LETTERS TO THE EDITOR

To the Editor:

In "New Temperature Integral Approximation for Nonisothermal Kinetics" (pp. 1554-1557),[1] Cai et al. have retested the validity of the Wanjun-Yuwen equation of temperature integral approximation, and the results disagreed with that stated by Wanjun et al.[8] The Wanjun-Yuwen equation and its shortened expression

$$\int_0^T e^{-(E/RT)} dT = \frac{RT^2}{1.002E + 1.874RT} e^{-(E/RT)}$$

for the approximation of temperature integral, are critically analyzed. It is shown that the accuracy of Wanjun-Yuwen equation accords with that reported by Wanjun et al. We stress that the shortened Wanjun-Yuwen equation is also simple, accurate, and reliable, and can be used in nonisothermal kinetic analysis.

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In their recent article, Cai et al.[1] proposed a new approximation for the temperature integral

$$\int_0^T e^{-(E/RT)} dT = \frac{E}{R} P(u)$$

where E is the activation energy, R is the universal gas constant, T is the absolute temperature, $u = E/(RT)$, and

$$P(u) = \int_u^\infty \frac{e^{-u}}{u^2} du$$

The proposed approximation for the temperature integral has been validated by comparing with several known approximate formulas, which included Coats-Redfern[2], Gorbachev-Lee-Beck[3,4], Li Chung-Hsiung[5], Agrawal[6], Quanyin-Su[7] equations. The formula,[8] labeled as Wanjun-Yuwen equation, was also introduced for comparison. Cai et al.[1] reported that the deviation ratio of Wanjun-Yuwen equation was more than 0.1% in the range $15 \le u \le 80$. This obviously disagrees with the previous statement,[8] in which the deviation ratio of Wanjun-Yuwen equation was less than 0.1% in the range $u \ge 14$. The values of deviation ratio at $u = 5$ and 10 are different from that reported previously.[8]

To clarify the earlier discrepancy, the accuracies of the equations of Coats-Redfern[2], Gorbachev-Lee-Beck[3,4], Agrawal[6], Wanjun-Yuwen[8], together with that proposed by Cai et al.[1], are reanalyzed. A shortened Wanjun-Yuwen formula, which parameters have just three significant figures after radix point, is proposed for the first time. The precision of the shortened Wanjun-Yuwen equation has been calculated as well. Their expressions and the corresponding approximations are listed in Table 1. An expression of Wanjun-Yuwen equation with "clerical error", in which parameter 1.00198882 is miswritten with 1.000198882, is also listed in Table 1. $P(u)$ has been determined as a function of u by numerical integration by MATLAB 6.5. The corresponding relative

Table 1. Expression for Some Proposed Approximations for the Temperature Integral

Author	$\int_0^T e^{-(E/RT)} dT$	$P(u)$
Coats-Redfern[2]	$\frac{RT^2}{E}\left(1 - \frac{2RT}{E}\right)e^{-(E/RT)}$	$\frac{e^{-u}}{u^2}\left(1 - \frac{2}{u}\right)$
Gorbachev-Lee-Beck[3,4]	$\frac{RT^2}{E + 2RT} e^{-(E/RT)}$	$\frac{e^{-u}}{u}\frac{1}{u+2}$
Agrawal[6]	$\frac{RT^2}{E}\left[\frac{1 - 2\left(\frac{RT}{E}\right)}{1 - 5\left(\frac{RT}{E}\right)^2}\right]e^{-(E/RT)}$	$\frac{e^{-u}}{u^2}\left(1 - \frac{2}{u}\right)\Big/\left(1 - \frac{5}{u^2}\right)$
J. Cai et al.[1]	$\frac{RT^2}{E}\frac{E + 0.66691RT}{E + 2.64943RT} e^{-(E/RT)}$	$\frac{e^{-u}}{u^2}\frac{u + 0.66691}{u + 2.64943}$
Wanjun-Yuwen[8]	$\frac{RT^2}{1.00198882E + 1.87391198RT} e^{-(E/RT)}$	$\frac{e^{-u}}{u}\frac{1}{1.00198882u + 1.87391198}$
Wanjun-Yuwen/shortened	$\frac{RT^2}{1.002E + 1.874RT} e^{-(E/RT)}$	$\frac{e^{-u}}{u}\frac{1}{1.002u + 1.874}$
Wanjun-Yuwen/clerical error	$\frac{RT^2}{1.000198882E + 1.87391198RT} e^{-(E/RT)}$	$\frac{e^{-u}}{u}\frac{1}{1.000198882u + 1.87391198}$

Table 2. Percentage Deviation from Numerical Result for Some Approximations at Various *u*

u	Coats-Redfern[2]	Gorbachev-Lee-Beck[3,4]	Agrawal[6]	Cai, et al.[1]	Wanjun-Yuwen[8]	Wanjun-Yuwen/ shortened	Wanjun-Yuwen/ clerical error
5	−18.858128	−3.402533	1.427341	0.186918	−1.772747	−1.774801	−1.644876
10	−5.175813	−1.224805	−0.185066	−0.046774	−0.342841	−0.344515	−0.192637
15	−2.395500	−0.628903	−0.177216	−0.029834	−0.063049	−0.064561	0.095938
20	−1.378704	−0.382529	−0.130333	−0.012326	0.009835	0.008413	0.173481
25	−0.895519	−0.257165	−0.096289	−0.001642	0.025751	0.024385	0.192275
30	−0.628361	−0.184737	−0.073212	0.004627	0.022883	0.021557	0.191361
35	−0.465202	−0.139126	−0.057273	0.008318	0.013542	0.012244	0.183430
40	−0.358277	−0.108549	−0.045921	0.010492	0.002252	0.000976	0.173207
45	−0.284412	−0.087053	−0.037591	0.011751	−0.009207	−0.010465	0.162582
50	−0.231253	−0.071367	−0.031316	0.012442	−0.020133	−0.021378	0.152327
55	−0.191723	−0.059570	−0.026477	0.012775	−0.030276	−0.031509	0.142735
60	−0.161530	−0.050475	−0.022673	0.012878	−0.039578	−0.040802	0.133893
65	−0.137949	−0.043315	−0.019629	0.012833	−0.048067	−0.049282	0.125794
70	−0.119180	−0.037578	−0.017156	0.012692	−0.055803	−0.057011	0.118393
75	−0.103997	−0.032909	−0.015122	0.012490	−0.062856	−0.064058	0.111631
80	−0.091542	−0.029060	−0.013428	0.012250	−0.069298	−0.070494	0.105444
85	−0.081198	−0.025849	−0.012002	0.011987	−0.075193	−0.076385	0.099774
90	−0.072513	−0.023142	−0.010792	0.011713	−0.080602	−0.081790	0.094565
95	−0.065151	−0.020839	−0.009755	0.011433	−0.085578	−0.086761	0.089769
100	−0.058856	−0.018864	−0.008861	0.011153	−0.090166	−0.091347	0.085342

errors of various approximations for $P(u)$ have been included in Table 2.

Except for Wanjun-Yuwen equation, as shown in Table 2, values of the percentage deviation from numerical results for various approximations are identical to that reported by Cai et al.[1] Also, they agree well with the results obtained by Wanjun et al.[8] The values of percentage of Wanjun-Yuwen equation shows that it is indeed less than 0.1% in the range $u \geq 14$ which validates the former results.[8] Meanwhile, the shortened Wanjun-Yuwen equation shows quite similar values of error with the original one, which indicates the shortened Wanjun-Yuwen equation is simple, accurate, reliable, and suitable for the evaluation of kinetic parameters from nonisothermal analysis, too. This fact implies that the parameters in approximations are not necessary to keep too many significant figures. However, the values of the percentage deviation for Wanjun-Yuwen equation reported by Cai et al.[1] are equal to that from the equation with the clerical error (Table 1), which suggests that Cai et al. might use a Wanjun-Yuwen equation with the clerical error (Table 1) in evaluating its accuracy. Therefore, the accuracy values that Cai et al. have calculated for this approximation could be wrong.

In my opinion, the article by Cai et al. may drive the readers to the erroneous conclusion that Wanjun-Yuwen equation for temperature integral approximation should not produce enough precise values of kinetic parameters. By publishing this note I hope to alert the readers from falling into this wrong conclusion.

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