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New simulation app for hygrothermal knock-down analysis

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One of the major challenges in aerospace composite design is the accurate prediction of working stress and strain knock-down in hygrothermal conditions. It is a complex analysis field, where the composite material's mechanical response is directly related to (1) changes in the polymer matrix equation of state, and (2) commonly used micromechanics. This complex relation requires rigorous modelling and extensive calculations. Composite Agency has developed a new simulation app for this purpose: CheFEM®. The chemical-physical basis of the tool and its use are described briefly in this article.

CheFEM uses a fundamental approach to describe the thermodynamics of an absorbed chemical and matrix: the Sanchez-Lacombe Equation of State (SL EOS). Once a chemical name, temperature and pressure are set, the chemical SL EOS computes the properties of the determined state: liquid, vapour or (supercritical) gas. Mixtures (water-glycerol, Skydrol) can also be evaluated.

The extended matrix SL EOS includes handling of the matrix glass transition, the related matrix free volume and the effects of matrix crosslinks and crystallinity. As such, below-Tg thermosets (such as epoxies and polyurethanes) and semi-crystalline thermoplastics (such as PEEK and PPS) can be computed seamlessly.

The SL EOS referenced foundation parameters (critical temperature, compressed density, and related cohesive energy density, etc.) are hard-coded in the CheFEM EOS database.

User tweaking

The intuitive user interface (see Figure 1) allows setting basic geometries such as aerospace testing specimens, fuselages, etc. For the depicted laminate view, parameters can be fine-tuned at several different levels: (1) matrix (crystalline fraction, initial stiffness, strength, strain, etc.), (2) filler (filler material, volume, orientation, etc.), and (3) layer (stress-free temperature, microvoids, etc.). Note that CheFEM can handle multi-angle plies such as [π/4] (0°/+45°/90°/-45°/-45°/90°/+45°/0°)s in one layer. The program uses an internal 24-ply based code to bootstrap the laminate behaviour as one layer. This article considers a Fiberite 934 matrix reinforced with 68 vol% of Thornel 300 carbon fibres in [π/4] fully exposed to RTW (23°C, 100% RH) conditions.

Thermodynamic output

CheFEM's output is primarily divided into a thermodynamic view and a mechanical view. The thermodynamic results for layer 2 are shown in Figure

Fig. 1: The CheFEM user interface, with unexposed pristine Fiberite 934 defined in layer 1, and exposed filled Fiberite 934 defined in layer 2

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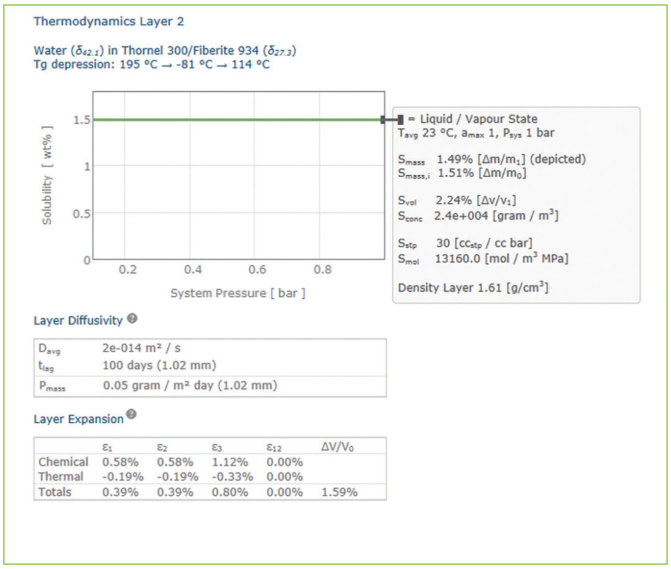

Fig. 2: CheFEM thermodynamic output with a selection of parameters for layer 2

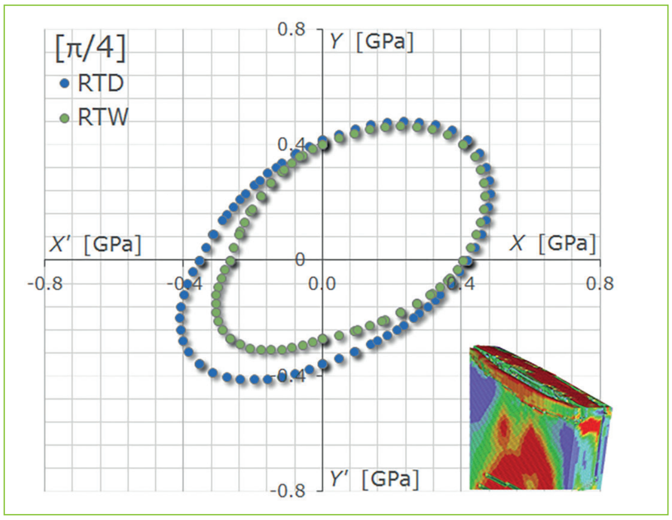

Fig. 3: Tsai-Wu failure envelopes generated by CheFEM. Inlay image: CheFEM data can be imported in other FEA packages for further fracture and application-oriented analysis

Tab. 1: CheFEM mechanical output for RTD and RTW conditions

Property	Unit	RTD (0% RH)	RTW (100% RH)
Filler			
Orientation	-	[π/4]	[π/4]
Volume	vol%	68	68
Matrix			
Water absorption	wt%	0.00	1.51
T*	**°C**	**23**	**104**
E @ **T***	GPa	4.6	3.5
S @ **T***	GPa	0.078	0.060
ε @ **T***	%	1.70	1.71
Composite stiffness			
Ex	GPa	62	60 (-3%)
Ey	GPa	62	60 (-3%)
Gxy	GPa	24	23 (-4%)
Composite strength			
X	GPa	0.42	0.40 (-5%)
X'	GPa	-0.36	-0.27 (-25%)
Y	-	0.42	0.40 (-5%)
Y'	GPa	-0.36	-0.27 (-25%)

2. The 50+ thermodynamic output properties include chemical uptake isotherm, chemical solubility, chemical-thermal swelling, glass temperature depression, diffusion coefficient, permeation rate, saturation times and eventual chemical degradation kinetics.

Mechanical output

CheFEM's mechanical output generates, among other properties, the chemically exposed stiffness and tensile parameters for the layer. A selection of this output for RTD (room temperature dry) and RTW (room temperature wet) conditions is listed in Table 1.

Note that T* (°C) is the temperature at which the matrix unexposed mechanical input properties (stiffness, strength and yield strain) must be taken. T* is derived from CheFEM thermodynamics, and based on the simulated matrix plasticizing and eventual chemical (equilibrium) reaction kinetics. As such, the described matrix properties are the only temperature-dependent mechanical input data that are needed for CheFEM. This data can usually be obtained from the matrix material producer or an experiment. All other properties, such as fibre stiffness and strength, can usually be determined at room temperature.

Failure envelopes

As a direct consequence of the above generated thermo-mechanical data, CheFEM can produce failure envelopes according to several failure criteria, such as maximum stress, maximum strain and Tsai's quadratic criteria. Figure 3 shows an example of the generated Tsai-Wu envelope. Moreover, CheFEM data can be imported in other (FEA) software packages. An example is the Abaqus Materials Library Manager, which can be used in conjunction with CheFEM.

Conclusion

The results demonstrated in this article correlate highly with the experimental work carried out on Thornel 300/Fiberite 934 composites in the 1970s and 1980s. Hence, CheFEM is definitely a useful tool to get a grip on the effects of environmental conditions (not only water) on composite materials. Besides aerospace, CheFEM is also used in other industries, e.g. for the analysis of seals, polymers and composites for oil & gas applications. The chemical-thermal cycling features of CheFEM will be discussed in the forthcoming part 2 of this article. □

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