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A PHYSICAL-INFORMED FE-NN METHODOLOGY FOR PREDICTING HIGHLY NONLINEAR THERMOMECHANICAL RESPONSE OF THERMOSET AND THERMOPLASTIC POLYMERS

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1 INTRODUCTION

Tension-Compression Asymmetry (TCA) and Glass Transition Sensitivity (GTS) are two critical nonlinear characteristics in polymers. TCA [1, 2] is a common phenomenon where materials exhibit different mechanical behaviour under tensile and compressive loading. In polymers, this is mainly due to their specific microstructure [3]. Additionally, the geometry of the test specimen, such as cylinder-shaped samples, can influence the TCA due to effects like barreling, which affects pressure dependence [4]. GTS is a critical effect in polymer marking the temperature θ_g at which a polymer shifts from a glassy to a rubbery state [5, 6]. This transition profoundly impacts the polymer's mechanical and physical properties, such as modulus, heat capacity, thermal expansion, and viscosity [17]. TCA and GTS significantly increase the complexity of developing accurate constitutive models.

Many researches were published to model TCA and GTS [1, 4, 7, 8]. However, for TCA, these models are discontinuous and require separate sets of parameters for tension and compression, complicating material application [1]. For GTS, most models are limited to a narrow temperature range and require multiple sets of parameters to account for different conditions [9, 10].

Recent advances in machine learning (ML) provide promising alternatives to traditional modeling approaches to break through the bottlenecks in material modeling [11, 12]. Aiming to improve the performance of ML-based models, physical knowledge is introduced into the neural network (NN) structure or replacing parts of classical models with NN-based methods [13, 14]. To our knowledge, these NN-implemented physical-based models focus on mechanical behaviour of metals and composites. Due to limited experimental data and the complex nature of inelastic mechanical behaviour, extending these models to polymers is challenging.

In this work, we make use of the theoretical foundations on constitutive modeling of polymers and propose a NN-based constitutive model for the nonlinear thermo-mechanical response of polymers. This model is implemented for the Finite Element (FE) analysis and a physical-informed FE-NN is proposed. This model accounts for temperature, strain rate dependencies,

and TCA, enabling accurate predictions of the mechanical response across the glass transition temperature. Epoxy Epon 862 and Polyamide 6 are utilized to evaluate the performance of this model. Figure 1 present the general scheme of the proposal approach.

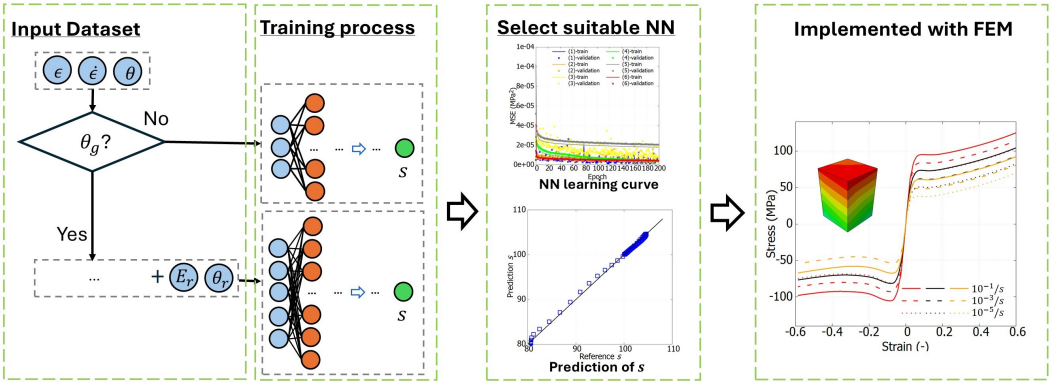

Figure 1: Overview of the stages required in this work to design a physical-informed FE-NN.

2 PHYSICAL-INFORMED FE-NN

The development of the FE-NN structure, model is based on a Unified Semi-Crystalline Polymer (USCP) model [15], which is a physically-based constitutive model simulate the mechanical response of thermosets and thermoplastics. The effective plastic strain rate is written as

$$\dot{\varepsilon} = \dot{\varepsilon}_0 \exp\left[-\left(\frac{A(s-\alpha\sigma_c)}{\theta}\right)\left(1-\left(\frac{\sigma_{eq}}{s-\alpha\sigma_c}\right)^m\right)\right], \tag{1}$$

where θ is the absolute temperature and variables m, $\dot{\varepsilon_0}$ and A are the rate-dependent sensitivity parameters. The magnitude $\sigma_c = tr(\sigma)$ is the trace of Cauchy stress, and α is the pressure sensitivity constant. The variable s is the key internal quantity controlling the hardening-softening features observed in the stress-strain response.

According to the USCP model, the phenomenological equation of the athermal resistance evolution $\dot{s}$ was written as:

$$\dot{s} = H_1\left(1-\frac{s}{s_1}\right)\dot{\varepsilon} + H_2\left(1-\frac{s}{s_2}\right)\dot{\varepsilon} + H_3\left(1-\frac{s}{s_3}\right)\dot{\varepsilon}, \tag{2}$$

where s_1 and s_2 are the athermal strengths related to the peak and lower yield, respectively. The athermal strength s_3 is the preferred stated of the crystalline phase, and it may depend on temperature, strain rate, crystallinity degree and humidity.

The time derivative of s, namely $\dot{s}$, requires several parameters, in which the Parameter Identification (PI) process demands at least two stress-strain curves at the same temperature. However, these set of parameters cannot be used to describe the dynamic shape changes in the stress-strain curve due to the rate and temperature sensitivity of polymers. To break this bottleneck, a pre-trained NN is used as a surrogate model to replace the calculation of s in the USCP model. Due to the NN's strong generalization capability, the model can be applied across a wide range of temperatures and strain rates. Figure 2 shows the main idea of replacing the classical constitutive model by the proposed NN-based model.

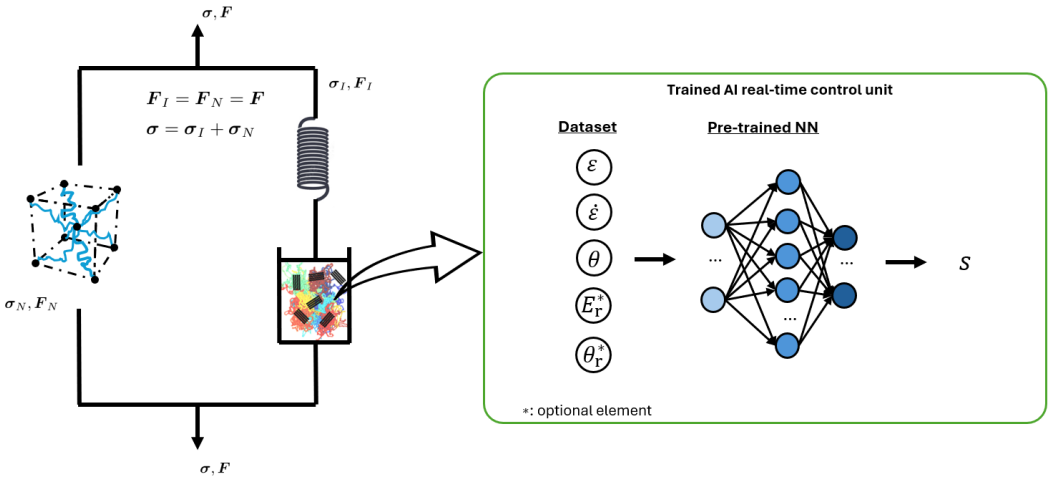

Figure 2: The rheological model incorporating NN as the surrogate method.

After the training process, this NN-based constitutive model is implemented in the Finite Element Method (FEM) for further simulations that can be used at structural level.

3 DETAIL OF NN TRAINING PROCESS

Epoxy exhibits clear TCA, whilst PA6 has a strong GTS across θ_g, and both polymers are utilized as two representative materials to evaluate the performance of the proposed FE-NN model. Experimental data from literature of epoxy [1] and PA6 [16] were used for PI process needed by the USCP model. Several sets of parameters and the USCP model were implemented in FEM using user-defined subroutine for dataset generation. The data used for NN training process is purely virtual data.

The general dataset used for NN training includes: the strain, strain rate and temperature as the input, the value of s as the output. To better describe the temperature sensitivity across θ_g, E_r and θ_r were added into the dataset. When $\theta > \theta_g$, $\theta_r = \theta_r$ and $E_r = E/(E_g - E_{max})$. When $\theta \leq \theta_g$, $\theta_r = \theta/(\theta_g - \theta_{min})$ and $E_r = E/(E_{min} - E_g)$. In this procedure, θ represented the current loading temperature, E_{max} and E_{min} were the maximum and minimum Young's modulus, respectively, while θ_{max} and θ_{min} were the maximum and minimum temperatures. After data generation and data normalization, the dataset was divided into two subsets: 80% for training and 20% for validation. The training subset was used to train the NN and the validation subset was used to evaluate the NN's performance.

A Back-Propagation NN was used to train the value of s. Two suitable NN structure were selected for epoxy Epon 862 and PA6 respectively. For TCA, NN includes three hidden layer (6-9-4). For GTS, NN includes seven hidden layer (7-9-12-15-8-4-2). In both cases, the mean squared error (MSE $= \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$) was selected as the loss function, with the tanh function chosen as the activation function. The learning rate was set to 0.0001, and the Adam optimizer, an adaptive learning rate optimization algorithm, was used. These NN structures were implemented using PyTorch 2.0.1 with Python 3.10. The value of s was replaced by the NN, and the equation is expressed as follows:

$$s = \begin{cases} f_{\mathrm{NN}}(\dot{\varepsilon}, \varepsilon, \theta), & \mathrm{TCA} \\ f_{\mathrm{NN}}(\dot{\varepsilon}, \varepsilon, \theta, E_{\mathrm{r}}, \theta_{\mathrm{r}}), & \mathrm{GTS} \end{cases} \tag{3}$$

After training, the pre-trained NN is implemented in FEM and replacing the calculation of s for further simulation.

4 VALIDATION OF PHYSICAL-INFORMED FE-NN

Figure 3 presents the comparison between FE-NN and experimental results under tensile and compressive conditions with a strain rate of 10^{-3}/s. FE-NN effectively captures the temperature- and strain rate- dependence of epoxy Epon 862. The pre-yielding, softening, hardening state of FE-NN are aligned with the experimental results.

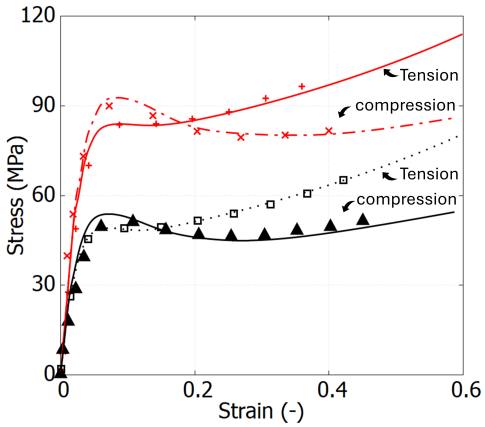

Figure 3: Comparison results between FE-NN and experimental data [1] of epoxy Epon 862 with a strain rate of under 10^{-3}/s. Red: 25°C, Black: 80°C. Symbol: experimental data, line: FE-NN.

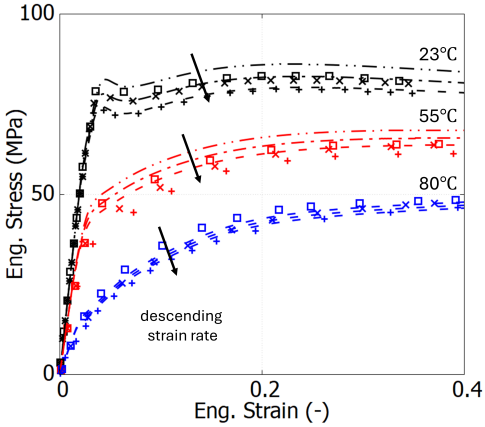

Figure 4: Comparison results between FE-NN and experimental results[1] for PA6.

Figure 4 displays the comparison between FE-NN and experimental results for PA6 under

tensile loading conditions. The results show that the FE-NN effectively captures the experimental observed mechanical features, including temperature and strain rate sensitivity spanning θ_g.

5 CONCLUSION

In this study, we propose a physical-informed FE-NN model to characterize the dynamic changes in rate- and temperature- sensitivity across the glass transition temperature and tension-compression asymmetry of polymers. The developed model approach relies on the USCP model, which is a physical-based constitutive model and it incorporates a NN-based approach to merge parameter sets and generate a unified function for athermal resistance, which is then fed back into the prescribed plastic strain rate. After training process of NN, this model is implemented within the FEM. The results show that this new FE-NN not only captures strain rate and temperature sensitivity phenomenon effectively but also the shape transition in stress-strain curves spanning the glass transition temperature θ_g.

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