 19.9                       | 19.8              | 18.4 | 18.4 | 16.8 | 16.8 | 15.3 | 15.3 | 13.8 | 13.8 |
| 25         | 18.4                       | 18.4              | 17.0 | 17.0 | 15.6 | 15.6 | 14.2 | 14.1 | 12.7 | 12.7 |
| 30         | 16.6                       | 16.6              | 15.3 | 15.3 | 14.0 | 14.0 | 12.8 | 12.7 | 11.5 | 11.4 |
| 35         | 14.5                       | 14.4              | 13.4 | 13.3 | 12.3 | 12.2 | 11.1 | 11.1 | 10.0 | 10.0 |
| 40         | 12.1                       | 12.0              | 11.2 | 11.0 | 10.2 | 10.2 | 9.3  | 9.2  | 8.4  | 8.3  |
| 45         | 9.5                        | 9.4               | 8.7  | 8.7  | 8.0  | 8.0  | 7.3  | 7.2  | 6.6  | 6.5  |
| 50         | 6.6                        | 6.6               | 6.1  | 6.1  | 5.6  | 5.6  | 5.1  | 5.1  | 4.6  | 4.5  |
| 55         | 3.4                        | 3.2               | 3.2  | 3.0  | 2.9  | 2.8  | 2.6  | 2.5  | 2.4  | 2.3  |
| 60         | 0                          | 0                 | 0    | 0    | 0    | 0    | 0    | 0    | 0    | 0    |

<sup>a</sup>This work.

<sup>b</sup>Reference 1.

approximate but satisfactory expression:

$$V_0 = 2000 - [R(T) - 300]. \quad (V)$$

The expansion of glass over the temperature range of interest can be neglected. Substitution of (V) into (IV) gives:

$$V_c(t) = V_T - V_t = [2300 - R(T)] [f(T) - f(t)] \quad (VI)$$

Finally, combining (I) and (VI) provides a general expression for SFI, namely:

$$\begin{aligned} \text{SFI} = & \frac{R(T) \cdot R(t) - [2300 - R(T)] [f(T) - f(t)]}{W} \\ & - \frac{R(T) - R(T') - [2300 - R(T)] [f(T) - f(T')]}{W} \\ & \times \frac{(T - t)}{(T - T')} \end{aligned} \quad (VII)$$

## RESULTS

Table I provides a comparison of volume corrections calculated from equation (VI) with those tabulated in the official method. The validity of equation (VI) is clearly evident. It should be noted that this expression is valid for reference temperatures other than 60 C; the temperature limits being dependent only on the limits for the coefficients of thermal expansion which are used. Thus, in situations

where programmable calculators or computers are not readily available for routine calculation, equation (VI) can be used to generate expanded tables of volume corrections for any reference temperature of interest.

## DISCUSSION

A general expression has been derived which allows direct machine calculation of SFI values from dilatometer readings. This expression is valid for calculation of SFI values within the limitations and assumptions inherent in the official dilatometric procedure. Considerable rearrangement and simplification is possible in situations where a general expression is not needed. This flexibility should be utilized to advantage when coding algorithms for use with a computer or programmable calculator. A completely general program for use with a Hewlett-Packard Model HP-65 calculator and tables of corrections for any reference temperature are available from the author on request.

## REFERENCES

1. "Official and Tentative Methods of the American Oil Chemists' Society," Third Edition, 1974, AOCS, Champaign, IL, Method Cd 10-57.

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