

**Additional data for “Understanding and predicting defect formation in automated fibre placement pre-preg laminates”, published in Composites
Part A: Applied Science and Manufacturing**

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A.1 Cure kinetics model

The cure reaction rate, \dot{x} of 8552 epoxy resin can be computed as follows [1]:

$$\dot{x} = \left(\frac{1}{\dot{x}_k} + \frac{1}{\dot{x}_d} \right)^{-1} \quad (1)$$

Here \dot{x}_k is the chemically controlled part of the reaction, defined as follows [1]:

$$\dot{x}_k = \left(\frac{1}{\dot{x}_{c1}} + \frac{1}{\dot{x}_{i2} + \dot{x}_{c2}} \right)^{-1} + \dot{x}_e \quad (2)$$

where for each reaction \dot{x}_{c1} , \dot{x}_{i2} , \dot{x}_{c2} and \dot{x}_e

$$\dot{x}_i = K_{0i} e^{-\frac{E_{a_i}}{RT}} (1-x)^{l_i} \left(\frac{1}{r} - x \right)^{m_i} (x^{n_{2i}} + b_i)^{n_i} \quad (3)$$

Here x is the instantaneous degree of cure.

\dot{x}_d expresses the diffusion controlled part of the reaction and is defined as follows [1]:

$$\dot{x}_d = k_{d_0} e^{-\frac{B}{f}} \quad (4)$$

where

$$f = a_f (T - T_g) + b_f \quad (5)$$

Here a_f and b_f are calculated as follows:

$$\begin{aligned} a_f &= a_1 & \text{if } T_g < T_{g_{a1}} \\ a_f &= S_a T_g + C_a & \text{if } T_{g_{a1}} < T_g < T_{g_{a2}} \\ a_f &= a_2 & \text{if } T_g > T_{g_{a2}} \end{aligned} \quad (6)$$

where

$$S_a = \frac{a_2 - a_1}{T_{ga2} - T_{ga1}} \quad (7)$$

and

$$C_a = a_2 - S_a T_{ga2} \quad (8)$$

Similarly,

$$b_f = \begin{cases} b_1 & \text{if } T_g < T_{gb1} \\ S_b T_g + C_b & \text{if } T_{gb1} < T_g < T_{gb2} \\ b_2 & \text{if } T_g > T_{gb2} \end{cases} \quad (9)$$

where

$$S_b = \frac{b_2 - b_1}{T_{gb2} - T_{gb1}} \quad (10)$$

and

$$C_b = b_2 - S_b T_{gb2} \quad (11)$$

Here T_g represents the glass transition temperature and is described by the DeBenedetto equation as follows:

$$T_g = T_{g0} + \frac{\lambda x (T_{g\infty} - T_{g0})}{1 - (\lambda - x)x} \quad (12)$$

The total heat of reaction, H_T of the resin system of this study is 600 J/g [1]. In addition an initial degree of cure, x_0 of 0.05 was assumed [1].

Table A.1 summarises all the parameters used in the Eqns. (1)-(12).

Table A.1. Cure kinetics parameters.

Parameter	Value				Units
	\dot{x}_{c1}	\dot{x}_{i2}	\dot{x}_{c2}	\dot{x}_e	
k_0	153900.5	1000	1000	3.963E+11	1/s
E_a	64.929.5	0	0	133168.3	J/mol
l	2.347	0	0	1.029	
r	1	1	1	1	
m	0	0	0	0	
n_2	1	0	0	1	
b	0.1594	1	1	0	
n	1.413	0	0	5.586	
k_{d0}	4				1/s
B	0.21				
a_1	4.8E-04				1/°C
a_2	4.8E-04				1/°C
T_{ga1}	0				°C
T_{ga2}	100				°C
b_1	0.021				
b_2	0.031				
T_{gb1}	120				°C
T_{g0}	195				°C
$T_{g\infty}$	-7				°C
T_{gb2}	250				°C
λ	0.78				

A.2 Specific heat capacity

The resin specific heat capacity is defined as follows [1]:

$$c_{pr} = c_{prb} + \frac{c_{pg} - c_{prb}}{1 - e^{k[(1-T_g)-\Delta T_c]}} \quad (13)$$

where

$$c_{pi} = (1 - x)c_{pi0} + xc_{pi\infty} \quad \text{for } i = rb, g \quad (14)$$

and

$$c_{pij} = s_{ij}T + c_{ij} \quad \text{for } i = rb, g \text{ and } j = 0, \infty \quad (15)$$

Here T is the temperature. The fibre specific heat capacity, c_{pf} is calculated as follows [2]:

$$c_{pf} = 750 + 2.05T \quad (16)$$

The specific heat capacity of the composite is expressed using the rule of mixtures:

$$c_p = w_f c_{pf} + (1 - w_f) c_{pr} \quad (17)$$

Here w_f is the fibre weight fraction and is defined as:

$$w_f = \frac{v_f \rho_f}{\rho} \quad (18)$$

where v_f is the fibre volume fraction, ρ_f and ρ is the fibre density and composite density, respectively. A v_f of 0.55 was assumed in this study. The composite density is computed using the rule of mixtures as follows:

$$\rho = v_f \rho_f + (1 - v_f) \rho_r \quad (19)$$

where ρ_r is the density of the resin. The parameters in Eqns. (13)-(19) are listed in Table A.2.

Table A.2. Specific heat capacity parameters.

Parameter	value	Units
ρ_r	1301	kg/m ³
ρ_f	1790	kg/m ³
s_{g0}	3.775	J/(kg °C ²)
c_{g0}	730	J/(kg °C)
$s_{g\infty}$	3.4	J/(kg °C ²)
$c_{g\infty}$	830	J/(kg °C)
s_{r0}	3.27	J/(kg °C ²)
c_{r0}	1088	J/(kg °C)
$s_{r\infty}$	2	J/(kg °C ²)
$c_{r\infty}$	1350	J/(kg °C)
k	0.278	1/°C
ΔT_c	-1.5	°C

A.3 Thermal conductivity

The thermal conductivity of the resin is calculated as follows [1]:

$$k_r = Ak_r + Bk_r T + Ck_r x \quad (20)$$

The fibre thermal conductivity in the longitudinal direction is defined as [2]:

$$k_{lf} = Ak_{lf} + Bk_{lf} T \quad (21)$$

The thermal conductivity of the fibre in the transverse direction is [2]:

$$k_{tf} = Ak_{tf} + Bk_{tf}T \quad (22)$$

The thermal conductivity of the composite in the longitudinal direction is computed using the rule of mixtures as follows:

$$k_{11} = v_f k_{lf} + (1 - v_f) k_r \quad (23)$$

In the transverse direction the thermal conductivity can be computed as follows [3]:

$$k_{22} = k_{33} = v_f k_r \left(\frac{k_{tf}}{k_r} - 1 \right) + k_r \left(\frac{1}{2} - \frac{k_{tf}}{2k_r} \right) + k_r \left(\frac{k_{tf}}{k_r} - 1 \right) \sqrt{v_f^2 - v_f + \frac{\left(\frac{k_{tf}}{k_r} + 1 \right)^2}{\left(\frac{2k_{tf}}{k_r} - 2 \right)^2}} \quad (24)$$

Table A.3 summarises all the parameters used in Eqns. (20)-(24).

Table A.3. Thermal conductivity parameters.

Parameter	value	Units
Ak_r	0.148	W/m/°C
Bk_r	3.43E-04	W/m/°C ²
Ck_r	6.07E-02	W/m/°C
Ak_{lf}	7.69	W/m/°C
Bk_{lf}	1.56E-02	W/m/°C ²
Ak_{tf}	2.4	W/m/°C
Bk_{tf}	5.07E-04	W/m/°C ²

A.4 Consolidation model parameters

The material parameters used in the model for consolidation of the material system IM7-8552 are given in Table A.4. The procedure for parameter extraction from simple consolidation tests is described in [4]. The parameters a and b control the behaviour of the rate dependent term of the apparent viscosity ($b_{squeeze}$ and b_{bleed} are the values of b before and after locking respectively). The parameter k controls the size of the inter-fibre channels at the micro-scale.

Table A.4. Consolidation model parameters.

Tempertaure (°C)	k	a	$b_{squeeze}$	b_{bleed}
30	0.949073376	-0.9302	-16.51	-33.24
40	0.919238734	-0.9124	-15.01	-31.74
50	0.884086642	-0.8822	-14.12	-30.85
60	0.850373593	-0.856	-13.58	-30.31
70	0.823853122	-0.8434	-13.27	-30
80	0.806058649	-0.8391	-13.08	-29.81
90	0.795357049	-0.8378	-12.96	-29.69

References

- [1] Johnston A. An integrated model of the development of process-induced deformation in autoclave processing of composite structures: University of British Columbia; 1997.
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- [3] Farmer J, Covert E. Thermal conductivity of a thermosetting advanced composite during its cure. Journal of Thermophysics and Heat Transfer(USA) 1996;10(3):467-475.
- [4] Belnoue JPH, Nixon-Pearson OJ, Ivanov D, Hallett SR. A novel hyper-viscoelastic model for consolidation of toughened prepregs under processing conditions. Mechanics of Materials. 2016;97:118-34.