Experimentally Validated Thermochemical Modelling Of Sustainable Composites In COMSOL Multiphysics®

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Abstract

Pultrusion of fibre-reinforced thermoplastic composites presents challenges due to the complexity of achieving uniform curing, particularly when transitioning from traditional thermosetting resins to sustainable, recyclable thermoplastic options. Effective control over parameters like die temperature, pultrusion velocity, and fibre volume fraction is critical to ensure product quality and efficiency.
In this study, we integrate different experimental measurements and advanced numerical modelling in COMSOL Multiphysics® to study thermochemical curing process during the pultrusion of fibre-reinforced thermoplastic composites. First, polymerisation kinetics are characterized through dynamic and isothermal differential scanning calorimetry (DSC) for a newly adopted reactive thermoplastic acrylic resin, named Elium® and a semi-empirical kinetic model is developed to capture the resin's curing behaviour.
The DSC-derived kinetic relation is used to inform a model developed in COMSOL Multiphysics ® which couples heat transfer and cure kinetics to represents the interaction between exothermic polymerisation reactions and thermal gradients during pultrusion.
Specifically, the transient heat equation is solved using the Heat Transfer in Solids module, while the curing reaction kinetics are modelled through the classical PDE interface. For enhanced numerical stability in curing simulations, a stabilised convection-diffusion equation is implemented to address instabilities arising from convective terms. Coupling between the heat transfer and curing kinetics interfaces is achieved via an internal heat generation term. This coupling ensures that heat generated by the exothermic curing reaction directly influences the temperature evolution. In turn, temperature affects the curing reaction rate through an Arrhenius-based reaction model combined with a logistic function. Within the curing kinetics module, the stabilised convection-diffusion equation incorporates the fitted kinetic model, derived from DSC experiments, as its source term.
The thermal predictions of this COMSOL model are validated through the temperature records of embedded thermocouples within the composite during actual manufacturing trials confirming the model accuracy in capturing temperature profiles and cure progression within the composite.
By using the validated model in COMSOL Multiphysics, a comprehensive parametric study is conducted to evaluate the effect of different process parameters on the thermal and curing behaviour. These parametric simulations highlighted significant influences of pultrusion velocity and die temperature on curing dynamics, with velocity notably impacting the required die length for complete curing. Fibre volume fraction showed a moderate yet notable influence, affecting peak temperatures and curing uniformity. Finally, practical design charts are derived, linking process parameters to the required die length for achieving complete and uniform curing.
This work not only uses experimental validations to highlight the capability of COMSOL Multiphysics® in modelling complex thermochemical processes but also provides practical insights and tools to enhance the pultrusion manufacturing of high-performance, recyclable thermoplastic composites.

Reference

A. A. Safonov et al., Mathematical simulation of pultrusion processes: A review, Composite Structures 184 (2018) 153–177.
K. Minchenkov et al., Thermoplastic pultrusion: A review, Polymers 13 (2) (2021) 180.

Figures used in the abstract

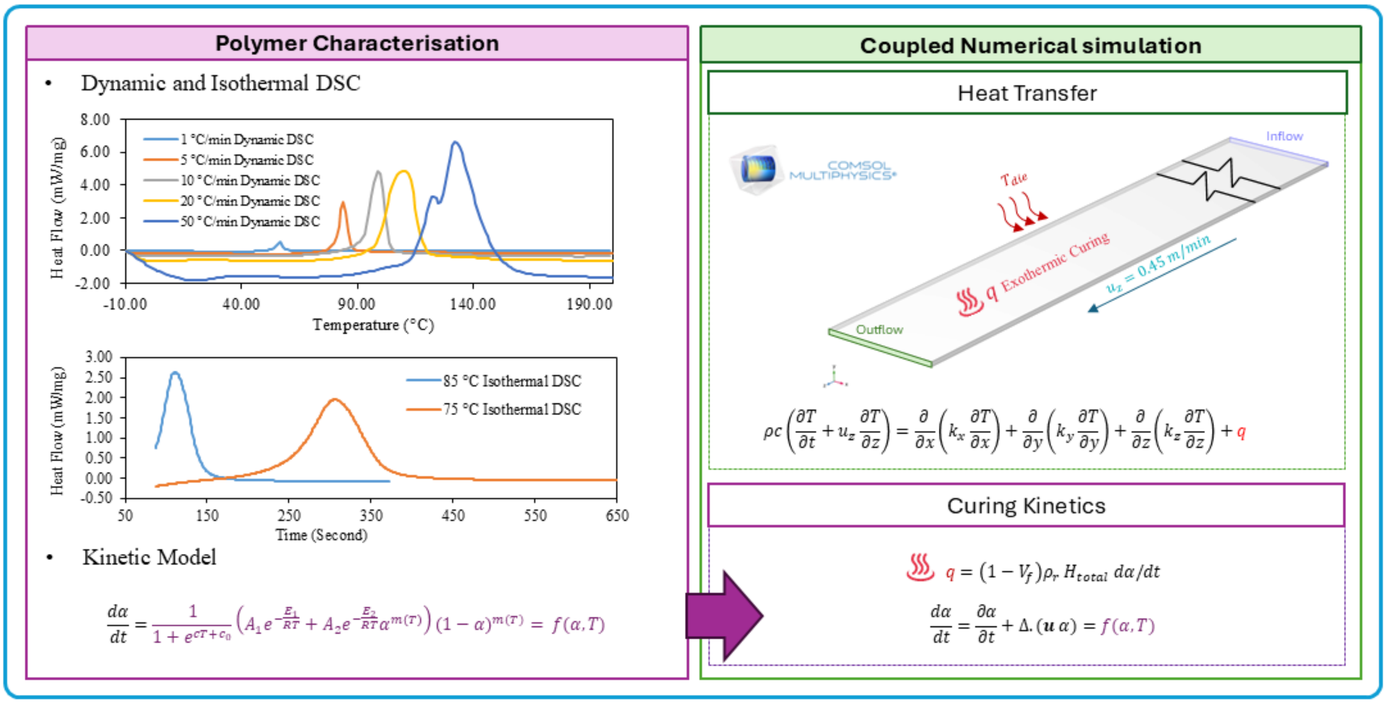

Figure 1 : The DSC-derived kinetic relation informs a model developed in COMSOL Multiphysics ® which couples heat transfer and cure kinetics

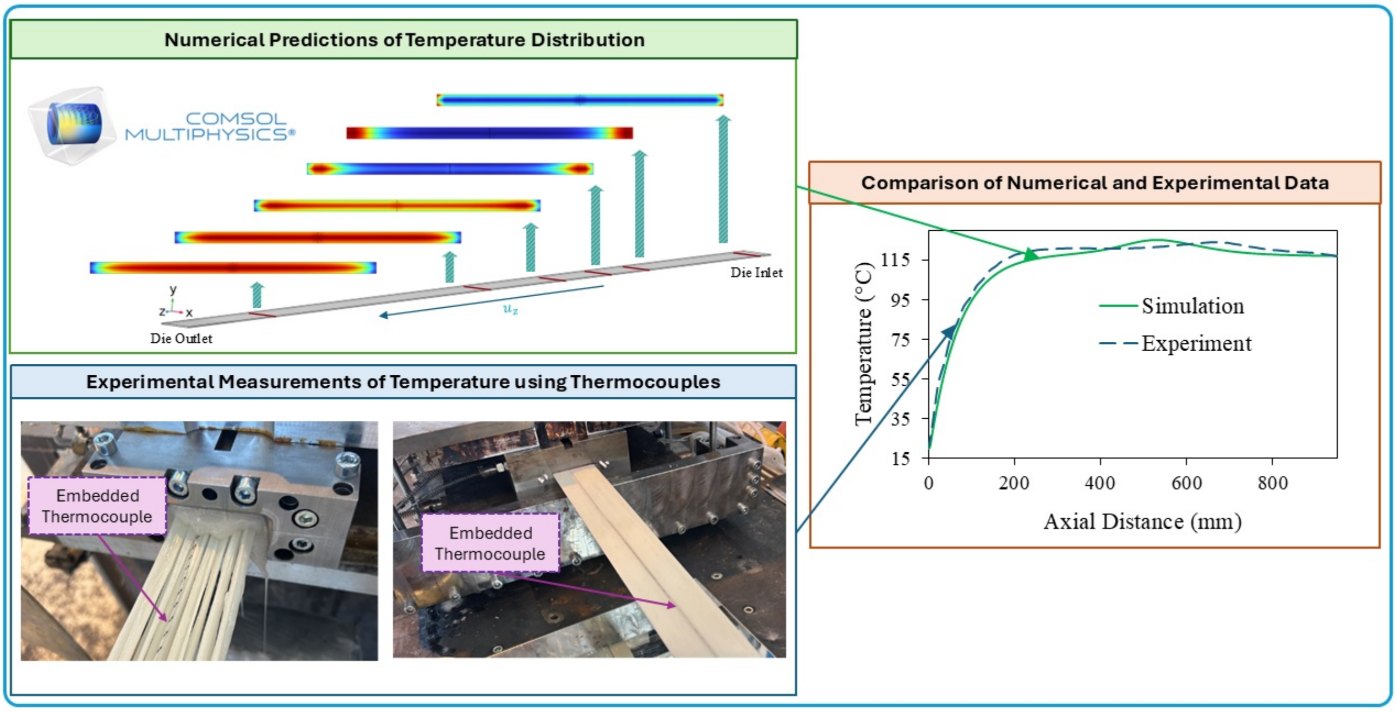

Figure 2 : Validation of the Numerical Model Using Experimental Measurements