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### **PREDICTION OF PROCESS-INDUCED DEFORMATIONS USING DEEP LEARNING INTERFACED FINITE ELEMENT CONSTITUTIVE MODELS**

Aravind Balaji<sup>1,2\*</sup>, Claudio Sbarufatti<sup>2</sup>, Antoine Parmentier<sup>1</sup>, David Dumas<sup>1</sup> and Francesco Cadini<sup>2</sup>

<sup>1</sup> Cenaero Research Center, Rue des Frères Wright 29, 6041 Gosselies, Belgium <sup>2</sup> Department of Mechanical Engineering, Politecnico di Milano, via La Masa 1, 20156 Milan, Italy

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#### **Abstract:**

The aim of the study is to improve the predictive capacity of a Finite Element (FE) tool in relation to a rheological thermo-chemo-viscoelastic constitutive model. This enhancement specifically focuses on accurately capturing the Process Induced Deformations (PID) resulting from the polymerization of the thermoset matrix. These deformations are due to the internal residual stress that arises from the material's inherent anisotropic properties, specifically the coefficients of thermal expansion and chemical shrinkage. The focus of the study is to accurately model the cure polymerization behaviour, which is known to have a significant impact on manufacturing defects. To account for the effect of process variables, such as maximum curing temperatures and temperature rates, a non-parametric neural network model is implemented







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# After vitrification Between gelation and vitrification **Prior to gelation**

**Differential Scanning Calorimetry (DSC) characterization tests :** 

DSC tests (rates of 1.5°C/min, 0.55°C/min, and 0.5°C/min & with isothermal dwells at 180°C, 175°C, and 185°C, respectively + some with partial curing) show that rates and dwells have an influence on the final state of the matrix. This raises the question of the interest for more representative kinetics models.

A new model should however ensure better general prediction and allow adapting to different resin formulations and variants.



**Parametric diffusion cure-kinetics (Cole, et al. [1991])** and DiBenedetto's model (Stutz, et al. [1990])

The cure kinetics model is implemented to describe the development of cure in terms of polymerization rate, as given by:

$$\frac{dX}{dt} = \frac{K X^{m} (1-X)^{n}}{1 + e^{C(X-X_{c})}}$$
  
where, K = Ae<sup>- $\Delta E/RT$</sup>  and X<sub>c</sub>=  $\iota_{0} - (\iota_{t}T)$ 

$$\frac{T_g - T_{g\infty}}{T_g} = \frac{\lambda X}{1 - (1 - \lambda) X}$$

#### **Parameters influencing the PIDs in thermoset parts**

Intrinsic parameters	Extrinsic parameters
Thermal conductivity	Mould
Mechanical properties	Friction properties
Coefficient of thermal expansion	Degree of vacuum
Coefficient of chemical shrinkage	Heating rates
Thickness	Cooling rates
Ply stacking sequence	Isothermal temperature dwells
Fibre volume fraction	Resin/fibre rich regions
Heat of reaction	



 $\psi$  and  $\psi'$  are the reduced time corresponding to spring and dashpot dependent on the curing state variables respectively and is defined as,

$$\psi = \int_{0}^{t} \frac{1}{a_{T}} dt'; \psi' = \int_{0}^{t} \frac{1}{a_{T}} d\tau'$$

The term a<sub>T</sub> corresponds to shift factor in the constitutive model and is assumed to be taken as a function approaching 0 and infinity in rubbery and glassy state, respectively.

Diffusion cure-kinetics interfaced constitutive model



viscoelastic constitutive model to make precise PID predictions. This modelling approach proves particularly useful when dealing with thick thermosets experiencing varying temperature gradients between the control temperature and the part temperature. The approach provides an accurate initial estimation of defects and facilitates the optimization of temperature profiles to reduce risks and enhance manufacturing quality.

Outlooks: The model could prove to be vital for characterizing complex resin formulations for newer thermoset materials without relying on Arrhenius formulations. Moreover, the model could be interfaced to conduct stochastic simulations, allowing for the quantification of uncertainties associated with cure temperature cycles.





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**Cenaero Research Center** Rue des Frères Wright 29, 6041 Belgium

#### Website: https://www.cenaero.be/



**Department of Mechanical Engineering** via La Masa 1, 20156 Milan, Italy

Website: https://www.polimi.it/