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Evaluation of the integral of the Arrhenius function by a series of Chebyshev polynomials — use in the analysis of non-isothermal kinetics

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Abstract

The Padé rational function in general use as an approximation for the $p(X)$ function or the Arrhenius integral seems to be in error. A corrected equation is given. Even the correct rational function, and other suggested approximating equations, are not accurate enough at low values of $X = E/RT$. Chebyshev polynomials offer a better solution, over the whole range of X values, to a greater precision than found in published tables. Relatively simple computer routines may be used to generate the coefficients required.

The Stander and van Vuuren/Zsakó method of analysis of non-isothermal data may be used to test the time of a typical calculation.

Keywords: Non-isothermal; Kinetics Arrhenius; Integral Chebyshev

1. Introduction

The simplest experiment to determine the kinetics of a thermal decomposition is thermogravimetry under non-isothermal conditions. If a computer is used to log the results, a large number of accurate readings are then available. Difficulties appear when these results have to be interpreted.

The evolution of the equations involved have been given many times, especially in the reviews [1–3]. The basic rate equation may be combined with the Arrhenius equation

$$\frac{d\alpha}{dt} = kf(\alpha), \quad k = Ae^{(-E/RT)}, \tag{1}$$

where α is the fraction of solid reacted at time t, k the rate constant (s^{-1}), $f(\alpha)$ a function of a depending on the mechanism of decomposition being obeyed. (One of the difficulties is finding a method to decide which of the possible functions is being obeyed, when well over 20 equations have been suggested. Summaries of some of the methods appear in [1–3].)

A is a pre-exponential function, dependent upon the rate of transfer of energy to a decomposition site, E the activation energy for the process, R the gas constant, and T the absolute temperature.

Assuming a rate of heating of b °/s and integrating and substituting $X = E/RT$ gives:

$$g(\alpha) = \frac{AE}{Rb}\int_{X_0}^{X} e^{-X}X^{-2}dX, \quad \text{where}$$

$$p(X) = \int_{X_0}^{X} e^{-X}X^{-2}dX, \tag{2}$$

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where $g(\alpha)$ is the integral of $1/f(\alpha)$. Unfortunately $p(X)$ cannot be integrated.

A large number of solutions to this problem, with varying complexity and precision, have been published [4–21]. In some cases the data has been tabular. Other authors have proposed approximating formulae which involve infinite series or so called rational functions. The authors were always seeking to prove how precise their formulae were by reference back to earlier tabulated values. Many papers just refer back to other workers in this field, which in turn refer back to earlier work, but there seem to be only a few original data sets available [4,5,22–25]. These early mathematical tables are themselves derived from some approximating infinite series, because there is, of course, no true value for the integral. The question is not only 'how precisely do the recent approximations fit the older standard tabulated data', but also, 'how reliable are the older data sets'.

Another step, often made in this problem, is to use integration by parts to get:

$$p(X) = \frac{e^{-X}}{X} - \int_X^{\infty} \frac{e^{-X}}{X} dX. \tag{3}$$

The integral part still cannot be evaluated, but it is a well known mathematical function called the integral of the exponential function, $E_1(X)$, which is numerically the same as another function $-E_i(-X)$ and approximating series and tables for their values have been published [22–25].

2. Approximating equations for $p(X)$

Amongst the approximating formulae that have appeared, are the ones put forward by Senum and Yang [11] which are known as rational or Padé approximations. If $p(X)$ is evaluated from Eq. (3), then the integral part, $E_1(X)$, may be found from the rational function given by the coefficients found in Table 4.3 of [26] (1st and 2nd parts, p. 111):

$$p(X) = \frac{e^{-X}}{X} - \frac{e^{-X}}{X} \frac{(X^4 + 19X^3 + 102X^2 + 154X + 24)}{(X^4 + 20X^3 + 120X^2 + 240X + 120)}. \tag{4}$$

This simplifies to:

$$p(X) = \frac{e^{-X}}{X} \times \frac{(x^3 + 18x^2 + 86x + 96)}{(x^4 + 20x^3 + 120x^2 + 240x + 120)}. \tag{5}$$

Senum and Yang [11] gave equations of this type with the degree of the polynomial in the denominator from 1 to 4, plus two other earlier approximating equations for comparison. They actually quoted results as a percentage error from standard data in [22], up to the 3rd degree equation only, for X from 0.5 to 100. They did give results for the 4th degree equation, seeming to prefer the 3rd degree equation. Many other workers have used this type of approximation using Senum and Yang's degree equation. Unfortunately, in their equation, they gave the coefficient of X on the top line as 88 and not the correct value of 86 as given in Eq. (5). This has, recently, also been noted by Flynn [21].

It is always possible that the coefficients in Table 4.3 of [26] are incorrect, but the equations to generate these coefficients are given in the same reference on p. 83. When tried, these gave exactly the coefficients of Table 4.3 of [26].

Table 1 shows the precision to be expected from the various approximation equations, compared with the tabulated values. This is similar to the table given by Senum and Yang [11] and shows the percentage error found for a reasonable number of X values, covering a range wide enough for any X value found in an analysis of kinetic results. This seems to be a simpler way of displaying the results than the complex error graphs given by other workers.

The error is given as literature table value of $p(X)$ minus the calculated value from an approximating equation. It may be seen that most errors are positive except for some Zsakó values and the incorrect 4th degree equation. Some values at $X = 100$ are also negative, but the value of $p(X)$ is here very small and also the absolute error is very low, and might be influenced by the precision of calculation on a particular computer.

It is unfortunate that Senum and Yang [11] did not put the error values for the 4th degree equation in their paper and also unfortunate that so many other workers

Table 1
$p(X)$ given by Zsakó and Padé approximations as percentage error relative to $p(X)$ calculated from the tables in [22]

$X = E/RT$	Zsako	1st degree	2nd degree	3rd degree	4th degree (Eq. (5))	4th degree (Senum/Yang)
0.5	−21.6	25.72	9.67	4.33	2.15	1.47
1.0	−2.91	17.42	4.72	1.58	0.608	−0.381
2.0	−0.157	9.86	1.66	0.370	0.0983	−1.05
5.0	−0.200	3.40	0.235	0.0239	3.13×10^{-3}	−0.905
10.0	0.155	1.22	0.0347	1.58×10^{-3}	9.93×10^{-5}	−0.532
20.0	0.185	0.383	3.75×10^{-3}	6.41×10^{-5}	1.65×10^{-6}	−0.235
40.0	0.0823	0.109	3.24×10^{-4}	2.13×10^{-6}	3.72×10^{-7}	−0.083
100.0	0.0172	0.019	1.03×10−5	-2.61×10^{-7}	-2.72×10^{-7}	−0.016

chose to use that equation blindly, without knowing if it worked. The error has now been propagated through many research publications [14,16,27–30] (and no doubt others).

Other previous methods of calculation of $p(X)$ have included asymptotic series such as Eq. (6) [9]:

$$p(X) = \frac{e^{-X}}{X^2} \times \left(1 - \frac{2!}{X} + \frac{3!}{X^2} - \frac{4!}{X^3} + \cdots + \frac{(-1)^n (n+1)!}{X^n}\right). \quad (6)$$

The problem with this type of equation is that the terms of the series need to decrease rapidly in value, so that a reasonable number of terms will give sufficient precision. At high values of X, i.e. >20, this is so. However, at low X the method fails, and the terms do not decrease rapidly enough. When $X = 10$ the terms first fall, then rise again, so evaluation is impossible. Even at $X = 20$ terms in the equation after the 19th begin to rise, so the evaluation should be stopped at that point, restricting precision to only seven significant figures. At $X = 10$ only the first nine terms decrease and the precision is restricted to two significant figures! Below $X = 10$ the method becomes impossible. This has been pointed out by Zsakó [12].

Another series suggested is shown in Eq. (7) [9]:

$$p(X) = \frac{e^{-X}}{X(X+1)}\left(1 - \frac{1}{X+2} + \frac{1}{(X+2)(X+3)} - \ldots + \frac{(-1)^{n+1}}{(X+2)\ldots(X+n)}\right). \quad (7)$$

This equation gives terms that are continuously becoming smaller, but the result is not all that close to the tabulated values of $p(X)$, giving only three significant figures of precision at the most.

Some other series have been suggested for low values of X such as the power series [11,12,22]:

$$p(X) = \frac{e^{-X}}{X} + \gamma + \ln(X) + \sum_{n=1}^{\infty} \frac{(-1^n n}{nn!}, \quad (8)$$

where γ is the Euler–Mascheroni constant, equal to 0.5772156649.

Unfortunately this function is only valid for $X < \pi$. This is pointed out in [11,22], but not in [12]. This equation is then of little use.

Only a few types of equations are mentioned here, but many others have been suggested [2–20] and reviewed [12,21,22].

The author decided to investigate new ways of calculating values of $p(X)$ with particular aims in mind.

1. The tables used in the past, for checking values obtained, are rather old and, considering the date of publication, must have been produced without the aid of computers, except for [22]. This may mean that they contain errors. A new set of values, computer-calculated, was needed.
2. The older tables often actually contained E_1 or E_i and so $p(X)$ must have been calculated from them, allowing the possibility of error again. $p(X)$ needed to be calculated and printed out or displayed directly.
3. The range of X covered by the tables was very variable from table to table. Only Ref. [22] was comprehensive. From an examination of literature

it seemed that the range $0.5 < X < 100$ should be covered.

4. The precision of the values of $p(X)$ was also variable between four significant figures for Doyle [5], five figures for Zsakó [4] to 8/10 figures in the standard tables [22–25]. It was decided to produce results at least as precise as the tables in [22–25] to allow comparisons to be made with these tables and to check the various suggested approximating formulae.
5. The evaluation of $p(X)$ should be placed in a procedure in a computer program, so that anyone who requires a value of $p(X)$, can call it in their own program, using their own favoured technique of non-isothermal analysis. If the program proves to be too slow, it should be possible, after testing at high precision, to cut back the precision to save time in the calculation.
6. The method of calculation used should be equally precise over all of the range of X values used. Many of the previous approximations are accurate at high X, but fail at low X, e.g. when $X < 5$.

3. Chebyshev polynomials

A better solution to the problem is to use Chebyshev polynomials. They provide values of $\exp(-X)/X$. E_1, from which E_1 and $p(X)$ may be calculated and are of similar precision throughout the range of X values. In a summation series, used in this method, the individual terms decrease continuously for almost all values of X. The variable X has to be converted into a normalised quantity, W/X, where W is a normalising factor and represents the smallest value of X that may be used, i.e. W/X must not exceed 1. There is no maximum X; the only limit imposed is in the precision of the computer (smallest numbers that may be stored as the terms and $p(X)$ value). In this application it is suggested that W, and thus the minimum X, is 0.5.

These polynomials are described in some detail in Luke's books [26,31].

The integral part of Eq. (3), or E_1, is given in [26] (p. 105):

$$E_1 = \int_X^\infty \frac{e^{-X}}{X}\,dX = \frac{e^{-X}}{X}\sum_{n=0}^{\infty} C_n T_n^*(W/X). \tag{9}$$

In this, C_n is a series of single coefficients of steadily decreasing size as n increases. This series is particular to the function being evaluated, E_1 here. T_n^* is a series of polynomials: as n rises the degree of the polynomial rises, as does the magnitude of the polynomial coefficients. T_0^* is a single constant, T_1^* is a first degree polynomial etc. There are several types of Chebyshev polynomials T_n. The particular set used here, T_n^*, is called shifted polynomials of the first kind and sets are listed in [26] (p. 462). This set is fixed and is used irrespective of the particular function being evaluated.

Values of the coefficients C_n for the integral E_1 are given in of [26] (p. 105), but these are for $W = 5$. The constants from the two tables in [26] could have been entered directly into a computer routine and used to evaluate $p(X)$. However, a large number of digits would have to be typed, with the risk of making a mistake. Secondly, the table given for C_n is for $W = 5$ and it is suggested that for the present application the set for $W = 0.5$ is used. Thirdly, the table for T_n^* stops at $n = 20$ and C_n stops at $n = 30$ and it was thought better to be able to try more terms, if the computer can hold them, at least for purposes of testing agreement with the older tables. For this reason it was decided to use routines to calculate the coefficients required, to store the coefficients and use them to evaluate $p(X)$. The coefficients C_n were found using the recurrence formula given on [26] (p. 218), shown here as Eq. (10). This has been slightly rearranged and symbols changed for Luke's program in [31] (p. 94):

$$\begin{aligned} C_n = {} & (n+1) \\ & \times \left[\left(2D - \frac{(2n+3)(n+\mathrm{ap}+1)(n+\mathrm{bp}+1)}{(n+2)} - 4W\right)\right. \\ & \times C_{n+1} + \left(\frac{D}{(n+1)} - 2(2n+3-2W)\right) \\ & \left. \times C_{n+2} - \left(\frac{(n+3-\mathrm{ap})(n+3-\mathrm{bp})}{(n+2)}\right) C_{n+3}\right]/D. \end{aligned} \tag{10}$$

where $D = (n+\mathrm{ap})(n+\mathrm{bp})$, $\mathrm{ap} = 1.0$, $\mathrm{bp} = 1.0$.

Since ap and bp are both 1.0, the formulae could have been simplified, but Luke's style of programming has been retained.

The recurrence was started from the end, i.e. putting $C_{n+3} = C_{n+2} = 0.0$ and $C_{n+1} = 1 \times 10^{-20}$, and working backwards.

There is also a rescaling procedure to make the sum of the absolute value of the coefficients equal to unity. The details of such a routine are given in [31] (p. 95).

The Chebyshev polynomial coefficients T_n^* were calculated using [26] (p. 432, Eq. (11); p. 436, Table B, the entry for T_n^*), and [31] (pp. 17 and 18). The orthogonal polynomials follow a recurrence formula:

$$q_{n+1}(X) = (a_n X + b_n)q_n(X) - c_n q_{n-1}(X)$$

$$\text{where} \quad q_n = \sum_{k=0}^{n} a_{k,n} X^k. \qquad (11)$$

$a_n = 4$, $b_n = -2$, $c_n = 1$ (note c_n is different to C_n above).

For the first polynomial, degree zero, the constant is 1. For the second polynomial, degree one, the constant is 2 and the coefficient of X^1 is -1. The recurrence formula then gives the coefficients for the other polynomials, one more coefficient for each successive polynomial. The values for the first 21 equations ($n = 0$–20) are given in [26] (p. 462, Table 11.4). In this case, the sum of the coefficients for any one polynomial should equal unity. If it does not, then the computer has lost some of the digits of precision because it is at the limit of its capacity.

4. Computer program

A computer program was written in FORTRAN 77 and was run using a compiler and executing system produced by Salford Software Ltd at Salford University. One subroutine calculates the values of C_n and stores them for later use. Similarly another subroutine finds the coefficients of the Chebyshev polynomials, T_n^* and stores them. These routines only need to be called once. To get the required precision the normal length *Real* variables were too short, so *Double Precision* real variables were used throughout. The coefficients in the T_n^* polynomials are all integer in value but rise to very large numbers. Single precision *Integer* variables would not hold these large numbers. Double sized integers were tried, but were still too small. It was necessary to declare the array to hold the coefficients as *Double Precision* real, even though it only held integer quantities. If more and more terms are used then eventually the array of coefficients will have truncated quantities because the precision limit is reached. It was found that the maximum number of terms that could be used was 40 before the coefficients in one polynomial did not add up to unity, i.e. digits were lost.

A further evaluation routine returned the value of E_1 for the value of X fed to it. A main program was provided for test purposes only. It asked for an X value and number of terms, i.e. the highest degree polynomial to be used. It displayed the result as $-E_i(-X)$ [or $E_1(X)$], Xe^{-X} E_1, $p(X)$ and $\log p(X)$, for convenience, because the tables available for checking against [4,5,22–25] give results in these various forms. The test program was tried by comparison against the tables, using $W = 0.5$. It gave perfect agreement with Doyle [5] and Zsakó [4] (tables with limited precision). It also gave perfect agreement with the other tables, which were of greater precision. The agreement for all values of $X > 1$ was perfect, as long as sufficient number of terms was taken. The program actually gives a more precise result (17/18 significant figures) than any of the tables. For $0.5 < X < 1.0$ the situation was more complicated, as shown in Table 2.

As might be expected, the agreement improves as the number of terms is raised, but as n reaches 40, and W/X approaches 1.0, the error rises to a large value. This is true to some extent for $n = 30$ as well. The situation is improved if the program is re-written in Pascal, which points to a precision fault or truncation of variables, Pascal variables being more precise than FORTRAN. Examination of intermediate calculations in the FORTRAN program showed that some variables were being truncated in value. The result for $X = 0.5$ and $n = 40$ is fortuitously accurate. When $W/X = 1.0$ exactly, there is some cancelling of intermediate values and no truncation of variables occurs.

It would appear better to restrict n to a maximum of 25 to preserve the highest precision down to $X = 0.5$. In practice it is highly unlikely that an agreement of anything as close as 10^{-5}% would be required and $n = 15$ or $n = 20$ would suffice.

The choice of how precisely to calculate $p(X)$ could be decided by the precision of experimental results. The mass readings would normally be known to four significant figures for a 10 mg sample, and the temperature to a similar precision, given that there is always random noise on a thermocouple EMF at the μV level. This means that 15 terms might be sufficient, but time of calculation should be considered as well.

Table 2
Values of E_1 calculated by Chebyshev compared with the published table values [22] as percentage error values summarised to show the range of power of 10[a]

N-terms	$X = 0.5$	$X = 0.6$	$X = 0.7$	$X = 0.8$	$X = 0.9$	$X = 1.0$
10	$<10^{-2}$	$<10^{-2}$	$<10^{-2}$	$<10^{-2}$	$<10^{-2}$	$<10^{-2}$
	$<10^{-3}$	$<10^{-3}$	$<10^{-3}$	$<10^{-3}$	$<10^{-3}$	$<10^{-3}$
15	$<10^{-3}$	$<10^{-3}$	$<10^{-3}$	$<10^{-3}$	$<10^{-3}$	$<10^{-3}$
	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$
20	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$	$<10^{-4}$
	$<10^{-5}$	$<10^{-5}$	$<10^{-5}$	$<10^{-5}$	$<10^{-5}$	$<10^{-5}$
25	$<10^{-5}$	$<10^{-5}$	$<10^{-5}$	$<10^{-5}$	$<10^{-5}$	$<10^{-5}$
	$<10^{-6}$	$<10^{-6}$	$<10^{-6}$	$<10^{-6}$	$<10^{-6}$	$<10^{-6}$
30	$<10^{-5}$	$<10^{-2}$	$<10^{-4}$	$<10^{-4}$	$<10^{-6}$	0
	$<10^{-8}$	$<10^{-7}$	$<10^{-7}$	$<10^{-8}$	$<10^{-7}$	0
40	$<10^{-5}$	1273	11	0.096	$<10^{-2}$	0
	$<10^{-8}$	$<10^{-1}$	$<10^{-1}$	$<10^{-4}$	$<10^{-5}$	0
Padé degree 18	$<10^{-2}$	$<10^{-2}$	$<10^{-3}$	$<10^{-3}$	$<10^{-3}$	$<10^{-3}$

[a] This is for the low range of X only. For higher X the agreement is perfect. The first line is from the FORTRAN program and the second line is from the Pascal program.

Senum and Yang [11] suggested that more terms could be used in the Padé or rational function, if greater precision were required. The constants for this, in the table in Luke's book [26] (p. 111), go up only to 6th degree. To go beyond this requires the constants calculating by the recurrence formula (12) [26] (p. 111). The constants become very large as the degree of the equation rises. The largest term has roughly the same number of digits as the degree. Thus to avoid errors it is best to calculate and use the equations inside a computer program. If such a program is used, and the degree of the equation is raised, the precision of the value of $p(X)$ improves with each step of degree up to the 18th degree equation. On stepping to the 19th equation, the result is obviously faulty, with errors of up to 100%. This is because the FORTRAN program cannot hold the variable required to a high enough precision. The results for a rational or Padé equation of degree 18 are shown in Table 2 on the bottom row. The precision is of the order of the same result for the Chebyshev equations with $n = 10$. This shows the superiority of the Chebyshev results.

5. Time taken for an evaluation of $p(X)$

A main program was set up to find how long it took to find a value of $p(X)$ for a given value of X using the Chebyshev polynomial method compared with Eq. (5). The computer used was a PC with a 486 DX4 100 processor chip (486 with integral floating point processor, running at 100 MHz). The time taken to repeatedly evaluate $p(20)$ 5000 times is shown in Table 3.

The increase in time between $n = 15$ and 20 is not great and would be worth allowing to achieve a greater precision of one more significant figure. The time taken for the Padé equation of degree 18, explained above, is also shown. Although it is faster than the Chebyshev polynomials, it is of the same order of

Table 3
Time for the evaluation of $p(X)$ $\{X = 20\}$ 5000 times (comparision of Chebyshev and Padé methods)

n (degree of polynomial)	Chebyshev polynomials (s)	Eq. (5) (Padé degree 4) (s)	Padé degree 18 (s)	Time per $P(x)$ (Chebyshev) (s)
40	14.451	0.055	0.495	2.890×10^{-3}
20	3.956	0.055		7.912×10^{-4}
15	2.582	0.055		5.164×10^{-4}

speed, so the Chebyshev method is worth using for the greater precision obtained. The difference in time between Chebyshev polynomials and Eq. (5) is large, but this could be tolerated if, when the $p(X)$ evaluation is used in a complete non-isothermal analysis, it does not occupy a time that is too much out of proportion to the rest of the calculations.

To test this, the Chebyshev method was incorporated into the author's favoured method of analysis. The first step in this program is to find the slope, $\tan\beta$, of $\log(g(\alpha))$ versus $1/T$, where $g(\alpha)$ is the integral function of α. The value of $\tan\beta$ was inserted into the equation of MacCallum and Tanner [8] (see Šesták [9]), allowing for a change from calorie to Joule.

This gave a starting point for the value of E. A value for X was next obtained, using an average temperature of T_{av}. This was then used in an iterative procedure, as first suggested by Škvára and Šesták [32]:

$$E = RX^2 e^X p(X) \tan\beta. \quad (12)$$

This equation was printed incorrectly in references [32,34], but the theory is given correctly in references [9,10].

The new E was used to obtain a new X, etc. This was continued until successive E values were within 1 J/mol of each other. In this method only one $p(X)$ has to be evaluated per iteration. The value of E obtained will not be quite correct because the iteration Eq. (12) uses $\tan\beta$ which cannot be a true value because $\log(g(\alpha))$ versus $1/T$ is not a true straight line.

An alternative calculation is that advocated by Stander and van Vuuren [33], based on an idea by Zsakó [4].

If the correct $g(\alpha)$ function has been chosen, then the E obtained is the true value and the two curves $g(\alpha)$ and $p(X)$ versus T are parallel.

The problem with this method is that it requires an evaluation of $p(X)$ for each data point for each iteration, which is considerably more than in the first method.

A compromise is to use the first iterative method to get an approximate E and then to use Stander and van Vuuren's method, at the end, for a last adjustment of the E value.

A program was written using the strategy described, with Chebyshev polynomials used to evaluate $p(X)$, testing 25 possible kinetic equations divided between six graph plots. The number of times $p(X)$ was evaluated using the Škvára and Šesták method was about 400, and if the Stander and van Vuuren method was added at the end, the evaluations were about 90 000 times. However, this was to check theoretical data made up from a known equation and known values of E and A. The value of E was calculated to the nearest 1 J/mol and it had to agree with the starting value of E. In practical use, there is probably no reason to require E to this precision, bearing in mind that mass is only recorded to four significant figures. If the precision in E is reduced, then the number of $p(X)$ evaluations would be reduced. In changing from the Padé ratio approximation to Chebyshev polynomials, for the Škvára and Šesták method the time increased from 3 to 4 s. Most of the time was used for the rest of the calculation, graph plotting, output of results etc. For the combined calculation, adding Stander and van Vuuren's method, the time went up from 5 to 60 s. Using another PC with no floating point processor (floating point calculations emulated within the FORTRAN library), running at 25 MHz, the times went up considerably, of the order of 80 times longer. Under these conditions the calculation is probably too slow to tolerate.

6. Conclusions

The speed of computers is still rising and modern processor chips all have a built-in floating point unit. In that case it is possible to use the calculations described on a reasonable time scale. There is, in that case, no longer the need to use approximating functions for $p(X)$, but to use Chebyshev polynomials, which provide $p(X)$, as precisely as required by the user, over the whole range of X values, with no errors appearing at low X, unlike all of the previously published equations.

Stander and van Vuuren/Zsakó's method of analysis seems to be able to pick out the correct kinetic equation from one non-isothermal experiment, only if the data are recorded to a high degree of precision.

The program mentioned is also available in Pascal and BASIC as well as FORTRAN 77. A copy in either language may be obtained from the author, if required, by sending a 3.5 inch floppy disc to the given address or e-mail to roger_heal@yehoo.cor.

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