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Article

Thermal Hazard Simulation of Carbon Nanotubes

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Abstract: This study investigates the high temperature hazard of carbon nanotube failure under different temperature levels, by modeling semi-parametric or parametric hazards relying on a numerical simulation system where temperature-dependent degradation trajectories are generated using Arrhenius-based simulations, producing realistic failure time data for NTS. Three methods were applied to estimate temperature hazards, namely the Cox model of relative hazards for the purpose of evaluating the effect of thermal and material covariates on failure hazards, then the Piecewise exponential model was applied (segmented) for the purpose of capturing the interval-specific hazard differences and the Spline-Based Hazard Regression model to estimate the smooth hazard function over time and for each model the hazard was derived for carbon nanotubes using probability, and then compared the three models between these methods using a simulation system based on comparison scales where it was found that the Cox model is better than the rest of the models used in this study to analyze the hazard of The heat on the carbon nanotubes.

Keywords: Carbon Nanotubes, Thermal Hazard, Hazard Models, Cox model, Piecewise exponential model, Spline-Based Hazard Regression model.

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1. Introduction

Carbon nanotubes (CNTs) have emerged as one of the promising nanomaterials due to their exceptional properties in the fields of mechanics, electricity, and heat.These one-dimensional nanostructures are defined by the possibilities to withstand tensile stress, thermal conductivity, and outstanding electronic characteristics, which can be used in many applications as nanoelectronics, composite materials, thermal sensors [1], and energy storage devices. Regardless of these strengths, the performance and reliability of systems built on carbon nanotubes are extremely influenced by the environmental factors and in particular, high temperatures. High temperatures may cause structural damage, the appearance of defects in the atomic lattice, the development of microcracks [2], and the alteration of the mechanical stiffness, which will impact the functional performance and make the probability of failure higher. Thus, the hazards that can be linked to the effects of heat on (CNTs) are important to comprehend in order to design safe and efficient systems and secure their work in practice [3].

It is a big challenge to model the failure of carbon nanotubes at thermal stress because the processes at the nanoscale level are stochastic. Complex failure behaviours are due to the effect of both thermal and non-uniform stress distribution and the diversity of network structures. In situations where the conventional strategies are unable to capture these complexities [4], and where experimental strategies fail to give proper predictions in different thermal conditions. Thus, semi-parametric hazard models including the Cox proportional hazards model, sliding window regression and the partial exponential model are a powerful tool to study the failure behavior by combining variables like heating rate and initial temperature such that it is possible to have a flexible estimation of hazard and influence of temperature on the probability of failure [5].

This study involved the generation of thermal degradation pathways of carbon nanotubes using simulation on the basis of Arrhenius kinetics. The degradation as a function of time and temperature was modelled to obtain the actual estimates of the failure times at the definite thermal conditions [6]. Combining semi-parametric failure hazard models with modeled failure data. The paper offers a holistic examination of how the changes in temperature affect the hazard of bursting of pipes. The Cox proportional hazards model gives information regarding the influence of variables in the hazard rate, the piecewise exponential model depicts the dynamics of the hazard across periods and the sliding window hazard model depicts how hazard changes over a period of tim [7].

The suggested method will involve both theoretical hazard modelling and practical simulation that will enable the quantitative estimation of hazards of carbon nanofibers under thermal stress [8]. Such a combination of statistical modelling and computing simulation offers a complete statistical prediction of reliability, safety margin, and the mechanism of creating equipment that utilizes carbon nanotubes to work in high thermal conditions. It is possible to apply the methodology to other nanomaterials and other environmental factors to give an overall outline to understand the thermal hazard in nanostructured systems [9].

This study is based on the integration of the sophisticated semi-empirical hazard models and the degradation analysis based on simulation to obtain the complete evaluation of thermal hazards in carbon nanotubes. The intended purpose of the study is to ascertain the chances of failure, examine the influence of shared variables and offer predictive value on the dependability of these tubes, which will in turn help in safe and optimal practice of such tubes in the engineering and technological sectors of life [10].

2.Methods : Modeling and Estimation

1.2 Cox Proportional Hazards Model

These unidimensional nanostructuThe Cox proportional hazard model is a semi-parametric regression analysis which tends to measure the effects of covariates on the hazard function. It is also an appropriate model to model the wear of carbon nanotubes, because there is no need to determine the basis hazard parameter [11]. The model is a product of the exponential of shared variables and the base hazard function. The hazard function is determined in the following way:

$$h(t \mid X) = h_0(t) exp(\beta^\top X)$$

With $h(t \mid X)$ being the hazard at time t, depending on the explanatory variables X, and $h_0(t)$ being the baseline hazard, and β being the regression coefficients [12]. Suppose the failure times observed are ordered in the following way , $t_{(1)} < t_{(2)} < \cdots < t_{(m)}$,we define the hazard set at time $t_{(j)}$ as follows :

$$R(t_{(j)}) = \{i : t_i \geq t_{(j)}\}$$

the Contribution of the partial probability of failure j-th as form $L_j(\beta) = \frac{\exp(\beta^\top X_{(j)})}{\sum_{i \in R(t_{(j)})} \exp(\beta^\top X_i)}$

09u The total partial probability of everything is, as regards the complete probability is $L(\beta) = \prod_{j=1}^{m} \frac{\exp(\beta^\top X_{(j)})}{\sum_{i \in R(t_{(j)})} \exp(\beta^\top X_i)}$The log-partial likelihood can be expressed as follows [13] , is :

$$\ell(\beta) = \sum_{j=1}^{m} \left[\beta^\top X_{(j)} - \log \sum_{i \in R(t_{(j)})} \exp(\beta^\top X_i) \right]$$

The score function and is the gradient of the log-partial likelihood with respect to β , is:

$$U(\beta) = \frac{\partial \ell}{\partial \beta} = \sum_{j=1}^{m} \left[X_{(j)} - \bar{X}_j(\beta) \right]$$

where weighted is $\bar{X}_j(\beta)$ is defined as $\bar{X}_j(\beta) = \frac{S_j^{(1)}(\beta)}{S_j^{(0)}(\beta)}$ [22] , is :

$$S_j^{(k)}(\beta) = \sum_{i \in R(t_{(j)})} X_i^{\otimes k} \exp(\beta^\top X_i)$$

with tensor powers defined as $X_i^{\otimes 0} = 1, X_i^{\otimes 1} = X_i, X_i^{\otimes 2} = X_i X_i^\top$ The observed information matrix (negative Hessian) [2], is :

$$H(\beta) = -\frac{\partial^2 \ell}{\partial \beta \, \partial \beta^\top} = \sum_{j=1}^{m} \left[\bar{X}_j^{(2)}(\beta) - \bar{X}_j(\beta) \bar{X}_j(\beta)^\top \right]$$

with $\bar{X}_j^{(2)}(\beta) = \frac{S_j^{(2)}(\beta)}{S_j^{(0)}(\beta)}$ The regression coefficients are estimated by solving the score equation $U(\beta) = 0$ using Newton-Raphson iterations is $\beta^{(k+1)} = \beta^{(k)} + H(\beta^{(k)})^{-1} U(\beta^{(k)})$ [14] , the asymptotic variance of the estimated coefficients $\hat{\beta}$ is $\mathrm{Var}(\hat{\beta}) = H(\hat{\beta})^{-1}$For time-dependent covariates $X_i(t)$Xi(t), the score function generalizes as :

$$U(\beta) = \sum_{j=1}^{m} \left[X_{(j)}(t_{(j)}) - \frac{\sum_{i \in R(t_{(j)})} X_i(t_{(j)}) \exp(\beta^\top X_i(t_{(j)}))}{\sum_{i \in R(t_{(j)})} \exp(\beta^\top X_i(t_{(j)}))} \right]$$

The martingale representation for subject i is :

$$M_i(t) = N_i(t) - \int_0^t Y_i(u) \exp(\beta^\top X_i(u)) \, d\Lambda_0(u)$$

where $N_i(t)$ is the counting process of failures, $Y_i(u)$Yi(u) is the at-hazard indicator, and $\Lambda_0(t)$ is the cumulative baseline hazard, A penalized Cox model can be applied to ensure numerical stability [15] , is :

$$\ell_{\text{pen}}(\beta) = \ell(\beta) - \frac{\lambda}{2} \parallel \beta \parallel^2$$

with penalized score and Hessian

$$U_{\text{pen}}(\beta) = U(\beta) - \lambda\beta, H_{\text{pen}}(\beta) = H(\beta) - \lambda I$$

This framework allows for an accurate estimation of the impact of thermal variables on the hazard of failure of carbon nanotubes, taking into account the constrained observations [16].

2.2. Piecewise Exponential Hazard Model

The partial exponential hazard model will be used and the basis of the hazard function is constant within prescribed intervals and thus, flexible in tracking alterations in hazard with time with simple parameters in each interval. The model is especially appropriate in the context of the study of the thermal degradation process as the hazard may abruptly shift because of the appearance of a certain phase or the appearance of a certain temperature stress. These intervals are separated into K intervals [17] , as :

$$[0, \tau_1), [\tau_1, \tau_2), \ldots, [\tau_{K-1}, \infty)$$

The hazard is assumed to be constant in each interval and is denoted as $h(t) = \lambda_k$ for , $t \in [\tau_{k-1}, \tau_k)$ where is the subject i experiencing a failure time t_i and an event indicator δ_i in the event [18]. In the position where $d_{ik} = 1$ is the case when failure has taken place within the interval k (0 if no failure occurs) and y_{ik} is the time of hazard at the interval k. Contribution to probability of subject i :

$$L_i(\lambda) = \prod_{k=1}^{K} \lambda_k^{d_{ik}} \exp(-\lambda_k y_{ik})$$

By aggregating all n of the subjectsthe, the likelihood factorizes by interval:

$$L(\lambda) = \prod_{k=1}^{K} \lambda_k^{d_k} \exp(-\lambda_k Y_k)$$

Where $d_k = \sum_{i=1}^{n} d_{ik}, Y_k = \sum_{i=1}^{n} y_{ik}$, The log-likelihood is $\ell(\lambda) = \sum_{k=1}^{K} [d_k \log\lambda_k - \lambda_k Y_k]$, The maximum likelihood estimator (MLE) for λ_k is $\hat{\lambda}_k = \frac{d_k}{Y_k}$, with variance $\mathrm{Var}(\hat{\lambda}_k) = \frac{d_k}{Y_k^2}$, If covariates X are included, we can assume a multiplicative form is :

$$h(t \mid X) = \lambda_k \exp(\beta^\top X) \qquad , t \in \text{interval } k$$

This can be fitted using Poisson regression by stacking interval-level data, with an offset $\log Y_k$logYk and log-link [19]:

$$\log E[d_k] = \log Y_k + \log\lambda_k + \beta^\top X$$

Bayesian estimation can also be performed by assuming a prior $\lambda_k \sim \mathrm{Gamma}(\alpha_k, \beta_k)$ and updating the posterior:

$$\lambda_k \mid \text{data} \sim \mathrm{Gamma}(\alpha_k + d_k, \beta_k + Y_k)$$

The periods $\{\tau_k\}$ are chosen according to the reduction of AIC/BIC models or loss of prediction with the help of cross-validation so that the hazard changes under the influence of thermal effects were properly represente [20].

3.2 Spline-Based Hazard Regression

Spline-based regression allows for flexible modelling of the baseline hazard as a smooth function of time, accommodating non-linear shapes without imposing a specific parametric model [21], the automatic curves capture gradual or sudden changes in hazard due to temperature fluctuations. The log hazard is represented as follows:

$$\log h(t \mid X) = B(t)^\top \gamma + \beta^\top X$$

where $B(t) = (B_1(t), \ldots, B_m(t))^\top$B(t)=(B1(t),…,Bm(t))⊤ is a vector of spline basis functions, γ are the spline coefficients, and ββ are regression coefficients for covariates, partial log-likelihood [22], is :

$$\ell(\gamma, \beta) = \sum_{j=1}^{m} \left[B(t_{(j)})^\top \gamma + \beta^\top X_{(j)} - \log \sum_{i \in R(t_{(j)})} \exp\left(B(t_i)^\top \gamma + \beta^\top X_i\right) \right]$$

A penalised partial likelihood function is used to avoid overfitting:

$$\ell_p(\gamma, \beta) = \ell(\gamma, \beta) - \frac{\lambda}{2} \gamma^\top \Omega \gamma$$

where Ω is a penalty matrix, typically the integrated squared second derivative of the spline basis $\Omega_{ab} = \int B_a''(t) B_b''(t)\, dt$ .The score functions are :

$$U_\gamma = \frac{\partial \ell}{\partial \gamma} - \lambda \Omega \gamma, U_\beta = \frac{\partial \ell}{\partial \beta}$$

The block Hessian matrix is :

$$H = \begin{pmatrix} H_{\gamma\gamma} + \lambda\Omega & H_{\gamma\beta} \\ H_{\beta\gamma} & H_{\beta\beta} \end{pmatrix}$$

and parameter updates are obtained via Newton-Raphson :

$$H\Delta = -U, \Delta = (\Delta\gamma, \Delta\beta)$$

The smoothing penalty ensures smooth hazard estimates, and the penalty factor λ selected using Cross-Validation (GCV) or REML. The variance of the estimates (γ^,β^) is approximated using the modified inverse observed information matrix [23].

3.Results

1.3 Simulation System

A numerical modelling framework was created to estimate the thermal hazards of carbon nanotubes (CNTs). This model generates degradation pathways based on temperature and failure times of individual nanotubes, which are then examined using semi-parametric hazard models. Thermal developments, degradation accumulation, and failure criteria are integrated into the simulation: the thermal profile of the nanotube is updated at discrete time steps either by a linear increase in temperature or at a heat rate of any rate chosen by the use [24] ,is :

$$T(t + \Delta t) = T(t) + \gamma \Delta t$$

where T (t) is the temperature at time t, γ is the heating rate, and Δt is the time step of the simulation:The thermal stress degradation of the nanotube can be described through an Arrhenius-type reaction rate [25] , is :

$$D(t+\Delta t) = D(t) + k(T)\Delta t \quad \text{and} \quad k(T) = A\exp\left(-\frac{E_a}{RT(t)}\right)$$

where $D(t)$ is the cumulative degradation, A is the pre-exponential factor, E_a is the activation energy, R is the universal gas constant, and $k(T)$ is the temperature-dependent degradation rate ,The cumulative degradation attains a critical D_c [13] , is :

$$T_f = \min\{t: D(t) \geq D_c\}$$

In this case, T_f denotes the simulated failure time of the nanotube,The simulated failure times $\{T_f^{(i)}\}_{i=1}^{n}$ of n nanotubes are the inputs of hazard estimation by the Cox Proportional Hazards, Piecewise Exponential [17] , and Spline-Based Hazard models. Covariates may include heating rate γor nanotube diameter d:

$$h(t \mid X_i) = h_0(t)\exp(\beta^T X_i)$$

In which X_i is the covariate vector of the irth nanotube, λ_k is the hazard of the k-th interval in the Piecewise model, and $B(t)$ is the spline basis of the Spline-Based model.

This simulation model enables systematic analysis of thermal hazard in conditions with different temperatures, heating rates, and material characteristics, which gives a solid input to further statistical analysis of nanotube failure [24].

2.3 Data Generation

The simulated data is a physics-based hazard analysis project on the thermal degradation of 100 carbon nanotubes (CNTs) at different temperatures under different temperature stresses. The temperature ramp rate (temp rate) is randomly applied to each CNT and the time-to-failure is modeled as a process of Arrhenius-type damage buildup [25], with an Arrhenius-type rate coefficient of temperature dependence and a time-dependent hazard of failure. The time column observed is the actual failure time or the censoring time (981.5 units), and it is right-censored at about 30% meaning that about 30% of the data is right-censored (event = 0) which is a simulation of the real world experimental restrictions in which not all samples fail during the experiment. The true time column is the actual generation of physical failure time through the simulation whereas temp rate standard is a standardized heating rate that may be used in statistical modelling. The existence of a significant negative association (≈ -0.926) between temp rate and true time is a validation of a highly plausible and monotonic relationship: higher thermal stress decreases hazard rate significantly, and decreases time-to-failure. The realistic synthetic data facilitates strong testing of hazard regression models, including Cox Proportional Hazards, Piecewise Exponential and Spline regressions, in controlled conditions, simulating material fatigue dynamics, and makes it ideal in testing and measuring the model performance, convergence and interpretability in estimating and comparing the thermal hazard function as a covariate.

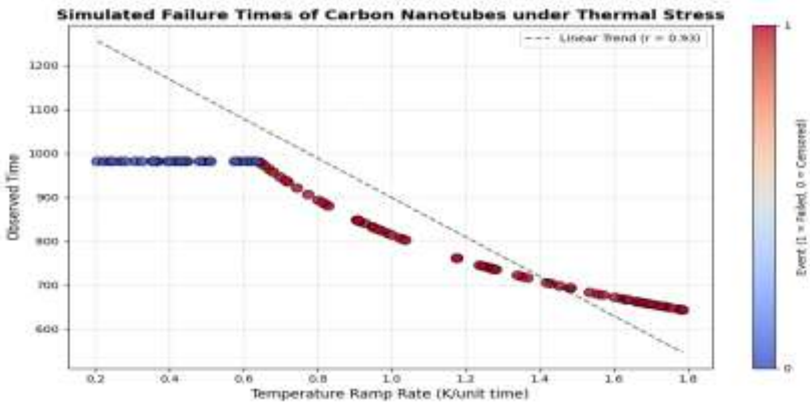

Figure 1. Represents the Data Generation form of the Simulation System

4. Discussion

In this part, the results obtained from the simulation system will be analyzed using Python libraries :

Table 1: Represents the Results of the Cox Proportional Hazards Model

covariate	coef	exp(coef)	se(coef)	coef lower 95%	coef upper 95%	exp(coef) lower 95%	exp(coef) upper 95%	cmp to	z	p	-log2(p)
temp_rate	1.965755	7.140299	0.233261	1.508572	2.422937	4.520273	11.27894	0	8.427292	3.54E-17	54.65002

The Cox Proportional Hazards model was able to estimate the influence of the temperature ramp rate (temp rate) on the failure time of carbon nanotubes. The temp rate value of 1.9658 ($p < 0.001$) showed that the rate of heating and the hazard of failure showed a strongly significant positive relationship. The hazard ratio (exp(coef) = 7.14) suggests that one extra unit of the temperature ramp rate yields the current hazard of failure by 7.14 times. The model had the Concordance Index of 1.000 or perfect discrimination - the pairs of nanotubes ranked correctly with respect to failure order due to thermal stress exerted on the nanotube. The high, monotonic, and almost linear correlation between temperature and degradation could explain this outstanding performance as the correlation between true survival time and temp rate is high (-0.926). The partial AIC value of 505.99 shows that it fits well with a least complex .

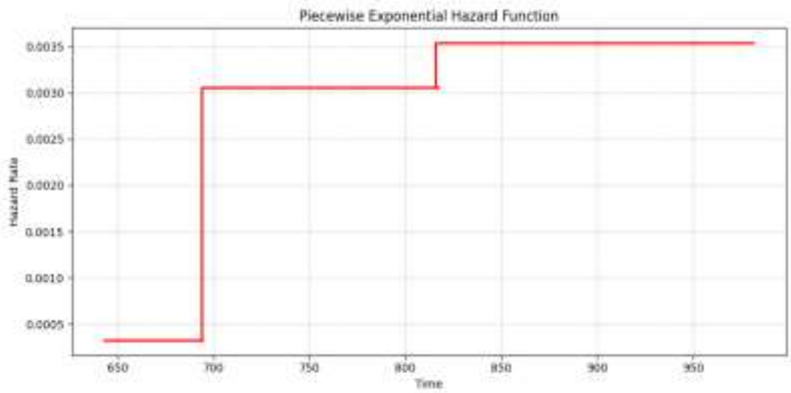

Figure 2: Represents the Results of the Piecewise Exponential Model

The partial exponential model splits the time axis into different periods, and the hazard rate is assumed to remain constant in each of the time periods. The hazard function that was obtained exhibited three different stages, the first one with a low level of hazard (≈ 0.000325) then it is sharply increased at (t ≈ 694) (≈ 0.003055), and then slightly further increased at (t ≈ 817) (≈ 0.003543). This is a threshold-dependent behaviour, in which the

damage is initially slow, but increases much faster as the critical level is passed, which is consistent with what might happen in physical reasons, e.g. weakening of a bond or structural instability in carbon nanotubes subjected to long-term thermal loading.
However, the model does not incorporate common variables, such as the heating rate, which limits its ability to distinguish between nanowires subjected to different heating rates. As a result, the concordance index becomes undefined (NaN), and the model shows a very high AIC value (1051.75) due to the large number of parameters (100), indicating an overfitting problem.

Table 2: Represents the Results of the Spline-Based Cox model Model

covariate	coef	exp(coef)	se(coef)	coef lower 95%	coef upper 95%	exp(coef) lower 95%	exp(coef) upper 95%	cmp to	z	p	-log2(p)
spline_1	-0.851417017	0.42681	0.394061	-1.62376	-0.07907	0.197156	0.923973	0	-2.16063	0.030724	5.024475
spline_2	1.232087068	3.428377	0.410782	0.426968	2.037206	1.532604	7.669151	0	2.999366	0.002705	8.529933
spline_3	0.83781348	2.311308	0.206752	0.432587	1.24304	1.541239	3.466136	0	4.052258	5.07E-05	14.26692

The spline-based Cox model extends the standard proportional hazards model (Cox PH) by representing the effect of the temperature rate (temp_rate) using B-spline functions, allowing for the characterisation of potential nonlinear relationships between thermal stress and failure probability. The analysis results showed that two of the three spline components have clear statistical significance: spline_2 with a coefficient of **(**1.232**)** and a **(**$p = 0.0027$**)**, and spline_3 with a coefficient of **(**0.838**)** and **(**$p < 0.001$**)**. Both were associated with an increase in hazard ratios of **(**3.43 and 2.31**)**, respectively. These results indicate an increased likelihood of failure at medium and high levels of temperature rate. In contrast, the spline_1 component had a negative coefficient of **(**−0.851**)**, which reflects a decrease in hazard at lower heating rates , Although this model has a greater level of flexibility than the traditional Cox linear model, the level of statistical performance was not as high; the concordance index was **(**0.948**)**, whereas the basic Cox model had obtained an even higher value (1.000). It also obtained greater AIC value of **(**552.25**)** than **(**505.99**)** of the standard model where three extra parameters are needed. Therefore, the findings point to the fact that adding complexity to the model does not substantially increase the predictive power, and it is possible to assume that the basic connection between the rate of heat and the likelihood of failure hazards is linear.

Table 3: Represents the Results of Comparing Three Model

Model	Concordance Index	AIC	Log-Likelihood	Number of Parameters
Cox PH	0.999967	505.9895204	-251.9947602	1
Piecewise Exponential	0.8786543	1051.750386	-522.8751931	100
Spline-Based Cox	0.94809228	552.2525533	-273.1262767	3

In performing a thorough comparison of the three models one immediately knows that the Cox proportional hazards model is the best that can be used with the current set of data. It demonstrated an excellent concordance, the most minimal value of Akaike Information Criterion (AIC), as well as the largest value of log-likelihood, based on a single coefficient, which indicates strong simplicity to predictive power. Concerning the Cox model using spline, even though it was more flexible in meeting the possible nonlinear relationships, it could not perform any better than the linear Cox model, meaning that no nonlinear effects were significant in the data. This was experienced in the rise in its AIC value and the reduction in the concordance index attributed to the rise in the number of parameters used.

Concerning the partial exponential model, though this model is efficient in explaining the variation of the hazard with time, it has major constraints, i.e., it does not take into consideration the accompanying variable, which limits its power to give individual hazards or compare one group of people with another. The extremely high AIC value and poor fit make its use unsuitable within the framework of regression models.

In general, the choice of statistical method should depend on the primary objective of the research; if the focus is on predicting and interpreting the effect of common variables, the Cox PH model is the most suitable. On the other hand, the partial exponential model can provide a deeper understanding of temporal hazard patterns only in the absence of common variables, but at the expense of interpretability. In the context of this study, the strong linear effect of temperature indicates that the Cox model is the optimal choice.

5. Conclusions

1. Cox proportional hazards model was found to be very effective in predicting the thermal failure of carbon nanotubes as the concordance index value of 1.000 proved that all the samples were properly ranked according to the failure time by the heating rate variable only. This dominance shows the quality of the unidirectional relationship of thermal stress and degradation mechanics, which ascertains that the higher the rate of heating, the faster the failure rate of the whole sample under the investigation.

2.Those findings also indicated that the approximate hazard ratio of the heating rate in the Cox model, which equalled 7.14, implies that there is a high probability that failure will occur as the intensity of the thermal loading increases. It indicates that a one-unit rise in heating rate results in over seven-fold rise in the instantaneous hazard of failure and this indicates the high sensitivity of the nanotubes to thermal conditions and this can serve as a dependable quantitative measure to determine the reliability of the material during a slow and gradual modification of thermal conditions.

3.Conversely, even though the Cox model could include the theoretical flexibility given by the spline in the representation of possible nonlinear relations it failed to show any significant improvement over the standard linear model. It found a decrease in the concordance index (0.948 versus 1.000) and an increase in the AIC value (552.25 versus 505.99) which means that the extra complexity of the spline terms does not have a significant statistical justification, and that the correlation between the heating rate and the hazard of a failure is linear enough.

4.With regards to the piecewise exponential model, it could determine key time intervals in the failure path, and it found steep rises in hazard at (t = about 694) and another at (t = about 817), which could represent physical limits to structural damage. Nonetheless, the lack of the accompanying variable (heating rate) in the model severely affects its applicability in the given context of prediction or group comparison leading to an undefined concordance index and a large AIC value, which is, therefore, not suitable when conducting a regression-based assessment.

5.The correlations between the conditional actual failure time and the heating rate are found to be highly negative (≈ -0.926) with realistically attenuation level (30 percent) which gives strong experimental foundation to compare the models and to give strength to their validation in the applications of nanomaterials science.

6.Overall, the findings verify that the conventional Cox model is the most effective in modeling the thermal hazards of carbon nanotubes that can be the most effective balance between predictive accuracy, mathematical simplicity, interpretability and statistical efficiency. As it is found in the results, critical aspect of the process of failure is the extent of thermal stress and its impact can be perfectly described with the help of simple linear predictor in the hazard function.

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