

Prediction of Yellowing of Polystyrene Materials under Natural Weathering Exposures

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Abstract

The polystyrene (PS) materials tend to yellow over time. The yellowing phenomenon is an indicator of the material's reduced performance and structural integrity. In the natural environment, sunlight is a major contributor to the yellowing, and elevated temperatures can accelerate the chemical reactions that lead to yellowing. The natural environmental factors are difficult to control, making it challenging to predict the yellowing process accurately. In this paper, we established a model to quantify the relationship between the yellowing index and key factors, solar radiation and temperature, from outdoor monitored climatic data. The model is trained and tested by the datasets collected from atmospheric exposure test stations located in Guangzhou and Qionghai. Same kinds of PS materials were exposed to external natural environments at the stations for one year. The parameters were estimated by least squares method. The results indicated that the model fits training and testing datasets well with R^2 of 0.980 and 0.985, respectively.

Keywords

Polystyrene, Ageing, Yellowing, Least Squares Method, Arrhenius Equation, Natural Weathering Exposures

1. Introduction

The changes in physical, chemical, or molecular properties characterize material aging, which leads to reduced material quality, performance and safety. Research on material aging and anti-aging has become crucial for industries. One significant concern to the polymer industries is that of yellowing discoloration phenomenon.

Yellowing is often associated with the breakdown of polymer chains, and hence it is an indication of chemical changes occurring in the material. These changes can weaken the molecular structure of the material, making it more brittle and prone to damage.

The aging process of a polymer material is a complex phenomenon that occurs over time and is influenced by various environment factors, such as light, heat, humidity, and chemical substances [1] [2]. To investigate effects of time and environmental conditions, aging tests can be either accelerated or natural. Accelerated artificial aging techniques involve subjecting products to controlled conditions in a laboratory such as high temperatures, or chemical treatments to speed up the aging process. Due to the use of more stringent conditions than the actual environment, artificial aging may not fully replicate the environmental conditions in real life. As a result, the aging effects obtained may not accurately reflect the actual performance. However, natural aging is a complex phenomenon that occurs naturally over time. These natural environmental factors are difficult to control, making it challenging to predict and manage the aging process accurately.

The yellowing phenomenon can be caused by oxidation, exposure to light, heat, chemical contamination and biological activity [3] [4]. In the natural environment, sunlight is a major contributor to the yellowing of many materials. Long-term exposure to sunlight can induce photo-oxidation reactions. High temperatures can also cause direct thermal degradation. Materials stored or used in high-temperature environments are more likely to yellow. There are several predictive models for aging of polymer materials, such as regression models and Bayesian methods [5]-[7]. They proposed linear or polynomial regression models for a given exposure time and temperature [5] [6]. For prediction of aging of multiplex polymer systems under conditions, a physical-chemical model with complicated non-linear dependency on exposure time was constructed, and Bayesian method was applied to estimate the unknown parameters of the model [7]. However, predictive models on the yellowing are very few [3]. A predictive model under accelerated exposures was built, and the change in yellow index was modeled using linear regression model under predefined accelerated exposure conditions for a given exposure time and photo dosage of light [8]. In this paper, we focus on the natural yellowing phenomenon and investigate the non-linear combination effect of solar radiation and temperature in the natural aging process of polystyrene (PS) materials.

2. Method

2.1. Experimental Data

The experimental data were obtained from atmospheric exposure test stations under real-world atmospheric conditions. The test stations are located in Guangzhou (GZ) and Qionghai (QH) that represent subtropical and tropical monsoon climate regions, respectively. Same kinds of PS materials were exposed to external environments at the stations for one year starting on November 1, 2006 or October 1, 2005. Their physical properties and atmospheric factors are regularly monitored

and recorded during the one-year period. The color of the materials gradually becomes more yellow and we tracked the color change monthly measured by yellow index. The yellowing index quantified by a tristimulus colorimeter is calculated using the formula $YI = 100 (1.28X - 1.06Z)/Y$, where X (red), Y (green), Z (blue) are the CIE tristimulus values. The qualification of yellowing degree since exposing to the aging test stations was carried out according to $Y = YI - YI_0$, where YI and YI_0 are current and initial yellowing indices [4]. In addition, the atmospheric environmental factors, including temperature, and solar radiation, were daily monitored. Therefore, for each test station, we have 12 and 365 readings for yellowing degree and every environmental factor, respectively.

We use the data starting in 2006 as training set, and the data starting in 2005 as testing set. The yellow index change Y versus time curves are plotted in **Figure 1**. We see that the materials become increasingly yellow over time, and the curve for QH is positioned above the curve for GZ. **Figure 2** presents daily average temperature, and daily cumulative solar radiation and the trends in corresponding monthly average values. It shows that the radiations are mixed together, and most of the time, the temperature in QH are higher than those in GZ.

2.2. Mathematical Model

Figure 1 shows that the yellowing indexes rise with a rapid initial increase and slow down on the top. The curve for Qionghai is generally positioned above the curve for Guangzhou. It is observed in **Figure 2** that most of temperatures in Qionghai are consistently above those in Guangzhou. Natural yellowing is a process primarily related to the dose of absorbed photons, which mainly come from solar radiation, and high temperatures can accelerate the process. To qualify the combination effect of solar radiation temperature on yellowing degree, we consider

$$\frac{Y(t)}{100 - Y(t)} = \int_0^t c(T(s))R(s) ds,$$

where $Y(t), R(t), c(T(t))$ are yellowing degree change, solar radiation, and an accelerate factor from temperature at time t . When the yellowing degree goes to a certain extent, such as 100, it has undergone a qualitative change. Elevated temperatures can accelerate the chemical reactions that lead to yellowing. Arrhenius equation describes the effect of temperature on the rate of a chemical reaction, and the rate is exponentially dependent on the reciprocal of the temperature. Learn from Arrhenius law, we assume the accelerated effect term

$$c(T(t)) = \exp\left(\beta_0 - \beta_r \frac{296.15}{T(t) + 273.15}\right),$$

where $296.15/(T(t) + 273.15)$ is the ratio of temperature $T(t)$ to 23°C (296.15 K). From this equation when $\beta_r > 0$, it follows that the process proceeds faster under increased temperature.

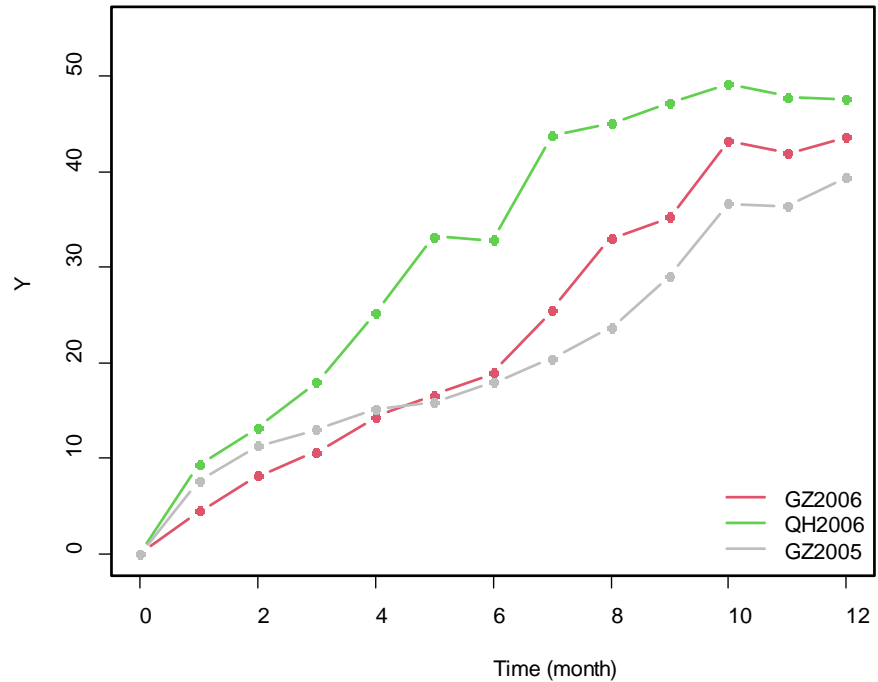


Figure 1. The change in yellow index (Y) for PS material exposed in Guangzhou (GZ) and Qionghai (QH) stations starting in 2006 or 2005.

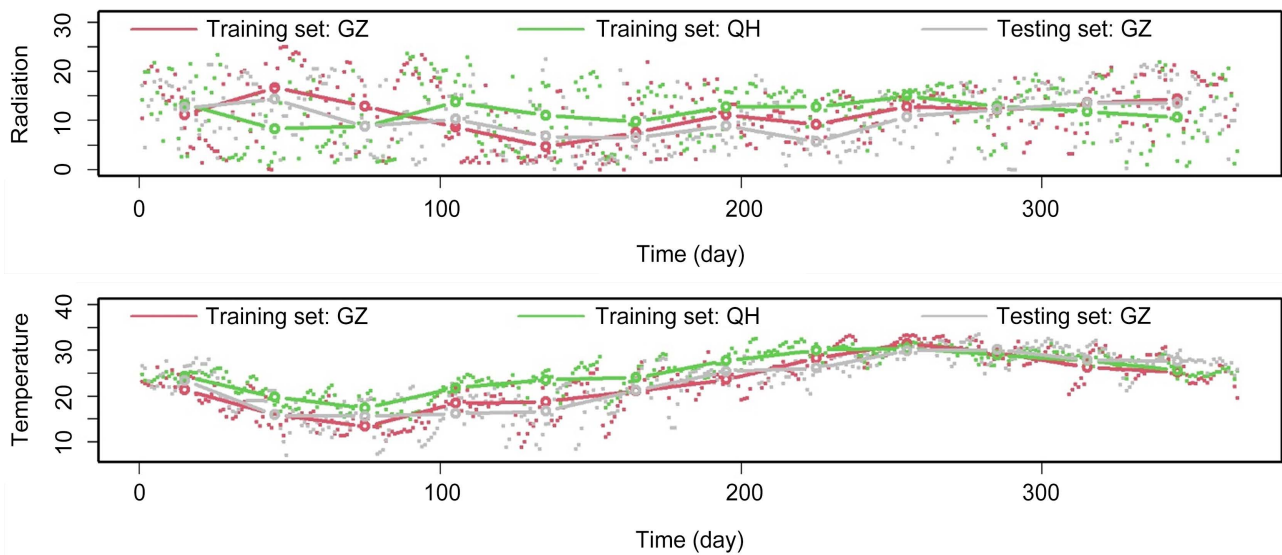


Figure 2. Daily and monthly average temperature ($^{\circ}\text{C}$), and solar radiation (MJ/m^2) in Guangzhou (GZ) and Qionghai (QH) stations.

3. Analysis and Results

With observed $\{Y(t_{k1}), Y(t_{k2}), \dots, Y(t_{k,12})\}$ and more densely environmental measurements $\{R(s_{k1}), T(s_{k1}), R(s_{k2}), T(s_{k2}), \dots, R(s_{k,365}), T(s_{k,365})\}$, for station GZ ($k=1$) and QH ($k=2$) in training dataset, the discrete version of the model is given by

$$\frac{Y(t_{ki})}{100 - Y(t_{ki})} = \sum_{s_{kj} \leq t_{ki}} R(s_{kj}) \exp\left(\beta_0 - \beta_T \frac{296.15}{T(s_{kj}) + 273.15}\right), \quad k = 1, 2; i = 1, 2, \dots, 12.$$

Adopt least squares method to estimate the parameters (β_0, β_T) , minimizing the sum of squared residuals $\sum_{k=1}^2 \sum_{i=1}^{12} (Y(t_{ki}) - \hat{Y}(t_{ki}))^2$, we obtain $\hat{\beta}_0 = -5.035$, $\hat{\beta}_T = 5.146$ which results in $R^2 = 0.980$. Applied to the trained model to testing dataset, the model also achieved good performance with $R^2 = 0.985$. The prediction results for training and testing datasets are illustrated in **Figure 3**.

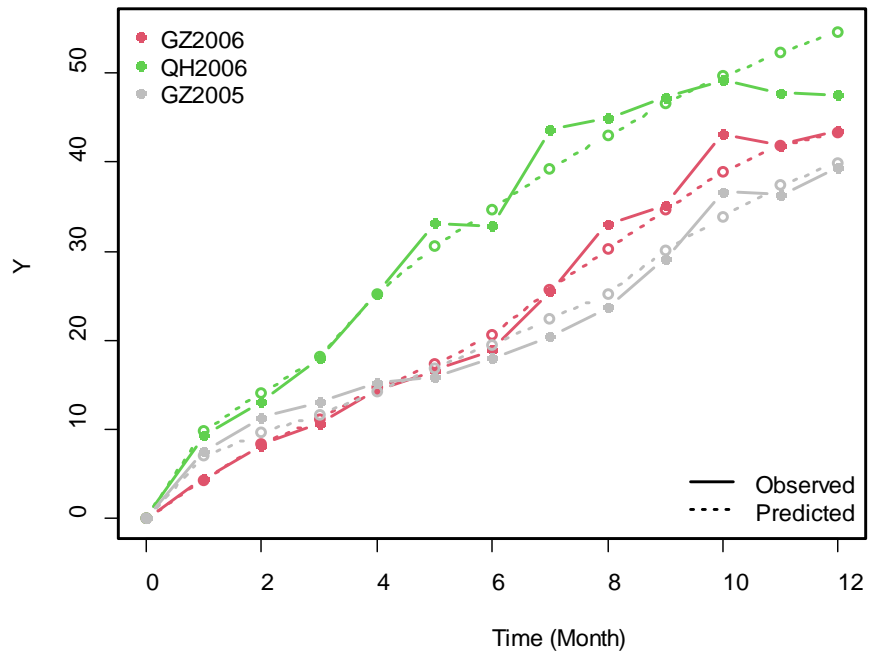


Figure 3. Observed and predicted values of the change in yellow index (Y) for training and testing datasets.

4. Conclusions and Further Research

In this study, we did outdoor weathering trials and had no stringent control of the exposure condition. We tracked the yellow indexes of PS materials and monitored outdoor climatic data. Yellowing discoloration is a complex process caused by processes of photo-degradation and thermal degradation. The yellowing index primarily depends on cumulative radiation, but the effect may vary under different temperature conditions. We established a model combined with an Arrhenius law for the temperature dependence to predict the change in yellowing index. The model provided a very high performance under natural weathering exposures. The results show the yellowing proceeds faster under increased radiation and temperature. To prevent yellowing, the PS materials are suggested to be stored in a place that is shielded from direct sunlight and has a relatively low temperature.

We only consider the effects of main contributors, solar radiation and temperature. Solar radiation is the electromagnetic energy emitted by the sun, including

Ultraviolet (UV) radiation, visible light (VL) and infrared radiation (IR). UV light has shorter wavelength and higher energy, and hence it might play a major role within solar radiation to yellowing process. In future work, we can consider more potentially relevant factors, such as UV and VL radiations, temperature and humidity, in the model and use more datasets to demonstrate its generalizability.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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