To the Editor:

In "New Temperature Integral Approximation for Nonisothermal Kinetics" (April 2006), Junmeng et al.[1] proposed a new approximation for the temperature integral (here we called it Junmeng-Fusheng approximation).

After some further researches, we have obtained a modification of Junmeng-Fusheng approximation for the temperature integral. The derivation of the modified approximation is shown later in this letter.

The following first degree rational approximation for the $Q(u)$ function is assumed

$$Q(u) = \frac{au + b}{u + c}$$

where a, b and c are underdetermined parameters, and $u=E/RT$.

By using the pattern search method, the values of a, b and c have been obtained: $a = 0.99962$, $b = 0.60462$, $c = 2.56879$. The corresponding approximations for the $P(u)$ function and the temperature integral are given below

$$P(u) = \frac{e^{-u}}{u^2}\frac{0.99962u + 0.60642}{u + 2.56879}$$

$$\int_0^T e^{-(E/RT)}dT = \frac{RT^2}{E}\frac{0.99962E + 0.60642RT}{E + 2.56879}e^{-(E/RT)}$$

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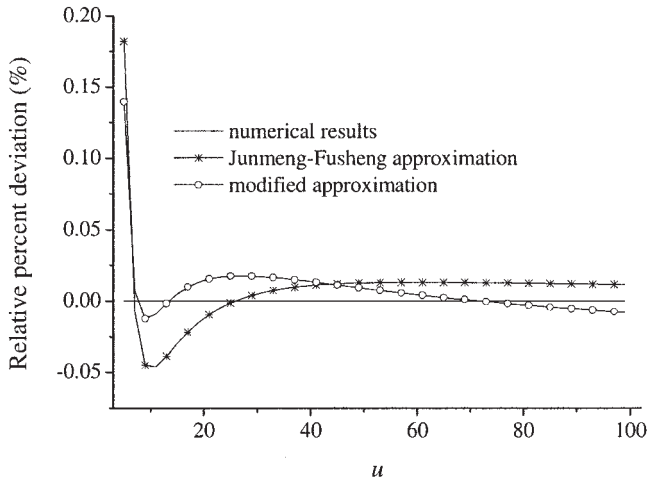

Figure 1. Comparison of the accuracy of Junmeng-Fusheng approximation and its modification.

Since $P(u)$ is the variable-transformed expression of the temperature integral, the accuracy evaluation of the temperature integral approximation is identical to that of the corresponding $P(u)$ approximation. The relative percent deviations associated with the use of the Junmeng-Fusheng approximation and its modification for a physical realistic domain of u are shown in Figure 1.

From Figure 1, we can observe that the modified approximation is more accurate than Junmeng-Fusheng approximation almost in the range of $5 \le u \le 100$ where most thermal decomposition reactions take place.

Literature Cited

1. Junmeng Cai, Fusheng Yao, Weiming Yi, Fang He. New temperature integral approximation for nonisothermal kinetics. *AIChE J.* 2006;52;4: 1554-1557.

Junmeng Cai
College of Power Engineering,
University of Shanghai for Science and Technology,
No. 516 Jungong Road, Shanghai 200093, P. R. China.
E-mail: caijunmeng7321@163.com

Fang He
School of Light Industry & Agriculture Engineering,
Shandong University of Technology,
No. 12 Zhangzhou Road, Zibo 255049, P. R. China
E-mail: hefang_sdut@163.com
hf@sdut.edu.cn