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Prediction of degree of impregnation in thermoplastic unidirectional carbon fiber prepreg by multi-scale computational fluid dynamics

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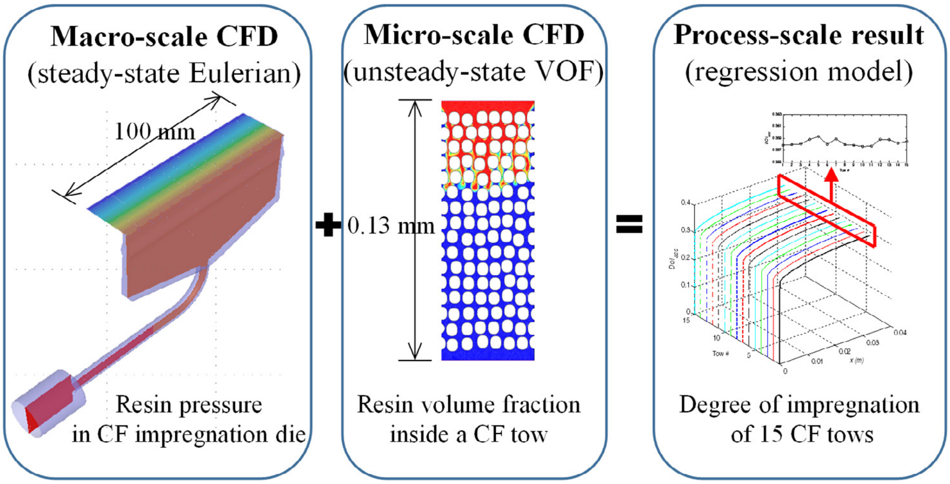
HIGHLIGHTS

- Degree of impregnation (DoI) for unidirectional carbon fiber prepreg (UD-CFP).
- Pressure profile of impregnation die obtained using macro-scale 3D Eulerian CFD model.
- DoI with time and pressure obtained from micro-scale 2D volume of fluid CFD model.
- Prediction of cumulative DoI for UD-CFP impregnation die by multi-scale CFD model.

GRAPHICAL ABSTRACT



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ABSTRACT

A multi-scale simulation approach was proposed to predict the degree of impregnation (DoI) in thermoplastic unidirectional carbon fiber prepreg (UD-CFP). The multi-scale approach included a two-dimensional (2D) micro-scale computational fluid dynamics (CFD) in a representative elementary volume (REV) of carbon fiber (CF) tow, a 3D macro-scale CFD of an entire impregnation die with 15 sliding CF tows, and a process-scale simulation assembling data from the micro- and macro-scale CFDs. In the macro-scale steady-state CFD, thermoplastic resin injection and CF tow insertion were considered for an impregnation die 10 cm in width. In the micro-scale transient CFD, impregnation mechanisms of resin into CF filaments 7 μm in diameter were identified in terms of surface coverage, capillary permeation, and penetration through CF filaments. The DoI as a function of pressure and time was obtained from the micro-scale CFD within a range of pressures found in the macro-scale CFD. In the process-scale simulation, the cumulative DoI of the 15 tows was predicted along the impregnation die length with the aid

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Abbreviations: 2D, two-dimensional; 3D, three-dimensional; CF, carbon fiber; CFD, computational fluid dynamics; CFRC, carbon fiber reinforced composite; CFP, carbon fiber prepreg; CSF, continuum surface force; DMSO, dimethyl sulfoxide; DoI, degree of impregnation; PA6, polyamide 6; REV, representative elementary volume; RMSD, root mean squared deviation; RoI, rate of impregnation; UD, uni-directional; VOF, volume of fluid.

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Nomenclature

a, b, c	constants of DoI function
A	cross sectional area (m^2)
C_2	inertial resistance coefficient (–)
C_a	capillary number (–)
c_p	heat capacity (J/kg/K)
d_H	hydraulic diameter (m)
DoI_{CFD}	DoI obtained from micro-scale CFD
DoI_{Cum}	cumulative DoI
DoI_{func}	DoI function obtained by regression of DoI_{CFD}
E	energy (J)
F	source term force (N)
$\vec{g}$	gravity vector (=9.81 m/s^2)
h	penetration depth (m)
H	temperature dependence term of viscosity (–)
$\vec{i}$	unit direction vector of x-axis
$\overline{\overline{I}}$	identity tensor (–)
$\vec{j}$	unit direction vector of y-axis
k	thermal conductivity (W/m/K)
K	permeability (m^2)
L	number index of times
L_P	length of wetted perimeter (m)
M	number index of pressures
n	power-law index
$\vec{n}$	normal vector (–)
N	number index of computational cells in 2D CFD domain
P	gauge pressure (Pa)
R	number index of computational cells in tow domain
R^2	correlation coefficient (–)
Re	Reynolds number (–)
t	time (s)
T	temperature (K or °C)
T_0	zero temperature (K)
T_{ref}	reference temperature (K)
u	velocity (m/s)
V	molar volume (cm^3/mol)
x	axial length (m)
x_{end}	end of impregnation die length (m)

Greek letters

α	volume fraction (–)
β	slope limiter value (–)
γ	shear rate (1/s)
ε	voidage (–)
η	viscosity (kg/m/s)
η_0	zero shear viscosity (kg/m/s)
η_∞	infinite shear viscosity (kg/m/s)
θ	contact angle (rad or °)
κ	surface curvature (1/m)
τ	time constant (s)
ρ	density (kg/m^3)
σ	surface tension (N/m)
$\overline{\overline{\tau}}$	stress tensor (Pa)
Φ	molar volume constant (–)

Subscripts

a	activation
D	DMSO
eff	effective
r	resin
$surf$	surface tension
T	tow
w	wall

of the micro- and macro-scale CFD results. Combining the multi-scale models gives a potential to predict the uniformity of the transverse resin amount in the final UD-CFP product.

1. Introduction

High strength fiber-reinforced composite materials have been widely applied in many structural and mechanical systems such as aerospace, automotive, sporting goods, biomedical, building, and infrastructure (Chang and Lees, 1988; Han et al., 2015; Ngo et al., 2017; Rodríguez-Tembleque and Aliabadi, 2016). Carbon fiber-reinforced composites (CFRCs) with thermoplastic matrices show excellent properties including light weight, high strength and modulus, good electrical and thermal conductivity, environmental resistance, and recyclability (Chang and Lees, 1988; Luo et al., 2014; Sakaguchi et al., 2000). However, the use of CFRCs with thermoplastic matrices suffers from drawbacks regarding their manufacture in industrial applications. Since the molten viscosity of thermoplastic resins is higher than that of thermoset resins, there are difficulties in impregnating thermoplastic resins into carbon fiber (CF) tows (Sakaguchi et al., 2000; Ye et al., 1995), where the tow is a bundle of strands (or filaments) having a diameter of a few micrometers. Understanding the impregnation mechanisms at the micro-scale is important to achieve a good quality of CFRCs (Hou et al., 1998; Ye et al., 1995).

The prepreg used to fabricate CFRC intermediates (Ngo et al., 2017) is ready to lay into the mold without the addition of any resin, because of pre-impregnation with a resin. Many researchers have presented impregnation and compaction behaviors of intermediate thermoplastic composites for commingled yarn (Hamada et al., 1993; Klinkmüller et al., 1995; Van West et al., 1991), powder-impregnated unidirectional fiber bundles (Kim et al., 1989), and prepreg tapes (Lee and Springer, 1987). The axial and transverse permeabilities were dependent on the microscopic characteristics and orientation of the fiber network (Gutowski et al., 1987). A comprehensive model describing the impregnation and consolidation mechanisms was developed for thermoplastic CFRCs under the assumption of an isothermal Newtonian fluid, porous media tow, and absence of capillary effect between the fluid and CF tow (Hou et al., 1998; Ye et al., 1995). Bijsterbosch and Gaymans (1993) studied the degree of impregnation (DoI) of glass fiber with polyamide 6 (PA6) in an impregnation bath, where the DoI experimentally obtained for various process and material parameters was expressed as a function of the square roots of time and pressure (Bijsterbosch and Gaymans, 1993). A resin permeability to CF filaments obtained at the micro-scale was used to calculate the resin velocity inside CFRC tows at the macro-scale, assuming that the CF filaments were entirely impregnated (Ngo et al., 2017). However, few studies have addressed the influence of the microscopic impregnation mechanism on the quality of CFRCs at the macro-scale.