

# CDS Complete Theory Manual

Release edition 3 October 2026

This manual explains the constitutive assumptions, governing equations and numerical limits behind CDS material, process, structural and electromagnetic studies. Start with the chapter for the physical problem, identify its required inputs and units, then compare its assumptions with the specimen or structure you intend to represent. A solved model is not by itself validated design data.

## Preface

Readers should be familiar with stress, strain, elementary heat transfer and matrix algebra. The opening chapters establish the common material and laminate description before introducing transport, structural response and failure. Read the assumptions beside each formulation before applying it to a new structure. A numerical solution can be internally consistent while the physical idealization remains inappropriate.

The chapter sequence follows the information used by the solver. Constituent data become effective ply properties; the stacking sequence determines laminate stiffness; boundary histories and loads determine the state from which stresses and failure measures are recovered. Electromagnetic models have their own property and excitation requirements and are presented as a separate branch. Worked operating instructions are collected in the Training and Exercise Manual.

## How to use this manual

Read the assumptions before choosing a model. Keep units consistent, inspect solver notices and use the recorded checks to distinguish a completed calculation from a validated result. Chapter links lead to the interactive website; exercise links open the Workbench. Account-controlled database downloads and classroom materials remain subject to their existing access rules.

Equations are editable Word mathematics. This PDF is exported from the same Word document. Historical reference chapters retain their stated scope; the current workflow and exercise chapters describe the available CDS implementation.

# Contents

|      |                                                                                 |     |
|------|---------------------------------------------------------------------------------|-----|
| 1    | Model hierarchy and solver foundations.....                                     | 4   |
| 1.1  | Framework and Scope .....                                                       | 4   |
| 1.2  | Assumptions and Limitations.....                                                | 6   |
| 2    | Material data and constitutive state .....                                      | 8   |
| 2.1  | Trusted material data from the source.....                                      | 8   |
| 2.2  | Thermoset cure kinetics .....                                                   | 9   |
| 2.3  | PEEK/PEKK crystallization pipeline.....                                         | 12  |
| 2.4  | AI Import.....                                                                  | 15  |
| 3    | Constituents to effective ply properties.....                                   | 16  |
| 3.1  | Micromechanics of Composites.....                                               | 16  |
| 3.2  | Elastic Micromechanics Theory .....                                             | 18  |
| 3.3  | Thermal Conductivity Micromechanics.....                                        | 36  |
| 3.4  | CTE Micromechanics .....                                                        | 41  |
| 3.5  | Semi-analytical aligned discontinuous-composite theory .....                    | 48  |
| 3.6  | Textile and Thermophysical Framework .....                                      | 54  |
| 3.7  | Fabric Micromechanics Theory .....                                              | 59  |
| 3.8  | Warp-Weft Averaging and Crimp Correction .....                                  | 70  |
| 3.9  | Filled Matrix Hybrid and Void Micromechanics .....                              | 81  |
| 3.10 | Effective Density and Specific Heat.....                                        | 90  |
| 3.11 | Orthotropic Thermophysical Property Assembly .....                              | 96  |
| 3.12 | Verification Validation and References .....                                    | 103 |
| 4    | Ply transformations and laminate constitutive response .....                    | 113 |
| 4.1  | Ply transformations and laminate constitutive response governing relation ..... | 113 |
| 4.2  | Laminate Analysis .....                                                         | 113 |
| 4.3  | Hygro-Thermo-Mechanical CLT and ABD .....                                       | 115 |
| 4.4  | Effective Laminate and Transport Properties.....                                | 117 |
| 4.5  | Common Ply Property Definition .....                                            | 119 |
| 4.6  | Micromechanics and Material Routing.....                                        | 121 |
| 4.7  | Uniform Transverse Traction and z-Response .....                                | 124 |
| 4.8  | Inputs and Model Selection .....                                                | 126 |
| 4.9  | Outputs and Event Histories.....                                                | 127 |
| 5    | Heat transport and polymer evolution.....                                       | 129 |
| 5.1  | Heat transport and polymer evolution governing relation .....                   | 129 |
| 5.2  | Heterogeneous 1D transient heat .....                                           | 129 |
| 5.3  | Trace temperature from properties to structural response .....                  | 133 |
| 5.4  | Connect process history to structural response .....                            | 134 |
| 5.5  | Resolve the thermal history before structural loading.....                      | 139 |
| 5.6  | Crystallization consolidation and interface bonding .....                       | 140 |
| 5.7  | Epoxy viscosity and cure .....                                                  | 144 |
| 5.8  | Thermoplastic prepreg processing.....                                           | 146 |
| 5.9  | PEEK crystallization Velisaris Seferis.....                                     | 147 |
| 5.10 | Intimate contact healing and coupled bonding.....                               | 151 |
| 5.11 | Laser heating for moving prepreg and AFP .....                                  | 155 |
| 5.12 | Void Consolidation Model .....                                                  | 160 |

|                                                                                |     |
|--------------------------------------------------------------------------------|-----|
| 5.13 Pultrusion heating and cooling dies .....                                 | 163 |
| 6 Moisture transport and environmental conditioning .....                      | 166 |
| 6.1 Moisture transport and environmental conditioning governing relation ..... | 166 |
| 6.2 Heterogeneous moisture diffusion .....                                     | 166 |
| 6.3 Connect moisture transport to stress response .....                        | 169 |
| 7 Geometry loads and structural response .....                                 | 171 |
| 7.1 Plate cylinder and beam models .....                                       | 171 |
| 7.2 Shear-deformable laminated plates .....                                    | 172 |
| 7.3 Constant-section shell cylinder .....                                      | 179 |
| 7.4 Hyer thick laminated cylinder .....                                        | 180 |
| 7.5 Process fields in progressive laminate failure .....                       | 182 |
| 7.6 Move from laminate mechanics to structural decisions .....                 | 186 |
| 7.7 Bonded roller contact width variants .....                                 | 187 |
| 8 Failure initiation damage and durability .....                               | 196 |
| 8.1 Failure Criteria .....                                                     | 196 |
| 8.2 Progressive Failure Algorithm .....                                        | 199 |
| 8.3 Fatigue S-N assessment .....                                               | 200 |
| 8.4 Specialized constitutive and structural models .....                       | 205 |
| 8.5 Damage and Failure Framework .....                                         | 209 |
| 8.6 Continuum Damage Mechanics .....                                           | 214 |
| 8.7 Composite Failure Criteria .....                                           | 222 |
| 8.8 Damage and Failure Workflow .....                                          | 231 |
| 8.9 Damage Degradation and Redistribution .....                                | 240 |
| 8.10 Mixed-Mode Cohesive Delamination .....                                    | 241 |
| 9 CREATE and DISCOVER design space interpretation .....                        | 244 |
| 9.1 CREATE and DISCOVER design space interpretation governing relation .....   | 244 |
| 9.2 From elastic response to a design study .....                              | 244 |
| 10 Verification interpretation and reproducibility .....                       | 249 |
| 10.1 Verification and Validation .....                                         | 249 |
| 10.2 Explore a test Understand its limits .....                                | 250 |
| 11 Electromagnetic response and specialized branches .....                     | 281 |
| 11.1 RF laminate shielding and transmission .....                              | 281 |
| Glossary and notation .....                                                    | 287 |
| References and further reading .....                                           | 288 |

# 1 Model hierarchy and solver foundations

## Online chapter

A CDS study is a dependency graph, not an isolated equation. Material records, constitutive models, ply definitions, geometry and boundary conditions determine which equations can be solved. Results belong to the input state used for that run; changing a linked record does not update an earlier stored solution.

Choose the physical idealization before choosing numerical resolution. A through-thickness transport model assumes in-plane uniformity. A laminate membrane model does not resolve local contact or a three-dimensional edge field. More nodes or smaller steps improve the numerical approximation within an idealization; they do not remove that idealization's limits.

Constituent and ply properties use material axes, while loading and geometry use structural axes. State the transformation convention, engineering shear convention, thickness direction and stress signs. Convert units at interfaces rather than mixing unit systems inside a stiffness or transport operator.

Resolve linked records and model compatibility, assemble material and laminate properties, apply initial and boundary conditions, advance the selected fields, recover stresses and evaluate failure measures. An unsupported coupling must remain explicitly excluded. A successful run is a numerical outcome, not evidence of design qualification.

## 1.1 Framework and Scope

CDS release r15 is a unified constituent-to-process-to-structure framework. Every physical ply may independently use automatic property resolution, embedded micromechanics, or direct measured properties; supply its own polymer process data; and enter the common damaged laminate and selectable plate, cylinder, or beam solution. Classical Lamination Theory supplies the membrane-bending foundation while mapped temperature, moisture, cure shrinkage, crystallization shrinkage, cohesive interfaces, and per-ply failure routing remain integrated without treating the stochastic short-fiber branch as the whole formulation.

### One connected property chain

Fiber, matrix, filler, void, architecture, and measured overrides resolve into the complete 3D elastic, strength, expansion, density, and transport definition for each ply.

### Independent source routing

Each ply can use a linked micromechanics recipe or measured material properties. Different plies may use different sources.

### Retained laminate foundation

Thin-laminate CLT, transformed orthotropic ply stiffness, full A-B-D coupling, and three-node-per-ply recovery remain the section-analysis foundation.

### Updated failure model

Each ply selects a compatible failure theory. New failures degrade only the activated fiber, matrix, or shear family before equilibrium is solved again at the same load.

### Environmental coupling

Temperature and moisture fields generate damaged force and moment resultants. They are recomputed after every stiffness change.

### Process-first solution

A heterogeneous 1D heat/moisture model uses independent top and bottom schedules, cure or crystallization kinetics, and per-ply transport properties before structural loading.

### Optional interface model

A mixed-mode cohesive law can represent delamination only when local interface separation history is supplied externally.

### Uniform 3D traction extension

Prescribed  $\sigma_z$ ,  $\tau_{xz}$ , and  $\tau_{yz}$  are recovered in global and local axes, contribute to failure, and add independent E3, G13, and G23 damage families.

### Multi-material laminate

Every active ply can use a different material, orientation, environmental state, strength set, and eligible failure criterion during the same progressive analysis.

### Optional Double-Double recommendation

Compatible equal-thickness master-ply stacks can be mapped to a stiffness-matched Tsai Double-Double family. The user chooses whether downstream analysis retains the supplied angles or uses the recommendation.

### Tsai Double-Double stiffness matching

For a compatible stack, CDS searches the staggered family  $[+\Phi/-\Psi/-\Phi/+\Psi]_{rT}$  on a  $0.5^\circ$  grid. The objective minimizes the normalized mismatch between the supplied laminate extensional stiffness and the candidate Double-Double stiffness while also reporting coupling and homogenization measures.

Equation 1. Tsai Double-Double stiffness matching

$$e_A(\Phi, \Psi) = \|A_{DD}(\Phi, \Psi) - A_{\text{original}}\|_F / \max(\|A_{\text{original}}\|_F, \epsilon)$$

### Meaning, notation and theory source

#### Definitions and derivation: Tsai Double-Double stiffness matching

Laminate flag 17 equals 0 to retain the supplied angles or 1 to use the compatible recommendation before all downstream laminate and progressive-failure calculations. Every ply row, material, thickness, property, and interface is preserved; only eligible ply angles are replaced. The Double-Double recommendation summarizes compatibility, recommended angles, coupling, homogenization, and stiffness error, while the ply-angle table reports original, recommended, and selected angles.

### Connected analysis sequence

- **1. Read one schema** Resolve eight scalar groups, constituent and ply tables, optional matrix shear laws, two surface histories, kinetics, loads, geometry, interfaces, and outputs.
- **2. Generate or accept each ply** Use the established resolver, embedded micromechanics, or direct measured properties independently. Preserve measured overrides.
- **3. Solve discontinuous RVEs when selected** Rebuild interaction segments, insert ordered Weibull breaks, couple RVE curves in series, and screen critical clusters.

- **4. Recommend or retain the layup** When compatible, calculate the stiffness-matched Double-Double candidate and use laminate flag 17 to retain or substitute its angles.
- **5. Solve and map process history** Interpolate schedules, solve heat/diffusion/polymer state, and form per-ply process resultants.
- **6. Assemble equilibrium** Integrate damaged A, B, and D and superimpose mechanical, thermal, moisture, process, and  $\sigma$ -Poisson actions.
- **7. Solve the structure** Select plate, shell/Hyer cylinder, or beam and recover stiffness, response, buckling, and frequency results.
- **8. Evaluate and redistribute** Check each ply independently, reduce newly failed families, and repeat equilibrium at the same load until stable.
- **9. Export** Return named engineering results with material lineage, process fields, structural results, detailed discontinuous events, properties, and matrices.

**Model intent:** this framework is a screening and research implementation. Calibration against the actual material system and target environment is required before design use.

## 1.2 Assumptions and Limitations

- The in-plane foundation is thin-laminate CLT with small strains and rotations. The r11 transverse extension prescribes uniform tractions and performs layerwise constitutive recovery; it is not a general 3D equilibrium solution.
- Hashin is the retained 2D plane-stress form; the model does not resolve 3D fiber kinking, fracture-plane rotation, or nonlinear matrix plasticity.
- Transport is one-dimensional through thickness. Lateral heat flow, edge drying, tool-contact geometry, damage-assisted diffusion, and spatial hot spots require a higher-fidelity model.
- Cure, crystallization, diffusion, saturation, reaction heat, and process shrinkage require material-grade and process-specific calibration; default kinetics rows are inert.
- Moduli, strengths, and fracture energies are not currently functions of temperature or moisture concentration.
- The cohesive branch requires externally supplied local kinematics and does not predict crack-front shape, migration, multiple finite-area delaminations, or contact.
- Conductivity and heat capacity are reported as pristine homogenized properties and are not degraded by cracks.
- Residual stiffness factors and stochastic short-fiber parameters require calibration and convergence studies.
- ROM/Reuss, Halpin-Tsai, approximate Mori-Tanaka, approximate self-consistent, fabric, filler, and directional-void branches are reduced-order engineering property generators; critical architecture-specific use requires calibration or a higher-fidelity RVE.
- Micromechanics generates pristine properties. Progressive damage is applied only in the laminate solver.
- Loss of numerical stiffness under load control is a collapse indicator, not a physical post-failure strain trajectory.

**Use boundary:** outputs support comparison, screening, calibration, and research. They are not material design allowables and do not replace test evidence or structural certification requirements.

## **Chapter review**

Resolve linked records and model compatibility, assemble material and laminate properties, apply initial and boundary conditions, advance the selected fields, recover stresses and evaluate failure measures. An unsupported coupling must remain explicitly excluded. A successful run is a numerical outcome, not evidence of design qualification.

## 2 Material data and constitutive state

### Online chapter

Every downstream prediction depends on the material definition. Separate measured values, fitted model coefficients, estimated properties and illustrative defaults. Record temperature, moisture condition, processing state, units and source with the values rather than treating a material name as a complete specification.

Elastic moduli, Poisson ratios and shear moduli define the stiffness response. Density, heat capacity, conductivity, moisture diffusivity and equilibrium uptake define different physical properties and cannot be inferred from stiffness alone. Orthotropic data must respect reciprocal compliance relationships and a physically admissible stiffness matrix.

Cure and crystallization are internal state variables. Their kinetics, heat release and shrinkage require independent parameter definitions and calibration. A strength allowable does not automatically evolve because the elastic modulus or degree of cure changes. Use only the state dependencies implemented by the selected constitutive branch.

Document the applicable property range and interpolation policy. Extrapolation beyond measured temperatures, moisture levels or strain rates is a separate modeling assumption. Illustrative teaching records should remain labeled throughout the result and report.

### 2.1 Trusted material data from the source

Theories / Materials

Prepare traceable engineering records, calibrated thermoset cure kinetics, and semicrystalline thermoplastic crystallization models before the data enters micromechanics, processing, laminate, or structural analyses.

2 theory sections 2 polymer-state branches

Theory map

Models, equations, figures, and cross-references

01 / Thermosets

#### Cure heat and shrinkage

Connect kinetic rate laws with exotherm, vitrification, diffusion limits, and chemical shrinkage.

[Open cure theory →](#)

02 / Thermoplastics

#### Crystallization and morphology

Resolve Nakamura–Avrami crystallization, latent heat, and crystallization shrinkage for PEEK and PEKK.

[Open crystallization theory →](#)

Complete reference

One continuous sequence

## Thermoset cure kinetics

## Thermoplastic crystallization

## 2.2 Thermoset cure kinetics

### 05.1.2 / Materials

Define calibrated epoxy cure, heat release, and irreversible process shrinkage at the material/ply level before solving the laminate process history. Each equation is accompanied by its physical meaning, variables, units, model connection and source.

### State variable and model routing

Degree of cure  $\alpha$  is the reacted fraction of the available thermoset chemistry. R15 bounds  $\alpha$  to [0,1], prevents reverse reaction, and evaluates kinetics independently at every transport node. Each ply selects its own polymer family and kinetics model in the process definition. Select thermoset cure for a reacting resin or an inert material for a nonreacting layer.

Eq. 05.1.2-01 Arrhenius rate constant

$$k_i(T) = A_i \exp[-E_i/(RT)]$$

### Equation details Explanation · variables · model connection · reference +

Converts each calibrated kinetic prefactor and activation energy into a temperature-dependent reaction-rate constant. Absolute temperature must be used.

**Variables**  $k_i$  rate constant for reaction branch  $i$   $s^{-1}$   $A_i$  pre-exponential factor for branch  $i$   $s^{-1}$   $E_i$  activation energy for branch  $i$  J/mol  $R$  universal gas constant 8.314462618 J/(mol·K)  $T$  local nodal absolute temperature K

**Model connection** Evaluated from the current thermal iterate before the selected cure law is advanced; it therefore couples cure rate to the transient temperature field.

**Theory basis** [Sourour–Kamal cure kinetics](#)

### Selectable reaction laws

The model ID chooses one of four rate laws. These laws describe chemistry only after their coefficients have been fit to DSC or equivalent measurements for the actual resin formulation.

Eq. 05.1.2-02 Nth-order cure

$$\dot{\alpha} = k_1(T)(1 - \alpha)^n$$

### Equation details Explanation · variables · model connection · reference +

Represents a non-autocatalytic reaction whose rate decreases as the unreacted fraction is consumed.

**Variables**  $\alpha$  degree of cure dimensionless, 0–1  $\dot{\alpha}$  instantaneous cure rate  $s^{-1}$   $k_1$  Arrhenius rate constant from Eq. 05.1.2-01  $s^{-1}$   $n$  reaction-order exponent dimensionless

**Model connection** The nth-order cure law. The returned nonnegative rate is passed to the bounded irreversible state update.

## Theory basis [Thermoset kinetic model basis](#)

Eq. 05.1.2-03 **Kamal–Sourour autocatalytic cure**

$$\dot{\alpha} = [k_1(T) + k_2(T)\alpha^m](1 - \alpha)^n$$

### Equation details Explanation · variables · model connection · reference +

Adds an autocatalytic branch that grows with degree of cure to the nth-order branch, allowing an isothermal rate peak after the reaction begins.

**Variables**  $k_1$ ,  $k_2$  *non-autocatalytic and autocatalytic Arrhenius rate constants*  $s^{-1}$   $\alpha$  *degree of cure* dimensionless, 0–1  $m$  *autocatalytic exponent* dimensionless  $n$  *unreacted-fraction exponent* dimensionless  $\dot{\alpha}$  *instantaneous cure rate*  $s^{-1}$

**Model connection** The Kamal–Sourour cure law, also used as the base reaction law before vitrification limitation is applied.

## Theory basis [Sourour–Kamal autocatalytic model](#)

Eq. 05.1.2-04 **Prout–Tompkins cure**

$$\dot{\alpha} = k_1(T)\alpha^m(1 - \alpha)^n$$

### Equation details Explanation · variables · model connection · reference +

Uses a single autocatalytic rate constant with reacted- and unreacted-fraction powers. A small positive numerical floor on  $\alpha$  prevents a zero-to-a-negative-power singularity.

**Variables**  $k_1$  *Arrhenius rate constant*  $s^{-1}$   $\alpha$  *degree of cure* dimensionless, 0–1  $m$ ,  $n$  *autocatalytic and reaction-order exponents* dimensionless  $\dot{\alpha}$  *instantaneous cure rate*  $s^{-1}$

**Model connection** The Prout–Tompkins cure law. It shares the same bounded state update, heat source, and shrinkage mapping as the other cure laws.

## Theory basis [NASA composite cure-process formulation](#)

Eq. 05.1.2-05 **Diffusion-limited Kamal multiplier**

$$f_d = \{1 + \exp[s_v(\alpha - \alpha_v)]\}^{-1}, \dot{\alpha}_{\text{limited}} = f_d \dot{\alpha}_{\text{Kamal}}$$

### Equation details Explanation · variables · model connection · reference +

Suppresses the chemical Kamal–Sourour rate as cure passes a calibrated vitrification threshold. It is an empirical mobility correction, not an independently predicted glass-transition model.

**Variables**  $f_d$  *diffusion or vitrification rate multiplier* dimensionless, 0–1  $s_v$  *logistic vitrification slope* dimensionless  $\alpha_v$  *degree of cure at the logistic midpoint* dimensionless  $\dot{\alpha}_{\text{Kamal}}$  *unlimited rate from Eq. 05.1.2-03*  $s^{-1}$   $\dot{\alpha}_{\text{limited}}$  *mobility-limited cure rate*  $s^{-1}$

**Model connection** The diffusion-limited cure law. The limited rate, rather than the raw chemical rate, advances  $\alpha$  and produces reaction heat.

## Theory basis [Cure-process modeling and vitrification context](#)

### Irreversible state integration

Eq. 05.1.2-06 **Bounded exponential cure update**

$$r_\alpha = 1 - \alpha^n, \alpha^{n+1} = \min[1, \max(\alpha^n, \alpha^n + r_\alpha \{1 - \exp(-r^n \Delta t / r_\alpha)\})]$$

#### Equation details Explanation · variables · model connection · reference +

Advances cure over one transport step without consuming more than the remaining unreacted fraction. The outer bounds enforce irreversibility and  $\alpha \leq 1$ .

**Variables**  $\alpha^n$ ,  $\alpha^{n+1}$  *degree of cure at the old and new process times* dimensionless  $\mathbf{r}^n$  *selected row or diffusion-limited kinetic rate*  $s^{-1}$   $\Delta t$  *transport time increment*  $s$   $\mathbf{r}_\alpha$  *available unreacted fraction*,  $1 - \alpha^n$  dimensionless

**Model connection** Applied independently at every active thermoset node inside each staggered thermal/kinetic iteration. The reported rate is  $(\alpha^{n+1} - \alpha^n) / \Delta t$ .

**Theory basis** [Numerical cure-process integration context](#)

#### Reaction heat and chemical shrinkage

Eq. 05.1.2-07 Volumetric cure heat source

$$q_c = \rho H_c \dot{\alpha}$$

#### Equation details Explanation · variables · model connection · reference +

Converts cure progress and mass-specific total heat of reaction into a volumetric source for the one-dimensional heat equation.

**Variables**  $q_c$  *volumetric cure heat generation*  $W/m^3$   $\rho$  *local effective ply density*  $kg/m^3$   $H_c$  *total heat of cure per unit mass*  $J/kg$   $\dot{\alpha}$  *bounded cure rate over the current step*  $s^{-1}$

**Model connection** Included in the thermal right-hand side only when the cure-exotherm option is enabled and reported separately as cure heat generation.

**Theory basis** [NASA composite cure-process heat balance](#)

Eq. 05.1.2-08 Local cure-shrinkage free strain

$$\varepsilon_k^c = -s_k^c (\alpha - \alpha_0)$$

#### Equation details Explanation · variables · model connection · reference +

Maps the increase in degree of cure into an anisotropic contraction in the ply material axes. Positive calibrated shrinkage magnitudes therefore produce negative free strain.

**Variables**  $\varepsilon_k^c$  *cure-shrinkage free strain in material direction k* strain  $s_k^c$  *full-cure shrinkage magnitude in direction k* strain  $\alpha_0$  *initial degree of cure* dimensionless  $\mathbf{k}$  *local ply direction 1, 2, or 3* index

**Model connection** Stored at each process node, fitted across each ply, transformed to laminate axes, and optionally included in the process force and moment resultants.

**Theory basis** [NASA cure-induced residual-stress study](#)

**Calibration boundary.** Pre-exponential factors, activation energies, exponents, total reaction heat, vitrification controls, and shrinkage are resin-system data. R15 defaults to an inert row and does not represent a universal epoxy.

## Material inputs and outputs

**Table 1. Material inputs and outputs**

| Input family               | Purpose                                        | Primary output            |
|----------------------------|------------------------------------------------|---------------------------|
| $A_1, E_1, A_2, E_2, m, n$ | Temperature-dependent reaction rate            | Cure-rate history         |
| $H_c$                      | Total heat of cure per unit mass               | Cure-heat history         |
| $S^c_{1,2,3}$              | Full-process local shrinkage magnitudes        | Process-shrinkage history |
| $\alpha_0, \alpha_v, S_v$  | Initial state and optional mobility limitation | Degree-of-cure history    |

## Theory references

- Sourour and Kamal, “Differential scanning calorimetry of epoxy cure: isothermal cure kinetics,” *Thermochimica Acta* 14 (1976) 41–59.
- NASA, *Composite Cure Process Modeling and Simulations using Finite Element Analysis* (2016).
- NASA/TM–20205009287, residual stresses induced during matrix cure.

## 2.3 PEEK/PEKK crystallization pipeline

This section describes the coupled material-state formulation. The optional WB5 PEEK parallel and series history models use a different, one-way calculation without latent-heat or shrinkage feedback; see Crystallization consolidation and interface bonding in the processing chapter.

### 05.1.3 / Materials

Represent calibrated semicrystalline thermoplastic evolution with single- or double-branch Nakamura/Avrami-style kinetics, latent heat, and anisotropic crystallization shrinkage. Each equation is accompanied by its physical meaning, variables, units, model connection and source.

This page describes the coupled material-state formulation. The optional WB5 PEEK parallel and series models use a separate one-way history calculation, without latent-heat or shrinkage feedback. See [crystallization, consolidation and interface bonding](#) for those models and their implementation limits.

## State normalization and temperature window

Select thermoplastic crystallization for a semicrystalline polymer. Crystallinity  $X$  is bounded between its initial value and the user-supplied maximum  $X_{\max}$ . Kinetics are active only when the current nodal temperature lies strictly between the calibrated glass-transition and melting temperatures.

Eq. 05.1.3-01 **Normalized crystallinity**

$$\xi = X/X_{\max}, 0 \leq \xi \leq 1$$

### Equation details Explanation • variables • model connection • reference +

Expresses current absolute crystallinity as a fraction of the maximum crystallinity available to the selected thermoplastic grade.

**Variables**  $\xi$  *normalized crystallinity* dimensionless, 0–1  $X$  *current absolute crystallinity* dimensionless mass or volume fraction  $X_{\max}$  *calibrated maximum crystallinity* dimensionless mass or volume fraction

**Model connection** The normalized state is used by both Nakamura branches and the bounded integration rule; the crystallinity history retains the absolute crystallinity  $X$ .

**Theory basis** [Nakamura nonisothermal crystallization](#)

Eq. 05.1.3-02 **Temperature and undercooling factor**

$$K_j(T) = K_{0j} \exp[-E_{xj}/(RT)] [(T_m - T)/(T_m - T_g)]^p$$

**Equation details** **Explanation · variables · model connection · reference +**

Combines Arrhenius temperature dependence with a calibrated undercooling function that vanishes at the melting temperature and is evaluated only inside the  $T_g$ – $T_m$  process window.

**Variables**  $K_j$  *crystallization rate coefficient for branch  $j$*   $s^{-1}$   $K_{0j}$  *branch pre-exponential coefficient*  $s^{-1}$   $E_{xj}$  *branch activation energy* J/mol  $T_g$ ,  $T_m$  *glass-transition and melting temperatures* K  $p$  *undercooling exponent* dimensionless  $R$ ,  $T$  *gas constant and local absolute temperature* J/(mol·K), K

**Model connection** Evaluated at every active thermoplastic transport node using the current thermal iterate. Outside  $T_g < T < T_m$ , R15 sets the crystallization rate to zero.

**Theory basis** [PEEK dual-mechanism crystallization model](#)

**Nakamura/Avrami evolution**

Eq. 05.1.3-03 **Single-branch normalized crystallization rate**

$$\dot{\xi}_j = n_j K_j(T) (1 - \xi) [-\ln(1 - \xi)]^{(n_j - 1)/n_j}$$

**Equation details** **Explanation · variables · model connection · reference +**

Differentiates the Nakamura form of Avrami crystallization to obtain an instantaneous nonisothermal rate in the normalized state. Numerical floors protect the logarithm near  $\xi=0$  and  $\xi=1$ .

**Variables**  $\dot{\xi}_j$  *normalized crystallization rate of branch  $j$*   $s^{-1}$   $n_j$  *Avrami exponent for branch  $j$*  dimensionless  $K_j(T)$  *temperature-dependent branch coefficient*  $s^{-1}$   $\xi$  *normalized crystallinity* dimensionless

**Model connection** The single-branch crystallization law uses its calibrated rate directly. The rate is then advanced using the irreversible bounded update.

**Theory basis** [Nakamura rate formulation](#)

Eq. 05.1.3-04 **Double-branch crystallization rate**

$$\dot{\xi} = w \dot{\xi}_1 + (1 - w) \dot{\xi}_2$$

**Equation details** **Explanation · variables · model connection · reference +**

Blends two independently calibrated Nakamura branches to represent two-stage crystallization with one bounded weighting factor.

**Variables**  $\dot{\xi}$  *combined normalized crystallization rate*  $s^{-1}$   $\dot{\xi}_1$ ,  $\dot{\xi}_2$  *normalized rates of branches 1 and 2*  $s^{-1}$   $w$  *branch-1 weight* dimensionless, 0–1

**Model connection** The dual-branch crystallization law. The same combined rate controls crystallinity growth, latent heat release, and the subsequent shrinkage state.

## Theory basis [Velisaris–Seferis dual-mechanism PEEK model](#)

Eq. 05.1.3-05 Bounded irreversible crystallinity update

$$r_{\xi} = 1 - \xi^n \xi^{n+1} = \min[1, \max(\xi^n, \xi^n + r_{\xi}\{1 - \exp(-\xi^n \Delta t / r_{\xi})\})], X^{n+1} = X_{\max} \xi^{n+1}$$

### Equation details Explanation · variables · model connection · reference +

Integrates the normalized rate over the process step without consuming more than the remaining crystallizable fraction, then maps the state back to absolute crystallinity.

**Variables**  $\xi^n, \xi^{n+1}$  old and new normalized crystallinity dimensionless  $r_{\xi}$  remaining crystallizable fraction,  $1 - \xi^n$  dimensionless  $\xi^n$  selected single- or double-branch rate  $s^{-1}$   $\Delta t$  transport time increment  $s$   $X^{n+1}$  new absolute crystallinity dimensionless fraction

**Model connection** Applied independently at every active thermoplastic node. The crystallization-rate history reports  $(X^{n+1} - X^n) / \Delta t$  rather than the normalized branch rate.

## Theory basis [Nonisothermal Nakamura state evolution](#)

### Latent heat and crystallization shrinkage

Eq. 05.1.3-06 Crystallization heat source

$$q_x = \rho H_x \dot{X}$$

### Equation details Explanation · variables · model connection · reference +

Converts absolute crystallinity growth and the calibrated heat of crystallization into a volumetric heat source.

**Variables**  $q_x$  volumetric crystallization heat generation  $W/m^3$   $\rho$  local effective ply density  $kg/m^3$   $H_x$  heat of crystallization per unit mass  $J/kg$   $\dot{X}$  absolute crystallinity rate  $s^{-1}$

**Model connection** Included in the heat equation only when the crystallization-exotherm option is enabled and reported as crystallization heat generation.

## Theory basis [PEEK crystallization calorimetry basis](#)

Eq. 05.1.3-07 Local crystallization-shrinkage free strain

$$\varepsilon_k^x = -s_k^x (X - X_0) / X_{\max}$$

### Equation details Explanation · variables · model connection · reference +

Maps crystallinity gained after the initial state into an anisotropic contraction in each ply material direction.

**Variables**  $\varepsilon_k^x$  crystallization free strain in local direction  $k$  strain  $s_k^x$  full-crystallization shrinkage magnitude strain  $X_0$  initial absolute crystallinity dimensionless fraction  $X_{\max}$  maximum absolute crystallinity dimensionless fraction  $k$  local ply direction 1, 2, or 3 index

**Model connection** Stored in the process-shrinkage history, fitted through each ply, and optionally added to the laminate process resultants and local failure-stress recovery.

## Theory basis [Process-shrinkage residual-stress framework](#)

**Material-grade calibration is required.** PEEK and PEKK grade, molecular architecture, cooling history, prior melt state, reinforcement, and measurement method change the fitted kinetics. The pipeline is a model family, not a generic property card.

### Required validation data

- DSC-derived crystallization rate and heat over relevant cooling/heating histories.
- $T_g$ ,  $T_m$ , and maximum crystallinity for the selected grade.
- Dilatometry or dimensional data for local crystallization shrinkage.
- Verification against nonisothermal process cycles before residual-stress use.

### Theory references

- Nakamura et al., “Some aspects of nonisothermal crystallization of polymers. I,” *Journal of Applied Polymer Science* 16 (1972) 1077–1091.
- Velisaris and Seferis, “Crystallization kinetics of polyetheretherketone (PEEK) matrices,” *Polymer Engineering & Science* 26 (1986) 1574–1581.
- NASA composite process modeling reference for coupled heat generation, shrinkage, and residual response.

## 2.4 AI Import

Theories / 05.1.1 AI Import

Research with ChatGPT. Review sources, units and conditions in Workbench before creating new material records.

[Read the step-by-step material import guide](#)

Open Material → Find / Import with AI in Workbench to copy a research prompt, load research JSON, attach local datasheets for comparison, and selectively import reviewed properties. Existing records are not overwritten.

Web search and automatic PDF extraction are not connected inside CDS in this version. Unknown values remain absent; estimates require explicit approval. Save the resulting workspace as CDS\_DB and retain original source files separately.

### Chapter review

Document the applicable property range and interpolation policy. Extrapolation beyond measured temperatures, moisture levels or strain rates is a separate modeling assumption. Illustrative teaching records should remain labeled throughout the result and report.

## 3 Constituents to effective ply properties

### Online chapter

Micromechanics maps constituent properties and architecture to an effective ply. The calculation requires a representative reinforcement arrangement and volume fractions. It does not replace measured design allowables or establish that a manufactured material has the assumed architecture.

Mixture estimates, inclusion models and shear-lag models make different assumptions about load transfer, geometry and interaction. Continuous aligned fibers, short fibers, fabrics and particle-filled systems require different architecture descriptions. Verify constituent limits and the effect of orientation and aspect ratio before comparing a predicted effective modulus with a test.

Pass the effective elastic tensor, density and directional expansion and transport properties with their coordinate convention. Retain separate provenance for each property family. A model calibrated for elastic stiffness is not automatically calibrated for thermal conductivity, diffusion or strength.

### 3.1 Micromechanics of Composites

#### Current Workbench models and compatibility

This theory library includes wider research formulations. Check the [released model directory](#) for selectable models, required inputs, limits and exercises. The event-driven RVE branch is not enabled in hosted Workbench.

Theories / Micromechanics

The complete CDS theory chain: continuous and discontinuous fibers, mean-field homogenization, Chou orientation factors, textile architectures, fillers and voids, thermophysics, damage and failure, constituent-limit recovery, and the per-ply handoff into progressive laminate analysis.

15 theory sections 4 homogenization branches 3 per-ply property sources

Theory map

Models, equations, figures, and cross-references

01 / Elastic foundation

#### Constituent to effective stiffness

Continuous and discontinuous fibers; rule of mixtures, Halpin–Tsai, Mori–Tanaka, self-consistent formulations; aspect ratio; global orientation; Chou  $F_a/F_p$ ; constituent-limit recovery; compliance and stiffness matrices.

[Open elastic theory →](#)

02 / Discontinuous fibers

#### Random ends Weibull strengths and critical clusters

This reference describes the Henry–Pimenta event-driven RVE formulation. It is not enabled in hosted Workbench; the released Cox elastic short-fiber model has a narrower supported scope.

[Open discontinuous-fiber theory →](#)

03 / Textile architectures

### **Tows fabrics and architecture corrections**

Plain weave, 2×2 twill, 4/5/8-harness satin, basket, leno, biaxial NCF, and triaxial braid with warp–weft averaging, crimp, interlacing, stitch, binder, and bias-angle effects.

[Open fabric theory →](#)

04 / Multiphysics and defects

### **Fillers voids and thermophysical response**

Filled-resin and hybrid homogenization, explicit and dilute directional void treatment, density, specific heat, orthotropic conductivity, directional CTE, validation checks, and linked references.

[Open filler and void theory →](#)

05 / Damage and failure

### **CDM and composite failure**

Continuum damage mechanics, Tsai–Wu and Hashin criteria, recovered endpoint properties, degradation, and failure progression.

[Open failure theory →](#)

06 / Unified r15 handoff

### **Generated properties enter progressive laminates**

Each physical ply independently selects automatic property resolution, embedded constituent micromechanics, or direct measured data. The generated pristine 3D property set then enters the common damaged-ABD and failure-redistribution solver.

[Open unified material routing →](#)

Complete reference

One continuous sequence

## **Elastic Micromechanics Theory**

### **Aligned Discontinuous-Fiber Model**

### **Textile and Thermophysical Framework**

### **Fabric Micromechanics Theory**

### **Warp Weft Averaging and Crimp Correction**

### **Filled Matrix Hybrid and Void Micromechanics**

### **Effective Density and Specific Heat**

### **Thermal Conductivity Micromechanics**

### **CTE Micromechanics**

### **Orthotropic Thermophysical Property Assembly**

### **Verification Validation and References**

### **Damage and Failure Framework**

### **Continuum Damage Mechanics**

### **Composite Failure Criteria**

### **Damage and Failure Workflow**

## **3.2 Elastic Micromechanics Theory**

Volume I / Elastic Micromechanics Theory

### **Abstract**

A compact elastic micromechanics framework is described for predicting the effective orthotropic stiffness of continuous fiber, discontinuous fiber, woven, filler-reinforced, and general multiphase composite materials. The model permits selection among four main homogenization branches: rule of mixtures, Halpin–Tsai, Mori–Tanaka engineering approximation, and a self-consistent engineering approximation. Constituent properties are supplied through Workbench vector inputs, while microstructure descriptors are supplied through scalar flags and scalar parameters. Fiber architecture effects are represented using fiber volume fraction, aspect ratio, and Tsu-Wei Chou axial and planar architecture parameters, denoted  $F_a$  and  $F_p$ . The model outputs effective Young's moduli, shear moduli, Poisson ratios, and related quantities for use in subsequent laminate and structural studies.

## Nomenclature

Table 2. Nomenclature

| Symbol                         | Definition                                                | Units                 |
|--------------------------------|-----------------------------------------------------------|-----------------------|
| $E_1, E_2, E_3$                | Effective orthotropic Young's moduli                      | Pa                    |
| $G_{12}, G_{13}, G_{23}$       | Effective orthotropic shear moduli                        | Pa                    |
| $\nu_{12}, \nu_{13}, \nu_{23}$ | Effective major Poisson ratios                            | –                     |
| $V_f, V_m, V_p, V_v$           | Fiber, matrix, particle/filler, and void volume fractions | –                     |
| $E_f, E_m, E_p$                | Fiber, matrix, and particle moduli                        | Pa                    |
| $G_f, G_m, G_p$                | Fiber, matrix, and particle shear moduli                  | Pa                    |
| $AR$                           | Fiber or inclusion aspect ratio, usually $l/d$            | –                     |
| $\eta_L$                       | Fiber length efficiency factor                            | –                     |
| $\eta_o$                       | Orientation efficiency factor                             | –                     |
| $F_a$                          | Chou axial architecture factor                            | –                     |
| $F_p$                          | Chou planar/random architecture factor                    | –                     |
| $\xi$                          | Halpin–Tsai shape parameter                               | –                     |
| $\eta$                         | Halpin–Tsai contrast parameter                            | –                     |
| <b>C</b>                       | Stiffness matrix or fourth-order stiffness tensor         | Pa                    |
| <b>S</b>                       | Compliance matrix or Eshelby tensor depending on context  | $\text{Pa}^{-1}$ or – |
| <b>A</b>                       | Strain concentration tensor or matrix                     | –                     |
| $\bar{\sigma}$                 | Macroscopic stress                                        | Pa                    |
| $\bar{\epsilon}$               | Macroscopic strain                                        | –                     |
| $\theta$                       | Global material orientation angle                         | deg                   |

## Model Scope

The solver model predicts effective properties of composite materials from constituent properties and architecture descriptors. The main elastic outputs are the orthotropic engineering constants

Equation 1. 4 1. Model Scope

$$\{E_1, E_2, E_3, G_{12}, G_{13}, G_{23}, \nu_{12}, \nu_{13}, \nu_{23}\}.$$

### Meaning, notation and theory source

[Definitions and derivation: 4 1. Model Scope](#)

These properties are used to generate Abaqus material definitions. Choose from the following stiffness models:

**Table 3. Model Scope**

| Model branch                              |
|-------------------------------------------|
| Rule of mixtures                          |
| Halpin-Tsai                               |
| Mori-Tanaka engineering approximation     |
| Self-consistent engineering approximation |

Choose the material architecture independently of the stiffness model:

**Table 4. Model Scope**

| Architecture branch                       |
|-------------------------------------------|
| Continuous unidirectional fiber composite |
| Discontinuous fiber composite             |
| Woven fabric composite                    |
| General multiphase composite              |

This separation allows, for example, a discontinuous-fiber material to be evaluated using a simple rule-of-mixtures approximation or a more interaction-aware self-consistent approximation.

## Constituent Property Inputs

Specify the properties of each constituent. The fiber property vector contains anisotropic stiffnesses, strengths, density, and thermophysical values. In Volume I only the elastic terms are required:

Equation 2. 5 2. Constituent Property Inputs

$$\mathbf{x}_f = [E_{f1}, E_{f2}, E_{f3}, G_{f12}, G_{f13}, G_{f23}, \nu_{f12}, \nu_{f13}, \nu_{f23}, \rho_f, \dots]^T.$$

### Meaning, notation and theory source

[Definitions and derivation: 5 2. Constituent Property Inputs](#)