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Short Communication

A constitutive model of polyether-ether-ketone (PEEK)

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ABSTRACT

A modified Johnson–Cook (JC) model was proposed to describe the flow behaviour of polyether-ether-ketone (PEEK) with the consideration of coupled effects of strain, strain rate and temperature. As compared to traditional JC model, the modified one has better ability to predict the flow behaviour at elevated temperature conditions. In particular, the yield stress was found to be inversely proportional to temperature from the predictions of the proposed model.

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1. Introduction

Polyether-ether-ketone (PEEK) is a semi-crystalline polyromatic linear polymer with a good combination of strength, stiffness, toughness and environmental resistance (Lu et al., 1996; Jenkins, 2000). In recent years, with the confirmation of biocompatibility (Rivard et al., 2002), PEEK has been increasingly employed as an effective biomaterial for implantable medical devices such as orthopaedic, spinal and cranial implants (Toth et al., 2006; Kurtz and Devine, 2007; El Halabi et al., 2011). Compared to stainless steel and titanium, an implant made of PEEK has clear benefits on temperature sensitivity, weight reduction and radiology advantage (Green

and Schlegel, 2001; Wang et al., 2010). As a result, there has been an increased demand of PEEK for medical applications. In so doing, it is necessary to understand the mechanical properties of PEEK not only at room temperature but also under elevated temperature for favourable processing conditions. In the past two decades, there has been an increasing interest in mechanical properties of PEEK (Boyce and Arruda, 1990; Dahoun et al., 1995; Hamdan and Swallowe, 1996; Jaekel et al., 2011). A series of material models were developed to quantify mechanical behaviours of PEEK (El Halabi et al., 2011; Jaekel et al., 2011; El-Qoubaa and Othman, 2015; Garcia-Gonzalez et al., 2015). However, most of these work focused on the mechanical properties at room temperature. Little

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attention has been paid to develop constitutive models of PEEK under elevated temperature. In this short communication, a new phenomenological constitutive, i.e. a modified Johnson–Cook (JC), model was proposed. The developed model can not only describe the flow behaviour of PEEK at room temperature, but also predict the flow stress at elevated temperatures. Therefore the modified JC model allows detailed evaluation of the sensitivities of the strain rate and temperature.

2. Constitutive modelling of PEEK

The flow behaviour of PEEK 450G was tested by [Rae et al. \(2007\)](#) for different temperatures and strain rates with a constitutive model established based on the experimental data. In this study, cylindrical compression specimens of 6.375 mm diameter and 6.375 mm height were machined from a commercial plate of extruded PEEK 450G. MST 880 and MST 810 servohydraulic machines were used for strain rates lower than 10 s^{-1} and between $10\text{--}100\text{ s}^{-1}$, respectively. The machine can be operated with an exponential decay of actuator speed to give constant strain rate with straining. True strain and stress data were calculated automatically by assuming a constant sample volume. In order to reduce the friction impact, paraffin wax was used to lubricate the specimen ends. In order to secure temperature uniformity, the samples were held at the testing temperature between 30 and 45 min prior to testing.

[Fig. 1](#) shows the flow stress behaviours of PEEK 450G at room temperature under the strain rates from 10^{-4} s^{-1} – 10^2 s^{-1} ([Fig. 1a](#)) and at the temperature range from $-85\text{ }^\circ\text{C}$ to $200\text{ }^\circ\text{C}$ at a constant strain rate of 10^{-3} s^{-1} ([Fig. 1b](#)). From [Fig. 1a](#), it is obvious that the flow stress curves clearly show that the yield stress increases with the increase of strain rates at room temperature. From [Fig. 1b](#), it can also be found that thermal history has a significant effect on the true stress–strain curves. The yield and flow stresses decrease with increasing temperature. This is mainly due to the high dependence of the mechanical properties of semi-crystalline polymers upon their degree of crystallinity and molecular weight as well as the size and orientation of the crystalline regions ([Chivers and Moore, 1994](#); [Kurtz and Devine, 2007](#); [Rae et al., 2007](#)). At the same time, it can be seen that there is little strain hardening effect over a range of temperature conditions.

2.1. JC model

The traditional phenomenological JC model may be expressed as ([Johnson and Cook, 1985](#))

$$\sigma(\epsilon^p, \dot{\epsilon}^p, T) = [A + B(\epsilon^p)^n] \left[1 + C \ln\left(\frac{\dot{\epsilon}^p}{\dot{\epsilon}_{\text{reference}}^p}\right) \right] (1 - T^{*m}) \quad (1)$$

where σ is the flow stress, A is the yield stress at reference temperature and reference strain rate, B is the strain hardening coefficient, n is the strain hardening exponent, ϵ^p is true strain, $\dot{\epsilon}$ is strain rate and $\dot{\epsilon}_{\text{reference}}$ is the reference strain rate. T^* is homologous temperature and is expressed as,

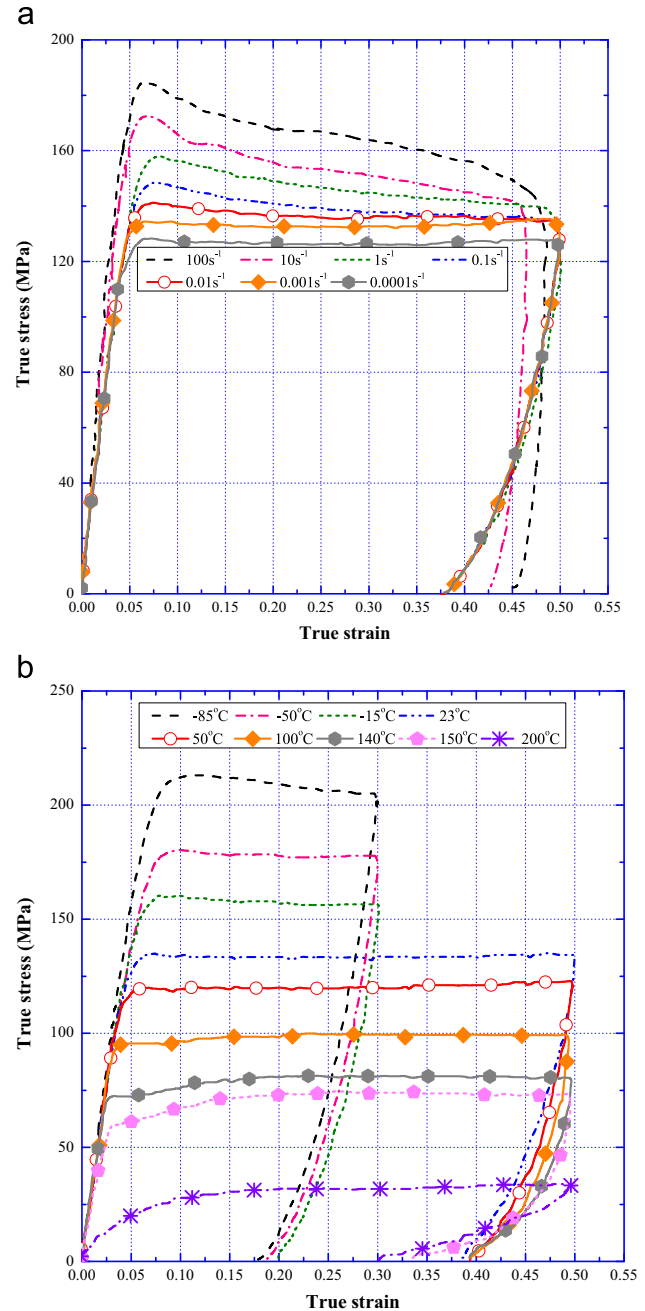


Fig. 1 – (a) Effect of strain rate on flow stress of PEEK at room temperature, and (b) effect of temperature on flow stress of PEEK at 10^{-3} s^{-1} ([Rae et al., 2007](#)).

Table 1 – JC model parameters ([Garcia-Gonzalez et al., 2015](#)).

Parameters	A (MPa)	B (MPa)	n	C	m
Values	132	10	1.2	0.034	0.7

$$T^* = \frac{T - T_{\text{reference}}}{T_{\text{melting}} - T_{\text{reference}}} \quad (2)$$

where T is temperature. $T_{\text{reference}}$ is the reference temperature. T_{melting} is the melting temperature of PEEK at 616 K. In Eq. (1), C and m are coefficients of strain rate hardening and

thermal softening exponent, respectively. Therefore, the total effect of strain hardening, strain rate hardening and thermal softening on the flow stress can be calculated by multiplication of these three terms in Eq. (1).

The temperature increase caused by deformation cannot be neglected when the strain rate is relatively high. The deformation-induced temperature increase can be estimated by assuming a conversion factor of 0.9 from deformation work into heat from an initial testing temperature T_0 ,

$$\int_{T_0}^T \rho C_p dT = 0.9 \int_0^{\epsilon^p} \sigma d\epsilon \quad (3)$$

where ρ is the density, C_p is the heat capacity, and ϵ is the strain. Assuming ρ and C_p are constants, therefore, Eq. (3) can be rearranged to,

$$T = T_0 + \Delta T = T_0 + \int_{T_0}^T dT = T_0 + \frac{0.9}{\rho C_p} \int_0^{\epsilon^p} \sigma d\epsilon \quad (4)$$

For PEEK material, $\rho = 1.304 \text{ g/cm}^3$, $C_p = 2.18 \text{ Jg}^{-1} \text{ K}^{-1}$. In this study, 296 K (room temperature) is taken as the reference temperature and 10^{-3} s^{-1} is taken as the reference strain rate.

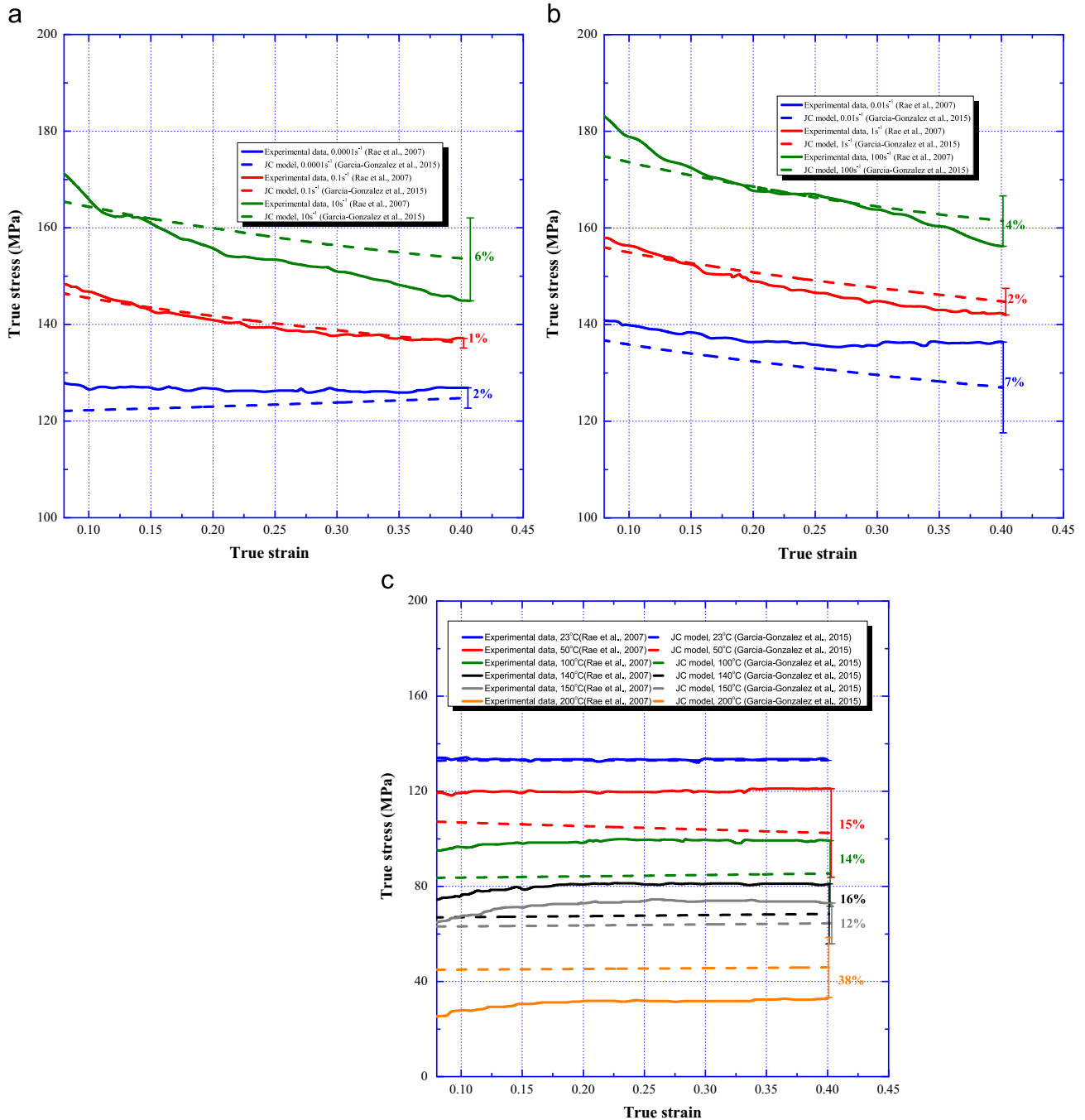


Fig. 2 – Comparisons of stress–strain of PEEK (a) and (b) at different strain rates at room temperature and (c) at different temperatures and strain rate of 10^{-3} s^{-1} .

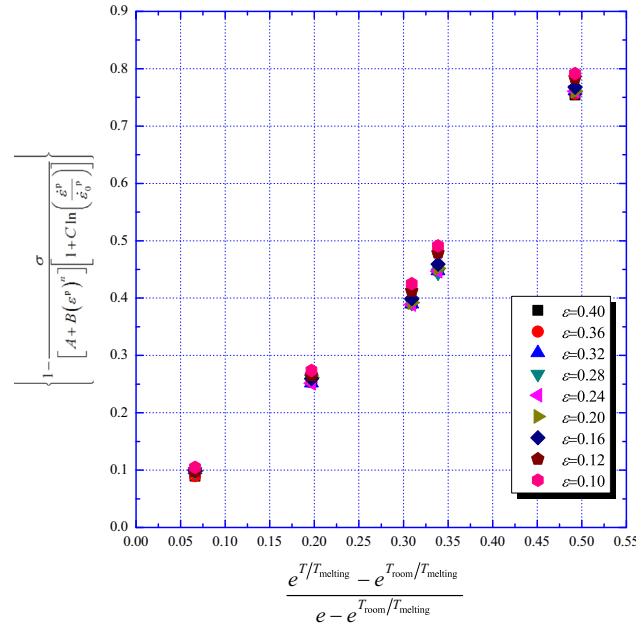


Fig. 3 – Determination of the value of λ .

At the reference strain rate of 10^{-3} s^{-1} , Eq. (1) reduces to,

$$\sigma(\epsilon^P, \dot{\epsilon}^P, T) = A + B(\epsilon^P)^n \quad (5)$$

The value of A is calculated from the yield stress (i.e. the stress at strain of 2×10^{-3}) of the flow curve at 296 K and 10^{-3} s^{-1} . Substituting the value of A in Eq. (5) and using the flow stress data at various strains for the same flow curves, $\ln(\sigma - A)$ vs $\ln \epsilon$ was plotted. B was calculated from the intercept of this plot while n was obtained from the slope.

At the reference temperature, there is no flow softening term, and so Eq. (1) can be expressed as

$$\sigma(\epsilon^P, \dot{\epsilon}^P, T) = [A + B(\epsilon^P)^n](1 - T^{*m}) \quad (6)$$

Using the flow stress data for a particular strain at different temperatures, the graph of $\ln\left[1 - \frac{\sigma}{A + B(\epsilon^P)^n}\right]$ vs $\ln T^*$ was plotted. The material constant m was obtained from the slope of this graph.

By using the experimental data (Rae et al., 2007), the parameters of the traditional JC model were obtained by Garcia-Gonzalez et al. (2015), as shown in Table 1.

Fig. 2 shows the comparisons between the predictions of JC model and experimental data. As can be seen from Fig. 2a and b, in the range of strain rates from 10^{-4} s^{-1} to 10^2 s^{-1} , the maximum deviation between the experimental data and JC model are less than 7%. Thus the developed JC model by Garcia-Gonzalez et al. (2015) can give an accurate prediction of the flow stress at room temperature. However, at elevated temperature, as shown in Fig. 2c, the maximum difference between the experimental data and JC model is 38%. Therefore, the traditional JC model cannot give good enough predictions under elevated temperatures. Hence it is highly desirable to develop new constitutive models that can be used to give improved prediction of the flow behaviour of PEEK at both room and elevated temperatures.

2.2. Modified JC model

Similar to the case of the traditional JC model, 296 K and 10^{-3} s^{-1} are taken as the reference temperature $T_{\text{reference}}$ and strain rate $\dot{\epsilon}_{\text{reference}}$, respectively, in deriving the modified JC model. By substituting the modified temperature term in the traditional JC model, the modified JC model is proposed as follows:

$$\sigma(\epsilon^P, \dot{\epsilon}^P, T) = [A + B(\epsilon^P)^n] \left[1 + C \ln\left(\frac{\dot{\epsilon}^P}{\dot{\epsilon}_{\text{reference}}^P}\right) \right] \times \left(1 - \lambda \frac{e^{T/T_{\text{melting}}} - e^{T_{\text{room}}/T_{\text{melting}}}}{e - e^{T_{\text{room}}/T_{\text{melting}}}} \right) \quad (7)$$

where A , B , n , C and λ are materials parameters. T_{room} is the room temperature, 296 K. Adopting the same method as mentioned above, the material constants can be obtained as, $A=132 \text{ MPa}$, $B=1.0797$, $n=0.06802$, $C=0.0207$. It is noteworthy that the values of B , n and C are different from the values obtained by Garcia-Gonzalez et al. (2015). This is mainly due to the mathematical treatment of the experimental data.

From Eq. (7), the following equation can be obtained:

$$1 - \frac{\sigma}{[A + B(\epsilon^P)^n] \left[1 + C \ln\left(\frac{\dot{\epsilon}^P}{\dot{\epsilon}_0^P}\right) \right]} = \lambda \frac{e^{T/T_{\text{melting}}} - e^{T_{\text{room}}/T_{\text{melting}}}}{e - e^{T_{\text{room}}/T_{\text{melting}}}} \quad (8)$$

By using the experimental data, the graph of $\left\{ 1 - \frac{\sigma}{[A + B(\epsilon^P)^n] \left[1 + C \ln\left(\frac{\dot{\epsilon}^P}{\dot{\epsilon}_0^P}\right) \right]} \right\}$ vs $\frac{e^{T/T_{\text{melting}}} - e^{T_{\text{room}}/T_{\text{melting}}}}{e - e^{T_{\text{room}}/T_{\text{melting}}}}$ was plotted, as shown in Fig. 3. The material constant is obtained from the slope of the graph to be 1.5343. Thus, the following modified JC model is obtained as

$$\sigma(\epsilon^P, \dot{\epsilon}^P, T) = [132 + 1.0797(\epsilon^P)^{0.06802}] \left[1 + 0.0207 \ln\left(\frac{\dot{\epsilon}^P}{\dot{\epsilon}_{\text{reference}}^P}\right) \right]$$

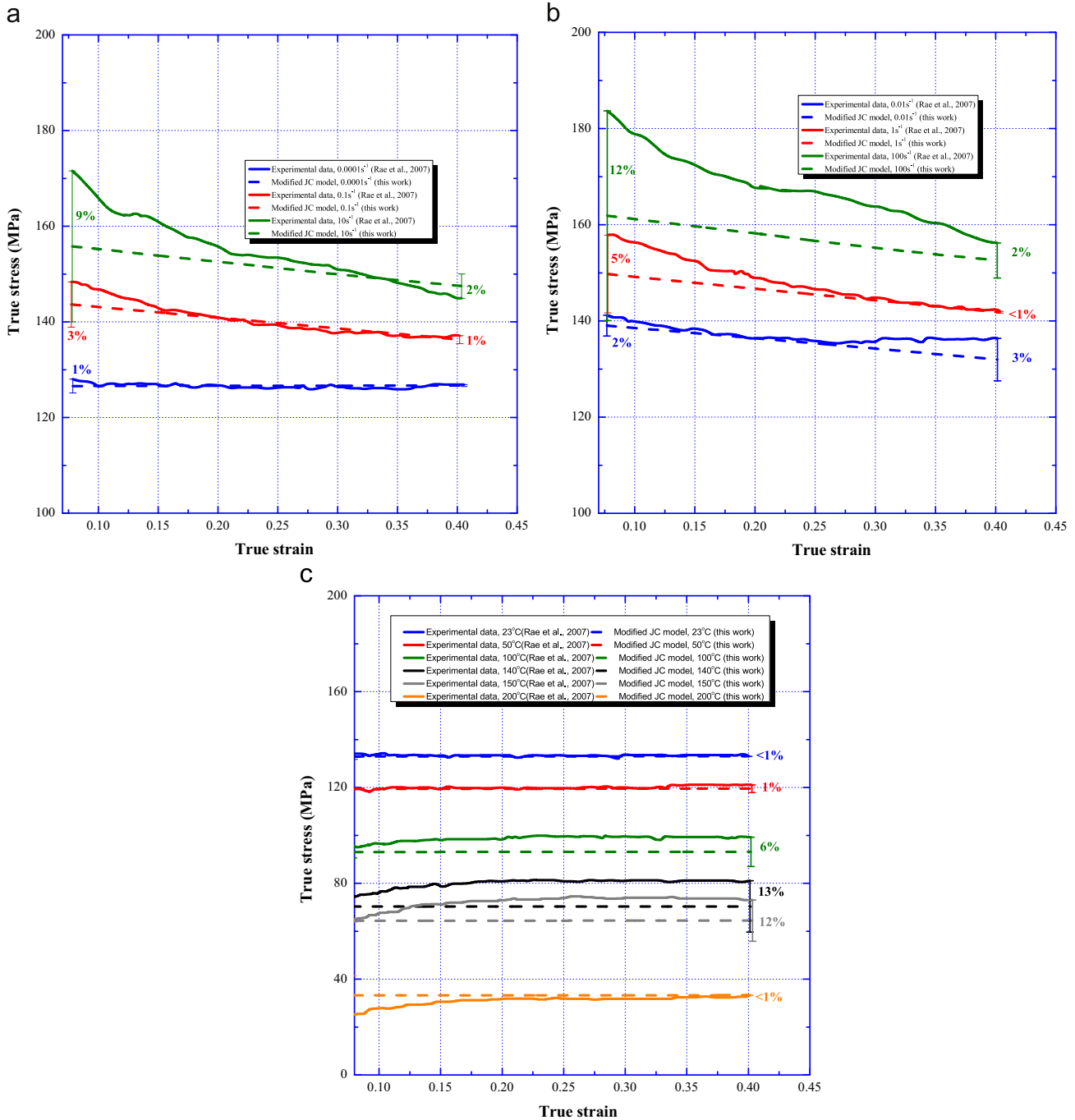


Fig. 4 – Comparisons of stress–strain of PEEK given by the experimental data and the modified JC model (a) and (b) at different strain rates and room temperature and (c) at different temperatures and strain rate of 10^{-3} s^{-1} .

$$\times \left(1 - 1.5343 \frac{e^{T/T_{\text{melting}}} - e^{T_{\text{room}}/T_{\text{melting}}}}{e - e^{T_{\text{room}}/T_{\text{melting}}}} \right) \quad (9)$$

Fig. 4 shows the comparisons between the predictions of the modified JC model and experimental data. As can be seen from Fig. 4a and b, in the range of strain rates from 10^{-4} s^{-1} to 10^2 s^{-1} , the differences between the experimental data and the modified JC model are less than 5% when the strain is about 0.4. The maximum difference is 12% when the strain is relative small, less than 0.1. However, the main advantage of

the modified JC model is that it gives a better prediction at elevated temperatures with a maximum deviation of 13%, as shown in Fig. 4c.

3. Strain rate and temperature sensitivity

Fig. 5 shows the strain rate and the temperature sensitivity of PEEK 450G material. From Fig. 5a, it is obvious that the yield stress is sensitive to the strain rate. In general, the yield

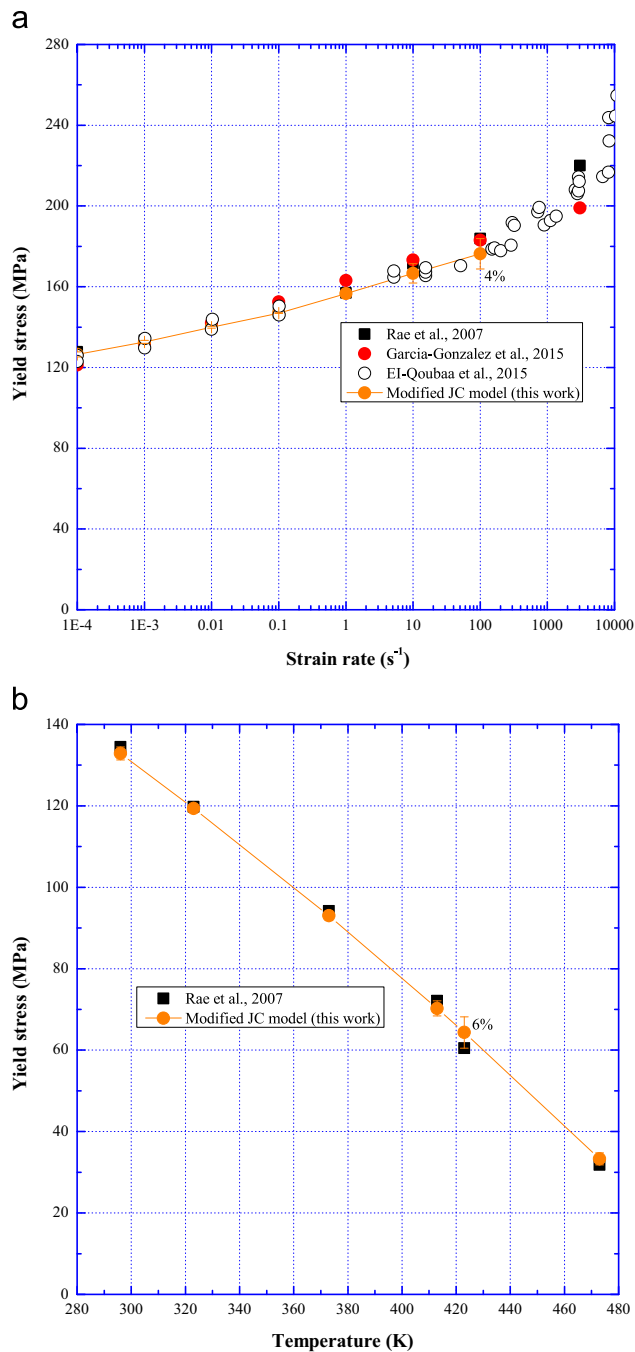


Fig. 5 – Strain rate (a) and temperature (b) sensitivity of PEEK.

stress increases with the increase of the strain rate. It can be found that PEEK 450G shows a largely constant strain rate dependence when the strain rate is less than $10^2 s^{-1}$ at room temperature. The strain rate sensitivity becomes non-linear when the strain rate is higher than $10^2 s^{-1}$. A good agreement is obtained between the experimental data and the modified JC model with a maximum deviation less than 4%. The yield stress is plotted in Fig. 5b as a function of temperature. As can be seen from the figure, the yield stress is inversely proportional to temperature. The differences between the experimental data and predictions by using the modified JC model are less than 6% showing a linear relationship between the yield stress and temperature.

4. Summary

The traditional JC model proposed by Garcia-Gonzalez et al. (2015) gives a reasonable prediction of the flow behaviour of PEEK at room temperature but this is not in the case of elevated temperatures. A modified JC model is proposed to describe the flow behaviour of PEEK not only at room temperature but also at elevated temperatures. The modified JC model correlates well with the experimental data in the entire range of strain rates and temperatures. The yield stress was found to be inversely proportional to the temperature.

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