*MAT_THERMAL

The *MAT_THERMAL cards allow thermal properties to be defined in coupled structural/thermal and thermal only analyses; see *CONTROL_SOLUTION. Thermal properties must be defined for all elements in such analyses.

Thermal material properties are specified by a thermal material ID number (TMID). This number is independent of the material ID number (MID) defined on all other *MAT_… property cards. In the same analysis identical TMID and MID numbers may exist. The TMID and MID numbers are related through the *PART card.

Available thermal materials are:

*MAT_THERMAL_ISOTROPIC

*MAT_THERMAL_ORTHOTROPIC

*MAT_THERMAL_ISOTROPIC_TD

*MAT_THERMAL_ORTHOTROPIC_TD

*MAT_THERMAL_DISCRETE_BEAM

*MAT_THERMAL_CHEMICAL_REACTION

*MAT_THERMAL_CWM

*MAT_THERMAL_ORTHOTROPIC_TD_LC

*MAT_THERMAL_ISOTROPIC_PHASE_CHANGE

*MAT_THERMAL_ISOTROPIC_TD_LC

*MAT_THERMAL_USER_DEFINED

*MAT_THERMAL_CHEMICAL_REACTION_ORTHOTROPIC

*MAT_THERMAL_ISOTROPIC

This is Thermal Material Type 1. With this material, isotropic thermal properties can be defined.

Card 1	1	2	3	4	5	6	7	8
Variable	TMID	TRO	TGRLC	TGMULT	TLAT	HLAT		
Type	A	F	F	F	F	F		

Card 2	1	2	3	4	5	6	7	8
Variable	HC	TC						
Type	F	F						

VARIABLE	DESCRIPTION
TMID	Thermal material identification. A unique number or label must be specified (see *PART).
TRO	Thermal density: EQ.0.0: Default to structural density
TGRLC	Thermal generation rate (see *DEFINE_CURVE). See Remark 2. GT.0: Load curve ID giving thermal generation rate as a function of time EQ.0: Thermal generation rate is the constant multiplier, TGMULT. LT.0: |TGRLC| is a load curve ID defining thermal generation rate as a function of temperature.
TGMULT	Thermal generation rate multiplier: EQ.0.0: No heat generation
TLAT	Phase change temperature
HLAT	Latent heat

VARIABLE	DESCRIPTION
HC	Specific heat
TC	Thermal conductivity

Remarks:

1. **Supported Load Curves.** *DEFINE_CURVE_FUNCTION is fully supported for *MAT_THERMAL_ISOTROPIC (added in revision 113488).

2. **Thermal Generation Rate.** TGRLC is similar to the volumetric heat generation rate in *LOAD_HEAT_GENERATION. It has units W/m^3 in the SI units system.

Example:

```
*MAT_THERMAL_ISOTROPIC
      1     2700.       210         1.0
      904.      222.
*define_curve_function
210
if(lc211,lc10,lc12,lc11)
*define_curve
211
0,-200
2.0,-200
*define_curve
10
0,1.43e+07
100,1.43e+07
*define_curve
11
0,2.43e+07
100,2.43e+07
*define_curve
12
0,3.43e+07
100,3.43e+07
```

*MAT_THERMAL_ORTHOTROPIC

This is Thermal Material Type 2. It allows orthotropic thermal properties to be defined.

Card 1	1	2	3	4	5	6	7	8
Variable	TMID	TRO	TGRLC	TGMULT	AOPT	TLAT	HLAT	
Type	A	F	F	F	F	F	F	

Card 2	1	2	3	4	5	6	7	8
Variable	HC	K1	K2	K3				
Type	F	F	F	F				

Card 3	1	2	3	4	5	6	7	8
Variable	XP	YP	ZP	A1	A2	A3		
Type	F	F	F	F	F	F		

Card 4	1	2	3	4	5	6	7	8
Variable	D1	D2	D3					
Type	F	F	F					

VARIABLE	DESCRIPTION
TMID	Thermal material identification. A unique number or label must be specified (see *PART).
TRO	Thermal density: EQ.0.0: Default to structural density

VARIABLE	DESCRIPTION
TGRLC	Thermal generation rate (see *DEFINE_CURVE). See Remark 1. GT.0: Load curve ID defining thermal generation rate as a function of time EQ.0: Thermal generation rate is the constant multiplier, TGMULT. LT.0: |TGRLC| is a load curve ID giving thermal generation rate as a function of temperature.
TGMULT	Thermal generation rate multiplier: EQ.0.0: No heat generation
AOPT	Material axes definition: EQ.0.0: Locally orthotropic with material axes by element nodes N1, N2 and N4 EQ.1.0: Locally orthotropic with material axes determined by a point in space and global location of element center EQ.2.0: Globally orthotropic with material axes determined by vectors EQ.3.0: Locally orthotropic with first material axis orthogonal to element normal (defined by element nodes N1, N2 and N4) and to a vector **d**. The third material direction corresponds to element normal. EQ.4.0: Local orthogonal in cylindrical coordinates with the material axes determined by a vector **d**, and an originating point, P, which define the centerline axis.
TLAT	Phase change temperature
HLAT	Latent heat
HC	Specific heat
K1	Thermal conductivity, K_1, in local x-direction
K2	Thermal conductivity, K_2, in local y-direction
K3	Thermal conductivity, K_3, in local z-direction
XP, YP, ZP	Coordinates of point p for AOPT = 1 and 4

VARIABLE	DESCRIPTION
A1, A2, A3	Components of vector **a** for AOPT = 2
D1, D2, D3	Components of vector **d** for AOPT = 2, 3 and 4

Remarks:

1. **Thermal Generation Rate.** TGRLC is similar to the volumetric heat generation rate in *LOAD_HEAT_GENERATION. It has units W/m^3 in the SI units system.

*MAT_THERMAL_ISOTROPIC_TD

This is Thermal Material Type 3. The isotropic properties can be temperature dependent. The temperature dependency is defined by specifying a minimum of two and a maximum of eight data points. You should define the properties for the temperature range that the material will see in the analysis.

Card 1	1	2	3	4	5	6	7	8
Variable	TMID	TRO	TGRLC	TGMULT	TLAT	HLAT		
Type	A	F	F	F	F	F		

Card 2	1	2	3	4	5	6	7	8
Variable	T1	T2	T3	T4	T5	T6	T7	T8
Type	F	F	F	F	F	F	F	F

Card 3	1	2	3	4	5	6	7	8
Variable	C1	C2	C3	C4	C5	C6	C7	C8
Type	F	F	F	F	F	F	F	F

Card 4	1	2	3	4	5	6	7	8
Variable	K1	K2	K3	K4	K5	K6	K7	K8
Type	F	F	F	F	F	F	F	F

VARIABLE	DESCRIPTION
TMID	Thermal material identification. A unique number or label must be specified (see *PART).

VARIABLE	DESCRIPTION
TRO	Thermal density: EQ.0.0: Default to structural density
TGRLC	Thermal generation rate (see *DEFINE_CURVE). See Remark 1. GT.0: Load curve ID giving thermal generation rate as a function of time EQ.0: Thermal generation rate is the constant multiplier, TGMULT. LT.0: |TGRLC| is a load curve ID defining thermal generation rate as a function of temperature.
TGMULT	Thermal generation rate multiplier: EQ.0.0: No heat generation
TLAT	Phase change temperature
HLAT	Latent heat
T1, …, T8	Temperatures: T1, ..., T8
C1, …, C8	Specific heat at: T1, …, T8
K1, …, K8	Thermal conductivity at: T1, …, T8

Remarks:

1. **Thermal Generation Rate.** TGRLC is similar to the volumetric heat generation rate in *LOAD_HEAT_GENERATION. It has units W/m^3 in the SI units system.

*MAT_THERMAL_ORTHOTROPIC_TD

This is Thermal Material Type 4. It allows temperature dependent orthotropic properties to be defined. The temperature dependency is defined by specifying a minimum of two and a maximum of eight data points. The properties must be defined for the temperature range that the material will see in the analysis.

Card Summary:

Card 1. This card is required.

TMID	TRO	TGRLC	TGMULT	AOPT	TLAT	HLAT	

Card 2. This card is required.

T1	T2	T3	T4	T5	T6	T7	T8

Card 3. This card is required.

C1	C2	C3	C4	C5	C6	C7	C8

Card 4. This card is required.

(K1)1	(K1)2	(K1)3	(K1)4	(K1)5	(K1)6	(K1)7	(K1)8

Card 5. This card is required.

(K2)1	(K2)2	(K2)3	(K2)4	(K2)5	(K2)6	(K2)7	(K2)8

Card 6. This card is required.

(K3)1	(K3)2	(K3)3	(K3)4	(K3)5	(K3)6	(K3)7	(K3)8

Card 7. This card is required.

XP	YP	ZP	A1	A2	A3		

Card 8. This card is required.

D1	D2	D3					

Data Card Definitions:

Card 1	1	2	3	4	5	6	7	8
Variable	TMID	TRO	TGRLC	TGMULT	AOPT	TLAT	HLAT	
Type	A	F	F	F	F	F	F	

VARIABLE	DESCRIPTION
TMID	Thermal material identification. A unique number or label must be specified (see *PART).
TRO	Thermal density: EQ.0.0: Default to structural density
TGRLC	Thermal generation rate (see *DEFINE_CURVE). See Remark 1. GT.0: Load curve ID defining thermal generation rate as a function of time EQ.0: Thermal generation rate is the constant multiplier, TGMULT. LT.0: |TGRLC| is a load curve ID defining thermal generation rate as a function of temperature.
TGMULT	Thermal generation rate multiplier: EQ.0.0: No heat generation
AOPT	Material axes definition (see *MAT_*OPTION*TROPIC_ELASTIC for a more complete description): EQ.0.0: Locally orthotropic with material axes by element nodes N1, N2 and N4 EQ.1.0: Locally orthotropic with material axes determined by a point in space and global location of element center EQ.2.0: Globally orthotropic with material axes determined by vectors EQ.3.0: Locally orthotropic with first material axis orthogonal to element normal (defined by element nodes N1, N2 and N4) and to a vector **d**- Third material direction corresponds to element normal.

VARIABLE	DESCRIPTION
	EQ.4.0: Local orthogonal in cylindrical coordinates with the material axes determined by a vector **d**, and an originating point, P, which define the centerline axis.
TLAT	Phase change temperature
HLAT	Latent heat

Card 2	1	2	3	4	5	6	7	8
Variable	T1	T2	T3	T4	T5	T6	T7	T8
Type	F	F	F	F	F	F	F	F

VARIABLE	DESCRIPTION
T1, …, T8	Temperatures: T1, …, T8

Card 3	1	2	3	4	5	6	7	8
Variable	C1	C2	C3	C4	C5	C6	C7	C8
Type	F	F	F	F	F	F	F	F

VARIABLE	DESCRIPTION
C1, …, C8	Specific heat at T1, …, T8

Card 4	1	2	3	4	5	6	7	8
Variable	(K1)1	(K1)2	(K1)3	(K1)4	(K1)5	(K1)6	(K1)7	(K1)8
Type	F	F	F	F	F	F	F	F

VARIABLE	DESCRIPTION
(K1)1, …, (K1)8	Thermal conductivity K_1 in the local x-direction at T1, …, T8

Card 5	1	2	3	4	5	6	7	8
Variable	(K2)1	(K2)2	(K2)3	(K2)4	(K2)5	(K2)6	(K2)7	(K2)8
Type	F	F	F	F	F	F	F	F

VARIABLE	DESCRIPTION
(K2)1, …, (K2)8	Thermal conductivity K_2 in the local y-direction at T1, …, T8

Card 6	1	2	3	4	5	6	7	8
Variable	(K3)1	(K3)2	(K3)3	(K3)4	(K3)5	(K3)6	(K3)7	(K3)8
Type	F	F	F	F	F	F	F	F

VARIABLE	DESCRIPTION
(K3)1, …, (K3)8	Thermal conductivity K_3 in the local z-direction at T1, …, T8

Card 7	1	2	3	4	5	6	7	8
Variable	XP	YP	ZP	A1	A2	A3		
Type	F	F	F	F	F	F		

VARIABLE	DESCRIPTION
XP, YP, ZP	Coordinates of point p for AOPT = 1 and 4
A1, A2, A3	Components of vector **a** for AOPT = 2

Card 8	1	2	3	4	5	6	7	8
Variable	D1	D2	D3					
Type	F	F	F					

VARIABLE	DESCRIPTION
D1, D2, D3	Components of vector **d** for AOPT = 2, 3 and 4

Remarks:

1. **Thermal Generation Rate.** TGRLC is similar to the volumetric heat generation rate in *LOAD_HEAT_GENERATION and has units W/m^3 in the SI units system.

*MAT_THERMAL_DISCRETE_BEAM

This is Thermal Material Type 5. It defines properties for discrete beams. It is only applicable when used with ELFORM = 6 on *SECTION_BEAM.

Card 1	1	2	3	4	5	6	7	8
Variable	TMID	TRO						
Type	A	F						

Card 2	1	2	3	4	5	6	7	8
Variable	HC	TC						
Type	F	F						

VARIABLE	DESCRIPTION
TMID	Thermal material identification. A unique number or label must be specified (see *PART).
TRO	Thermal density: EQ.0.0: default to structural density.
HC	Specific heat HC = (heat transfer coefficient) × (beam cross-sectional area) [W/K] = [W / m^2 K] × [m^2]
TC	Thermal conductance (SI units are W/K)

Remarks:

A beam cross-sectional area is not defined on *SECTION_BEAM for an ELFORM = 6 discrete beam. Heat transfer calculations require a beam cross-sectional area. Therefore, the cross-sectional area is lumped into the value entered for HC.

*MAT_THERMAL_CHEMICAL_REACTION

This is thermal material type 6. The chemical species making up this material undergo specified chemical reactions. A maximum of 8 species and 8 chemical reactions can be defined. The thermal material properties of a finite element undergoing chemical reactions are calculated based on a mixture law consisting of those chemical species currently present in the element. The dependence of the chemical reaction rate on temperature is described by the Arrhenius equation. Time step splitting is used to couple the system of ordinary differential equations describing the chemical reaction kinetics to the system of partial differential equations describing the diffusion of heat.

Card Summary:

Card 1. This card is required.

TMID	NCHSP	NCHRX	ICEND	CEND	GASC	FID	MF

Card 2. This card must be included but all parameters can be set to 0 if no filler material is present.

RHOf	LCCf	LCKf	VFf				

Card 3. Include one card for each of the NCHSP species.

RHO*i*	LCC*i*	LCK*i*	VF*i*	MW*i*			

Card 4. Include one card for each of the NCHSP species.

RC*i*1	RC*i*2	RC*i*3	RC*i*4	RC*i*5	RC*i*6	RC*i*7	RC*i*8

Card 5. Include one card for each of the NCHSP species.

RX*i*1	RX*i*2	RX*i*3	RX*i*4	RX*i*5	RX*i*6	RX*i*7	RX*i*8

Card 6. This card is required.

LCZ1	LCZ2	LCZ3	LCZ4	LCZ5	LCZ6	LCZ7	LCZ8

Card 7. This card is required.

E1	E2	E3	E4	E5	E6	E7	E8

Card 8. This card is required.

Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8

Data Card Definitions:

Card 1	1	2	3	4	5	6	7	8
Variable	TMID	NCHSP	NCHRX	ICEND	CEND	GASC	FID	MF
Type	A	I	I	I	F	F	I	I

VARIABLE	DESCRIPTION
TMID	Thermal material ID. A unique number or label must be specified (see *PART).
NCHSP	Number of chemical species (maximum 8)
NCHRX	Number of chemical reactions (maximum 8)
ICEND	Species number controlling reaction termination
CEND	Concentration for reaction termination. Reactions are terminated when concentration of species ICEND exceeds CEND.
GASC	Gas constant: 1.987 cal/(mol K), 8.314 J/(mol K)
FID	Function ID for user specified chemical reaction rate equation for a single reaction model with two species
MF	ODE solver method: EQ.0: Default EQ.1: An alternative ODE solver for stiff differential equations

Filler Material Properties. This card is used to the material properties for the filler material, such as carbon fiber mat. This card must be included but all parameters can be set to 0 if no filler material is present.

Card 2	1	2	3	4	5	6	7	8
Variable	RHOf	LCCf	LCKf	VFf				
Type	F	I	I	F				

VARIABLE	DESCRIPTION
RHOf	Density of the filler material
LCCf	Load curve ID specifying the specific heat as a function of temperature for the filler material
LCKf	Load curve ID specifying the thermal conductivity as a function of temperature for the filler material
VFf	Volume fraction of the filler material. The remaining volume is occupied by the reacting chemicals.

Chemical Species Cards. Include one card for each of the NCHSP species. These cards set species properties. The dummy index *i* is the species number and is equal to 1 for the first species card, 2 for the second, and so on.

Card 3	1	2	3	4	5	6	7	8
Variable	RHO*i*	LCC*i*	LCK*i*	VF*i*	MW*i*			
Type	F	I	I	F	F			

Reaction Cards. Include one card for each of the NCHSP species. Each field contains the species's coefficient for one of the NCHRX chemical reactions. See Card 3 for explanation of the species index *i*.

Card 4	1	2	3	4	5	6	7	8
Variable	RC*i*1	RC*i*2	RC*i*3	RC*i*4	RC*i*5	RC*i*6	RC*i*7	RC*i*8
Type	F	F	F	F	F	F	F	F

Reaction Rate Exponent Cards. Include one card for each of the NCHSP species. Each field contains the specie's rate exponent for one of the NCHRX chemical reactions. See Card 3 for explanation of the species index *i*.

Card 5	1	2	3	4	5	6	7	8
Variable	RX*i*1	RX*i*2	RX*i*3	RX*i*4	RX*i*5	RX*i*6	RX*i*7	RX*i*8
Type	F	F	F	F	F	F	F	F

VARIABLE	DESCRIPTION
RHOi	Density of the i^{th} species
LCCi	Load curve ID specifying the specific heat as a function of temperature for the i^{th} species
LCKi	Load curve ID specifying the thermal conductivity as a function of temperature for the i^{th} species
VFi	Initial fraction of the i^{th} species relative to the other reacting chemicals. Note that $\sum_i \mathrm{VF}_i = 1$.
MWi	Molecular weight of the i^{th} species
RCij	Reaction coefficient n_{ij} for species i in reaction j. Leave blank for undefined reactions
RXij	Rate exponent p_{ij} for species i in reaction j. Leave blank for undefined reactions.

Pre-exponential Factor Card. Each field contains the natural logarithm of its corresponding reaction's pre-exponential factor.

Card 6	1	2	3	4	5	6	7	8
Variable	LCZ1	LCZ2	LCZ3	LCZ4	LCZ5	LCZ6	LCZ7	LCZ8
Type	I	I	I	I	I	I	I	I

VARIABLE	DESCRIPTION
LCZj	Load curve defining data pairs of $(\text{temperature}, \ln Z_j)$ where Z_j is the pre-exponential factor for reaction j. Leave blank for undefined reactions.

Activation Energy Card. Each field contains the activation energy value for its corresponding reaction.

Card 7	1	2	3	4	5	6	7	8
Variable	E1	E2	E3	E4	E5	E6	E7	E8
Type	F	F	F	F	F	F	F	F

VARIABLE	DESCRIPTION
E*j*	Activation energy for reaction *j*. Leave blank for undefined reactions.

Heat of Reaction Card. Each field contains the heat of reaction value for its corresponding reaction.

Card 8	1	2	3	4	5	6	7	8
Variable	Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8
Type	F	F	F	F	F	F	F	F

VARIABLE	DESCRIPTION
Q*j*	Heat of reaction for reaction *j*. Leave blank for undefined reactions.

Rate Model for a Single Reaction:

Chemical reactions are usually expressed in *chemical equation notation*; for example, a chemical reaction involving two reactants and two products is

$$a\mathrm{A} + b\mathrm{B} \rightarrow g\mathrm{G} + h\mathrm{H}, \tag{MT6.1}$$

where A, B, G, and H are chemical species such as NaOH or HCl, and a, b, g, and h are integers called *stoichiometric numbers*, indicating the number of molecules involved in a single reaction.

The rate of reaction is the number of individual reactions per unit time. Using a stoichiometric identity, which is just an accounting relation, the rate of reaction is proportional to the rate of change in the concentrations of the species involved in the reaction. For the chemical reaction in Equation (MT6.1), the relation between concentration and rate, r, is,

$$r = -\frac{1}{a}\frac{\mathrm{d}[\mathrm{A}]}{\mathrm{d}t} = -\frac{1}{b}\frac{\mathrm{d}[\mathrm{B}]}{\mathrm{d}t} = +\frac{1}{g}\frac{\mathrm{d}[\mathrm{G}]}{\mathrm{d}t} = +\frac{1}{h}\frac{\mathrm{d}[\mathrm{H}]}{\mathrm{d}t}, \tag{MT6.2}$$

where [X] denotes the concentration of species X, and the sign depends on whether or not the species is an input, in which case the sign is negative, or a product, in which case the sign is positive.

The Model

This thermal material model (T06) is built on the assumption that the reaction rate r_j of reaction j depends on the concentration of the input species according to

$$r_j = k_j(T)\prod_i [\mathrm{X}_i]^{p_{ij}} \ ,$$

where i ranges over all species, and, for each species, the exponent, p_{ij}, is determined by empirical measurement but may be approximated by the stoichiometric number associated with X_i. The proportionality constant, k_j, is related to the cross-section for the reaction, and it depends on temperature through the Arrhenius equation:

$$k_j = Z_j(T)\exp\left(-\frac{E_j}{RT}\right) \ ,$$

where $Z_j(T)$ is experimentally determined (see Card 6), E_j is the activation energy (see Card 7), R is the gas constant, and T is temperature.

As an example, for the chemical reaction of Equation (MT6.1)

$$r = Z(T)\exp\left(-\frac{E}{RT}\right)[\mathrm{A}]^{\alpha}[\mathrm{B}]^{\beta} \ ,$$

where the stoichiometric numbers have been used instead of experimentally determined exponents.

The rate of heat generation (exothermic) and absorption (endothermic) associated with a reaction is calculated by multiplying the heat of reaction, Q_i, by its rate.

User-Defined Single Reaction Model:

In addition to the standard model described in the previous section this material model also allows the user to specify a chemical reaction rate equation. In case of a single reaction model with two species, the equation can be defined using the *DEFINE_FUNCTION keyword. Here, the equation can be given as function of the current temperature and concentration of the second species. Consequently, the input may read as follows:

```
*DEFINE_FUNCTION
1, reaction rate
chemrx(temp,conc)= …
```

Note that in this case the actual argument names are used for the interpretation of the function: the material model expects the temperature argument to be names "temp" and the concentration of the second species to be denoted by "conc".

Rate Model for a System of Reactions:

For a system of coupled chemical reactions, the change in concentration of a species is the sum of all the contributions from each individual chemical reaction:

$$\frac{\mathrm{d}[\mathrm{X}_i]}{\mathrm{d}t} = \sum_j n_{ij} r_j \ .$$

The index j runs over all reactions; n_{ij} is the stoichiometric number for species X_i in reaction j; and r_j is the rate of reaction j. The sign of n_{ij} is positive for reactions that have X_i as a product and negative for reactions that involve X_i as an input.

Example:

Consider the following system of reactions (three reactions and three species):

$$\mathrm{A} \rightarrow \mathrm{B} \quad \Rightarrow \quad r_1 = -\frac{\mathrm{d}[\mathrm{A}]}{\mathrm{d}t} = \frac{\mathrm{d}[\mathrm{B}]}{\mathrm{d}t} = k_1[\mathrm{A}] \quad \Rightarrow \quad \boxed{\begin{aligned} \dot{\overline{[\mathrm{A}]}} &= -k_1[\mathrm{A}] \\ \dot{\overline{[\mathrm{B}]}} &= +k_1[\mathrm{A}] \end{aligned}}$$

$$\mathrm{A} + \mathrm{B} \rightarrow \mathrm{C} \quad \Rightarrow \quad r_2 = -\frac{\mathrm{d}[\mathrm{A}]}{\mathrm{dt}} = -\frac{\mathrm{d}[\mathrm{B}]}{\mathrm{d}t} = \frac{\mathrm{d}[\mathrm{C}]}{\mathrm{d}t} = k_2[\mathrm{A}][\mathrm{B}] \quad \Rightarrow \quad \boxed{\begin{aligned} \dot{\overline{[\mathrm{A}]}} &= -k_2[\mathrm{A}][\mathrm{B}] \\ \dot{\overline{[\mathrm{B}]}} &= -k_2[\mathrm{A}][\mathrm{B}] \\ \dot{\overline{[\mathrm{C}]}} &= +k_2[\mathrm{A}][\mathrm{B}] \end{aligned}}$$

$$2\mathrm{B} \rightarrow \mathrm{C} \quad \Rightarrow \quad r_3 = -\frac{1}{2}\frac{\mathrm{d}[\mathrm{B}]}{\mathrm{d}t} = \frac{\mathrm{d}[\mathrm{C}]}{\mathrm{d}t} = k_3[\mathrm{B}]^2 \quad \Rightarrow \quad \boxed{\begin{aligned} \dot{\overline{[\mathrm{B}]}} &= -2k_3[\mathrm{B}]^2 \\ \dot{\overline{[\mathrm{C}]}} &= +k_3[\mathrm{B}]^2 \end{aligned}}$$

The identities $\mathrm{X}_1 = A$, $\mathrm{X}_2 = B$, and $\mathrm{X}_3 = C$ allow deducing the rate exponents p_{ij}, where both indices i (species) and j (reaction) range from 1 to 3. The nonzero values are

$$\begin{aligned} p_{11} &= 1.0 \\ p_{12} &= 1.0 \\ p_{22} &= 1.0 \\ p_{23} &= 2.0 \end{aligned} \tag{MT6.3}$$

These values are needed as input parameters RX_{ij} (see card 5 in example input below).

The time evolution equations are,

(MT6.4)

$$\frac{d[B]}{dt} = \sum n_{2j} r_j = +k_1[A] - k_2[A][B] - 2k_3[B]^2$$
$$\frac{d[C]}{dt} = \sum n_{3j} r_j = \qquad + k_2[A][B] + \ k_3[B]^2.$$

Equivalent Units (Normalized Units):

The concentrations are often scaled so that each unit of reactant yields one unit of product. Systems for which each species is assigned *its own* unit of concentration based on stoichiometric considerations are *equivalent unit systems*.

Being unit-agnostic, LS-DYNA is capable of working in equivalent units. However, care must be taken so that units are treated consistently, as applying a unit scaling to the time evolution equations can be nontrivial.

1. For each reaction, the experimentally measured pre-exponential coefficients carry units that depend on the reaction itself. For instance, the pre-exponential factors Z_1, Z_2, and Z_3 for the reactions $A \rightarrow B$, $A + B \rightarrow C$, and $2B \rightarrow C$ respectively will have units of

$$[Z_1] = \frac{1}{[\text{time}]} \times \frac{1}{[\text{Concentration of A}]}$$
$$[Z_2] = \frac{1}{[\text{time}]} \times \frac{1}{[\text{Concentration of A}]} \times \frac{1}{[\text{Concentration of B}]}$$
$$[Z_3] = \frac{1}{[\text{time}]} \times \left\{\frac{1}{[\text{Concentration of B}]}\right\}^2.$$

Note that each pre-factor has a different dimensionality.

2. The equations in (MT6.2), which relate rate to concentration change, are logically inconsistent unless all species are measured using the *same* units for concentration. A species-dependent system of equivalent units would require the insertion of additional conversion factors into (MT6.2) thereby changing the form of the time-evolution equations.

To avoid unit consistency issues, we recommend that reactions be defined in the same unit system that was used to measure their empirical values.

Example of Equivalent Units:

The following system of reactions:

$$A \rightarrow B$$
$$A + B \rightarrow C$$
$$2B \rightarrow C$$

changes species A into species C through an intermediate which is species B. For each unit of species C that is produced, the reaction consumes two units of species A (1 unit from the 1st and 1 unit from the 2nd equation). Since this set of chemical formulae corresponds to the curing of epoxy, which is a nearly volume-preserving process, it is customary to work in a system of equivalent units that correspond to species volume fractions.

The following set of equivalent units, then, is used in the published literature:

1. Whatever the starting concentration of species A is, all units are uniformly rescaled so that $[A] = 1$ at time zero. Per the boxed remark above, since the constants were measured with respect to these units, this consideration does not introduce new complexity.

2. Since the process preserves volume, and since one particle of species C replaces two particles of species A (and one particle of B replace one of A), the units of concentration for species C are doubled.

$$\tilde{C} = 2[C]$$

Under this transformation the rate relation for C is

$$r_2 = r_3 = \frac{d[C]}{dt} = \frac{1}{2}\frac{d\tilde{C}}{dt} \; .$$

The time evolution Equations (MT6.4) become, (note [C] has been replaced by $\tilde{C}$):

$$\begin{aligned}
\frac{d[A]}{dt} &= \sum n_{1j} r_j &&= -k_1[A] - k_2[A][B] \\
\frac{d[B]}{dt} &= \sum n_{2j} r_j &&= +k_1[A] - k_2[A][B] - 2k_3[B]^2 \\
\frac{d\tilde{C}}{dt} = 2\frac{d[C]}{dt} &= 2\sum n_{3j} r_j = \sum \tilde{n}_{3j} r_j &&= +2k_2[A][B] + 2k_3[B]^2
\end{aligned}$$

The coefficients n_{ij} or $\tilde{n}_{ij}$, respectively, should be identically copied from the above system as reaction coefficients RC_{ij} (for Card 4):

Variable	RC11	RC12	RC13	RC14	RC15	RC16	RC17	RC18
Value	-1	-1	0					

Variable	RC21	RC22	RC23	RC24	RC25	RC26	RC27	RC28
Value	+1	-1	-2					
Variable	RC31	RC32	RC33	RC34	RC35	RC36	RC37	RC38
Value	0	+2	+2					

The exponents RX_{ij} are likewise picked off (Equations (MT6.3)) for next set of cards in format 5:

Variable	RX11	RX12	RX13	RX14	RX15	RX16	RX17	RX18
Value	+1	+1	0					
Variable	RX21	RX22	RX23	RX24	RX25	RX26	RX27	RX28
Value	0	+1	+2					
Variable	RX31	RX32	RX33	RX34	RX35	RX36	RX37	RX38
Value	0	0	0					

*MAT_THERMAL_CWM

This is Thermal Material Type 7. It is a thermal material with temperature dependent properties that allows for material creation triggered by temperature. The acronym CWM stands for Computational Welding Mechanics and the model is intended to be used for simulating multistage weld processes in combination with the mechanical counterpart, *MAT_CWM.

Card 1	1	2	3	4	5	6	7	8
Variable	TMID	TRO	TGRLC	TGMULT	HDEAD	TDEAD	TLAT	HLAT
Type	A	F	F	F	F	F	F	F

Card 2	1	2	3	4	5	6	7	8
Variable	LCHC	LCTC	TLSTART	TLEND	TISTART	TIEND	HGHOST	TGHOST
Type	F	F	F	F	F	F	F	F

VARIABLE	DESCRIPTION
TMID	Thermal material identification. A unique number or label must be specified (see *PART).
TRO	Thermal density: EQ.0.0: Default to structural density
TGRLC	Thermal generation rate (see *DEFINE_CURVE): GT.0: Load curve ID defining thermal generation rate as a function of time EQ.0: Thermal generation rate is the constant multiplier, TGMULT. LT.0: |TGRLC| is a load curve ID defining thermal generation rate as a function of temperature. This feature is similar to the volumetric heat generation rate in *LOAD_HEAT_GENERATION and has units W/m^3 in the SI units system.

VARIABLE	DESCRIPTION
TGMULT	Thermal generation rate multiplier: EQ.0.0: No heat generation
HDEAD	Specific heat for inactive material before birth time
TDEAD	Thermal conductivity for inactive material before birth time
TLAT	Phase change temperature
HLAT	Latent heat
LCHC	Load curve (or table) for specific heat as function of temperature (and maximum temperature up to current time)
LCTC	Load curve for thermal conductivity as function of temperature
TLSTART	Birth temperature of material start
TLEND	Birth temperature of material end
TISTART	Birth time start
TIEND	Birth time end
HGHOST	Specific heat for ghost (quiet) material
TGHOST	Thermal conductivity for ghost (quiet) material

Remarks:

This material is initially in a quiet state, sometimes referred to as a *ghost material*. In this state the material has the thermal properties defined by the quiet specific heat (HGHOST) and quiet thermal conductivity (TGHOST). These should represent the void, for example, by picking a relatively small thermal conductivity.

However, the ghost specific heat must be chosen with care since the temperature must be allowed to increase at a reasonable rate due to the heat from the weld source. When the temperature reaches the birth temperature, a history variable representing the indicator of the welding material is incremented. This variable follows

$$\gamma(t) = \min\left[1, \max\left(0, \frac{T_{\max} - T_l^{\text{start}}}{T_l^{\text{end}} - T_l^{\text{start}}}\right)\right] ,$$

where $T_{\max} = \max\{T(s)|s < t\}$.

The effective thermal material properties are interpolated as

$$\tilde{c}_p = c_p(T, T_{\max})\gamma + c_p^{\text{quiet}}(1-\gamma)$$
$$\tilde{\mu} = \mu(T)\gamma + \mu^{\text{quiet}}(1-\gamma)$$

where c_p and μ are the specific heat and thermal conductivity, respectively. Here, the specific heat, c_p, is either a temperature dependent curve, or a collection of temperature dependent curves, ordered in a table according to maximum temperature $T_{\max}$.

The time parameters for creating the material provide additional formulae for the final values of the thermal properties. Before the birth time t_i^{start} of the material has been reached, the specific heat c_p^{dead} and thermal conductivity μ^{dead} are used. The default values, that is, the values used if no user input is given, are

$$c_p^{\text{dead}} = 10^{10} c_p(T, T_{\max})$$
$$\mu^{\text{dead}} = 0$$

Thus, the final values of the thermal properties read

$$c_p = \begin{cases} c_p^{\text{dead}} & t \le t_i^{\text{start}} \\ \tilde{c}_p \dfrac{t - t_i^{\text{start}}}{t_i^{\text{end}} - t_i^{\text{start}}} + c_p^{\text{dead}} \dfrac{t - t_i^{\text{end}}}{t_i^{\text{start}} - t_i^{\text{end}}} & t_i^{\text{start}} < t \le t_i^{\text{end}} \\ \tilde{c}_p & t_i^{\text{end}} < t \end{cases}$$

$$\mu = \begin{cases} \mu^{\text{dead}} & t \le t_i^{\text{start}} \\ \tilde{\mu} \dfrac{t - t_i^{\text{start}}}{t_i^{\text{end}} - t_i^{\text{start}}} + \mu^{\text{dead}} \dfrac{t - t_i^{\text{end}}}{t_i^{\text{start}} - t_i^{\text{end}}} & t_i^{\text{start}} < t \le t_i^{\text{end}} \\ \tilde{\mu} & t_i^{\text{end}} < t \end{cases}$$

These parameters allow you to control when the welding layer becomes active and thereby define a multistage welding process. Prior to the birth time, the temperature is kept more or less constant due to the large specific heat, and, thus, the material is prevented from being created

*MAT_THERMAL_ORTHOTROPIC_TD_LC

This is Thermal Material Type 8. With this model, orthotropic thermal properties that are dependent on temperature (and/or mechanical history variables and/or external variables) can be specified with load curves. The properties must be defined for the temperature (and/or history variable and/or external variable) range that the material sees in the analysis. See *LOAD_EXTERNAL_VARIABLE for defining external variables and Remark 2.

Card Summary:

Card 1a. Include this card if ITGHSV = 0 (see Card 2).

TMID	TRO	TGRLC	TGMULT	AOPT	TLAT	HLAT	

Card 1b. Include this card if |ITGHSV| > 0 (see Card 2).

TMID	TRO	TGRLC	TGMULT	AOPT	TLAT	HLAT	

Card 2. This card is required.

LCC	LCK1	LCK2	LCK3	ILCCHSV	ILCKHSV	ITGHSV	

Card 3. This card is required.

XP	YP	ZP	A1	A2	A3		

Card 4. This card is required.

D1	D2	D3					

Data Card Definitions:

Include this card if ITGHSV = 0 (see Card 2).

Card 1a	1	2	3	4	5	6	7	8
Variable	TMID	TRO	TGRLC	TGMULT	AOPT	TLAT	HLAT	
Type	A	F	I	F	F	F	F	

VARIABLE	DESCRIPTION
TMID	Thermal material identification. A unique number or label must be specified (see *PART).
TRO	Thermal density. EQ.0.0: Default to structural density
TGRLC	Thermal generation rate (see *DEFINE_CURVE). See Remark 1. GT.0: Load curve ID defining thermal generation rate as a function of time EQ.0: Thermal generation rate is the constant multiplier, TGMULT. LT.0: |TGRLC| is a load curve ID defining thermal generation rate as a function of temperature.
TGMULT	Thermal generation rate multiplier. EQ.0.0: No heat generation
AOPT	Material axes definition (see *MAT_*OPTION*TROPIC_ELASTIC for a more complete description): EQ.0.0: Locally orthotropic with material axes by element nodes N1, N2 and N4 EQ.1.0: Locally orthotropic with material axes determined by a point in space and global location of element center EQ.2.0: Globally orthotropic with material axes determined by vectors EQ.3.0: Locally orthotropic with first material axis orthogonal to element normal (defined by element nodes N1, N2 and N4) and to a vector **d**- Third material direction corresponds to element normal. EQ.4.0: Local orthogonal in cylindrical coordinates with the material axes determined by a vector **d**, and an originating point, P, which define the centerline axis.
TLAT	Phase change temperature
HLAT	Latent heat

Include this card if |ITGHSV| > 0 (see Card 2).

Card 1b	1	2	3	4	5	6	7	8
Variable	TMID	TRO	TGRLC	TGMULT	AOPT	TLAT	HLAT	
Type	A	F	I	F	F	F	F	

VARIABLE	DESCRIPTION
TMID	Thermal material identification. A unique number or label must be specified (see *PART).
TRO	Thermal density. EQ.0.0: Default to structural density
TGRLC	Thermal generation rate curve/table ID (see *DEFINE_CURVE). See Remark 1. GT.0: Load curve giving thermal generation rate as a function of the mechanical history variable specified by ITGHSV. EQ.0: Use mechanical history variable specified by ITGHSV times constant multiplier value TGMULT. LT.0: Table of load curves for different temperatures. Each curve gives the thermal generation rate as a function of the mechanical history variable specified by ITGHSV.
TGMULT	Thermal generation rate multiplier. Defines a volumetric heat rate (W/m^3 in SI units system). EQ.0.0: No heat generation
AOPT	Material axes definition (see *MAT_*OPTION*TROPIC_ELASTIC for a more complete description): EQ.0.0: Locally orthotropic with material axes by element nodes N1, N2 and N4 EQ.1.0: Locally orthotropic with material axes determined by a point in space and global location of element center EQ.2.0: Globally orthotropic with material axes determined by vectors EQ.3.0: Locally orthotropic with first material axis orthogonal to element normal (defined by element nodes N1, N2

VARIABLE	DESCRIPTION
	and N4) and to a vector **d**- Third material direction corresponds to element normal.
	EQ.4.0: Local orthogonal in cylindrical coordinates with the material axes determined by a vector **d**, and an originating point, P, which define the centerline axis.
TLAT	Phase change temperature
HLAT	Latent heat

Card 2	1	2	3	4	5	6	7	8
Variable	LCC	LCK1	LCK2	LCK3	ILCCHSV	ILCKHSV	ITGHSV	
Type	I	I	I	I	I	I	I	

VARIABLE	DESCRIPTION
LCC	Load curve ID defining specific heat as a function of temperature or external variable (see Remark 2), or if |ILCCHSV| > 0: GT.0: Load curve as a function of mechanical history variable specified by ILCCHSV. LT.0: Table of load curves for different temperatures. Each curve is a function of the mechanical history variable specified by ILCCHSV.
LCK*i*	Load curve ID defining thermal conductivity, K_i (i = 1,2,3), in the local (x, y, z)-direction as a function of temperature or external variable (see Remark 2), or if |ILCKHSV| > 0: GT.0: Load curve giving thermal conductivity in the local direction as a function of the mechanical history variable specified by ILCKHSV. LT.0: Table of load curves for different temperatures. Each curve gives thermals conductivity in the local direction as a function of the mechanical history variable specified by ILCKHSV.
ILCCHSV	Optional: GT.0: Mechanical history variable # used by LCC.

VARIABLE	DESCRIPTION
	LT.0: As above but |ILCCHSV| = 1 through 6 means the history variable is one of the six stress components, |ILCCHSV| = 7 means the history variable is the plastic strain, and |ILCCHSV| = 7 + k means the history variable is history variable k.
ILCKHSV	Optional: GT.0: Mechanical history variable # used by LCK1, LCK2, LCK3. LT.0: As above but |ILCKHSV| = 1 through 6 means the history variable is one of the six stress components, |ILCKHSV| = 7 means the history variable is the plastic strain, and |ILCKHSV| = 7 + k means the history variable is history variable k.
ITGHSV	Optional: GT.0: Mechanical history variable # used by TGRLC. LT.0: As above but |ITGHSV| = 1 through 6 means the history variable is one of the six stress components, |ITGHSV| = 7 means the history variable is the plastic strain, and |ITGHSV| = 7 + k means the history variable is history variable k.

Card 3	1	2	3	4	5	6	7	8
Variable	XP	YP	ZP	A1	A2	A3		
Type	F	F	F	F	F	F		

Card 4	1	2	3	4	5	6	7	8
Variable	D1	D2	D3					
Type	F	F	F					

VARIABLE	DESCRIPTION
XP, YP, ZP	Coordinates of point p for AOPT = 1 and 4

VARIABLE	DESCRIPTION
A1, A2, A3	Components of vector **a** for AOPT = 2
D1, D2, D3	Components of vector **d** for AOPT = 2, 3 and 4

Remarks:

1. **Thermal generation rate.** TGRLC is similar to the volumetric heat generation rate in *LOAD_HEAT_GENERATION and has units W/m^3 in the SI units system

2. **Effect of external variables.** By default, material properties can be defined as a function of the temperature field, but this material also supports material definitions based on a given distribution of an external variable (see *LOAD_EXTERNAL_VARIABLE). In that case, one or more of the load curves, LCC, LCK1, LCK2, and LCK3, are evaluated based on the external variable data instead of temperature. To do this, set ITMP on *LOAD_EXTERNAL_VARIABLE to the material property index for the desired thermal material property. The following table lists the material property indices:

Property index	Property name	Load curve
1	Specific heat	LCC
2	Thermal conductivity in the x-direction	LCK1
3	Thermal conductivity in the y-direction	LCK2
4	Thermal conductivity in the z-direction	LCK3

*MAT_THERMAL_ISOTROPIC_PHASE_CHANGE

This is Thermal Material Type 9. With this material, temperature dependent isotropic properties with phase change can be defined. The latent heat of the material is defined together with the solid and liquid temperatures. The temperature dependency is defined by specifying a minimum of two and a maximum of eight data points. The properties must be defined for the temperature range that the material will see in the analysis.

Card 1	1	2	3	4	5	6	7	8
Variable	TMID	TRO	TGRLC	TGMULT				
Type	A	F	F	F				

Card 2	1	2	3	4	5	6	7	8
Variable	T1	T2	T3	T4	T5	T6	T7	T8
Type	F	F	F	F	F	F	F	F

Card 3	1	2	3	4	5	6	7	8
Variable	C1	C2	C3	C4	C5	C6	C7	C8
Type	F	F	F	F	F	F	F	F

Card 4	1	2	3	4	5	6	7	8
Variable	K1	K2	K3	K4	K5	K6	K7	K8
Type	F	F	F	F	F	F	F	F

Card 5	1	2	3	4	5	6	7	8
Variable	SOLT	LIQT	LH					
Type	F	F	F					

VARIABLE	DESCRIPTION
TMID	Thermal material identification. A unique number or label must be specified (see *PART).
TRO	Thermal density: EQ.0.0: Default to structural density
TGRLC	Thermal generation rate (see *DEFINE_CURVE). See Remark 2. GT.0: Load curve ID defining thermal generation rate as a function of time EQ.0: Thermal generation rate is the constant multiplier, TGMULT. LT.0: |TGRLC| is a load curve ID defining thermal generation rate as a function of temperature.
TGMULT	Thermal generation rate multiplier: EQ.0.0: No heat generation
T1, …, T8	Temperatures: T1, …, T8
C1, …, C8	Specific heat at T1, …, T8
K1, …, K8	Thermal conductivity at T1, …, T8
SOLT	Solid temperature, T_S (must be < T_L)
LIQT	Liquid temperature, T_L (must be > T_S)
LH	Latent heat

Remarks:

1. **Phase Change.** During phase change, meaning between the solid and liquid temperatures, the specific heat of the material will be enhanced to account for the latent heat as follows:

$$c(t) = m\left[1 - \cos 2\pi\left(\frac{T - T_S}{T_L - T_S}\right)\right], \qquad T_S < T < T_L$$

Here m is a multiplier such that the latent heat λ is given by:

$$\lambda = \int_{T_S}^{T_L} c(T)dT \ .$$

Here $c(T)$ is the specific heat.

2. **Thermal Generation Rate.** TGRLC is similar to the volumetric heat generation rate in *LOAD_HEAT_GENERATION and has units W/m^3 in the SI units system.

*MAT_THERMAL_ISOTROPIC_TD_LC

This is Thermal Material Type 10. With this model, isotropic thermal properties that are dependent on temperature (and/or mechanical history variables and/or external variables) can be specified with load curves. The properties must be defined for the temperature (and/or history variable and/or external variable) range that the material sees in the analysis. See *LOAD_EXTERNAL_VARIABLE for defining external variables and Remark 2.

Card Summary:

Card 1a. Include this card if TGHSV = 0.

TMID	TRO	TGRLC	TGMULT	TLAT	HLAT		

Card 1b. Include this card if TGHSV ≠ 0.

TMID	TRO	TGRLC	TGMULT	TLAT	HLAT		

Card 2. This card is required.

HCLC	TCLC	HCHSV	TCHSV	TGHSV			

Data Card Definitions:

Include this card if TGHSV = 0 (see Card 2).

Card 1a	1	2	3	4	5	6	7	8
Variable	TMID	TRO	TGRLC	TGMULT	TLAT	HLAT		
Type	A	F	I	F	F	F		

VARIABLE	DESCRIPTION
TMID	Thermal material identification. A unique number or label must be specified (see *PART).
TRO	Thermal density. EQ.0.0: Default to structural density
TGRLC	Thermal generation rate (see *DEFINE_CURVE). See Remark 1. GT.0: Load curve ID defining thermal generation rate as a

VARIABLE	DESCRIPTION
	function of time EQ.0: Thermal generation rate is the constant multiplier, TGMULT. LT.0: |TGRLC| is a load curve ID defining thermal generation rate as a function of temperature.
TGMULT	Thermal generation rate multiplier. EQ.0.0: No heat generation
TLAT	Phase change temperature
HLAT	Latent heat

This card is included if |TGHSV| > 0 (see Card 2).

Card 1b	1	2	3	4	5	6	7	8
Variable	TMID	TRO	TGRLC	TGMULT	TLAT	HLAT		
Type	A	F	I	F	F	F		

VARIABLE	DESCRIPTION
TMID	Thermal material identification. A unique number or label must be specified (see *PART).
TRO	Thermal density. EQ.0.0: Default to structural density
TGRLC	Thermal generation rate curve/table ID (see *DEFINE_CURVE). See Remark 1. GT.0: Load curve specifying thermal generation rate as a function of the mechanical history variable specified by TGHSV. EQ.0: Use mechanical history variable specified by ITGHSV times constant multiplier value TGMULT. LT.0: Table of load curves for different temperatures. Each curve specifies the thermal generation rate as a function of the mechanical history variable specified by TGHSV.

VARIABLE	DESCRIPTION
TGMULT	Thermal generation rate multiplier. Defines a volumetric heat rate (W/m^3 in SI units system). EQ.0.0: No heat generation
TLAT	Phase change temperature
HLAT	Latent heat

Card 2	1	2	3	4	5	6	7	8
Variable	HCLC	TCLC	HCHSV	TCHSV	TGHSV			
Type	I	I	I	I	I			

VARIABLE	DESCRIPTION
HCLC	Load curve ID specifying specific heat as a function of temperature or external variable (see Remark 2), or, if |HCHSV| > 0: GT.0: Load curve specifying the specific heat as a function of the mechanical history variable specified by HCHSV. LT.0: Table of load curves for different temperatures. Each curve specifies the specific heat as a function of the mechanical history variable specified by HCHSV.
TCLC	Load curve ID specifying thermal conductivity as a function of temperature or external variable (see Remark 2), or if |TCHSV| > 0: GT.0: Load curve giving thermal conductivity as a function of the mechanical history variable specified by TCHSV. LT.0: Table of load curves for different temperatures. Each curve is a function of the mechanical history variable specified by TCHSV.
HCHSV	Optional: GT.0: Mechanical history variable # used by HCLC. LT.0: As above but |HCHSV| = 1 through 6 means that the variable is one of the six stress components, |HCHSV| = 7 means that the variable is the plastic strain, and

VARIABLE	DESCRIPTION
	$\lvert$HCHSV$\rvert = 7 + k$ means that the variable is history variable k.
TCHSV	Optional: GT.0: Mechanical history variable # used by TCLC. LT.0: As above but $\lvert$TCHSV$\rvert = 1$ through 6 means the variable is one of the six stress components, $\lvert$TCHSV$\rvert = 7$ means the variable is the plastic strain, and $\lvert$TCHSV$\rvert = 7 + k$ means that the variable is history variable k.
TGHSV	Optional: GT.0: Mechanical history variable # used by TGRLC. LT.0: As above but $\lvert$TGHSV$\rvert = 1$ through 6 means the variable is one of the six stress components, $\lvert$TGHSV$\rvert = 7$ means the variable is the plastic strain, and $\lvert$TGHSV$\rvert = 7 + k$ means that the variable is history variable k.

Remarks:

1. **Thermal generation rate.** TGRLC is similar to the volumetric heat generation rate in *LOAD_HEAT_GENERATION. It has units W/m^3 in the SI units system.

2. **Effect of external variables.** By default, material properties can be defined as a function of the temperature field, but this material also supports material definitions based on a given distribution of an external variable (see *LOAD_EXTERNAL_VARIABLE). In that case, HCLC and/or TCLC are evaluated based on the external variable data. To do this, set ITMP on *LOAD_EXTERNAL_VARIABLE to the material property index for the desired thermal material property. The following table lists the material property indices:

Property index	Property name	Load curve
1	Specific heat	HCLC
2	Thermal conductivity	TCLC

*MAT_THERMAL_USER_DEFINED

These are Thermal Material Types 11 - 15. You can supply your own subroutines. Please consult Appendix H for more information.

Card Summary:

Card 1. This card is required.

TMID	RO	MT	LMC	NVH	AOPT	IORTHO	IHVE

Card 1.1. This card is included if IORTHO = 1.

XP	YP	ZP	A1	A2	A3		

Card 1.2. This card is included if IORTHO = 1.

D1	D2	D3					

Card 2. Up to 4 of this card can be included to set LMC parameters. This input ends at the next keyword ("*") card.

P1	P2	P3	P4	P5	P6	P7	P8

Data Card Definitions:

Card 1	1	2	3	4	5	6	7	8
Variable	TMID	RO	MT	LMC	NVH	AOPT	IORTHO	IHVE
Type	A	F	F	F	F	F	F	F

VARIABLE	DESCRIPTION
TMID	Thermal material identification. A unique number or label must be specified (see *PART).
RO	Thermal mass density
MT	User material type (11-15 inclusive)
LMC	Length of material constants array. LMC must not be greater than 32.

VARIABLE	DESCRIPTION
NVH	Number of history variables
AOPT	Material axes option of orthotropic materials (see MAT_*OPTION*-TROPIC_ELASTIC for more details). Set if IORTHO = 1.0. EQ.0.0: Locally orthotropic with material axes by element nodes N1, N2 and N4 EQ.1.0: Locally orthotropic with material axes determined by a point, P, in space and global location of element center EQ.2.0: Globally orthotropic with material axes determined by vectors EQ.3.0: Locally orthotropic with first material axis orthogonal to element normal (defined by element nodes N1, N2 and N4) and to a vector **d**- Third material direction corresponds to element normal. EQ.4.0: Local orthogonal in cylindrical coordinates with the material axes determined by a vector **d**, and an originating point, P, which define the centerline axis. LT.0.0: The absolute value of AOPT is a coordinate system ID number (CID on *DEFINE_COORDINATE_NODES, *DEFINE_COORDINATE_SYSTEM or *DEFINE_COORDINATE_VECTOR).
IORTHO	Set to 1.0 if the material is orthotropic.
IHVE	Set to 1.0 to activate exchange of history variables between mechanical and thermal user material models.

Orthotropic Card 1. Additional card read in when IORTHO = 1.

Card 1.1	1	2	3	4	5	6	7	8
Variable	XP	YP	ZP	A1	A2	A3		
Type	F	F	F	F	F	F		

VARIABLE	DESCRIPTION
XP, YP, ZP	Coordinates of point P for AOPT = 1 and 4
A1, A2, A3	Components of vector **a** for AOPT = 2

Orthotropic Card 2. Additional card read in when IORTHO = 1.

Card 1.2	1	2	3	4	5	6	7	8
Variable	D1	D2	D3					
Type	F	F	F					

VARIABLE	DESCRIPTION
D1, D2, D3	Components of vector **d** for AOPT = 2, 3 and 4

Material Parameter Cards. Set up to 8 parameters per card. Include up to 4 cards. This input ends at the next keyword ("*") card.

Card 2	1	2	3	4	5	6	7	8
Variable	P1	P2	P3	P4	P5	P6	P7	P8
Type	F	F	F	F	F	F	F	F

VARIABLE	DESCRIPTION
P1	First material parameter
⋮	⋮
PLMC	LMCth material parameter

Remarks:

1. **IHVE.** The IHVE = 1 option makes it possible for a thermal user material subroutine to read the history variables of a mechanical user material subroutine defined for the same part and vice versa. If the integration points for the thermal and mechanical elements are not coincident, then extrapolation/interpolation is used to calculate the value when reading history variables.

2. **TITLE.** Option TITLE is supported

3. **Units Transformation.** Transformation of units using *INCLUDE_TRANSFORM is only supported for the RO field and the vectors on Cards 1.1 and 1.2.

*MAT_THERMAL_CHEMICAL_REACTION_ORTHOTROPIC

This is Thermal Material Type 17. The chemical species making up this material undergo specified chemical reactions. The chemical reaction kinetics is the same as for thermal material *MAT_T06, but the thermal conductivity is assumed to be orthotropic. A maximum of 8 species and 8 chemical reactions can be defined. The orthotropic thermal material properties of a finite element undergoing chemical reactions are calculated based on a mixture law consisting of those chemical species currently present in the element. The dependence of the chemical reaction rate on temperature is described by the Arrhenius equation. Time step splitting is used to couple the system of ordinary differential equations describing the chemical reaction kinetics to the system of partial differential equations describing the diffusion of heat.

Card Summary:

Card 1. This card is required.

TMID	NCHSP	NCHRX	ICEND	CEND	GASC	FID	MF

Card 2. This card is required.

AOPT	XP	YP	ZP	A1	A2	A3	

Card 3. This card is required.

D1	D2	D3					

Card 4. This card must be included, but all parameters can be set to 0 if no filler material is present.

RHOf	LCCf	LCK1f	LCK2f	LCK3f	VFf		

Card 5. Include one card for each of the NCHSP species.

RHO*i*	LCC*i*	LCK1*i*	LCK2*i*	LCK3*i*	VF*i*	MW*i*	

Card 6. Include one card for each of the NCHSP species.

RC*i*1	RC*i*2	RC*i*3	RC*i*4	RC*i*5	RC*i*6	RC*i*7	RC*i*8

Card 7. Include one card for each of the NCHSP species.

RX*i*1	RX*i*2	RX*i*3	RX*i*4	RX*i*5	RX*i*6	RX*i*7	RX*i*8

Card 8. This card is required.

LCZ1	LCZ2	LCZ3	LCZ4	LCZ5	LCZ6	LCZ7	LCZ8

Card 9. This card is required.

E1	E2	E3	E4	E5	E6	E7	E8

Card 10. This card is required.

Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8

Data Card Definitions:

Card 1	1	2	3	4	5	6	7	8
Variable	TMID	NCHSP	NCHRX	ICEND	CEND	GASC	FID	MF
Type	A	I	I	I	F	F	I	I

VARIABLE	DESCRIPTION
TMID	Thermal material identification. A unique number or label must be specified (see *PART).
NCHSP	Number of chemical species (maximum 8)
NCHRX	Number of chemical reactions (maximum 8)
ICEND	Species number controlling reaction termination
CEND	Concentration for reaction termination
GASC	Gas constant: 1.987 cal/(mol K), 8314. J/(mol K)
FID	Function ID for user specified chemical reaction rate equation for a single reaction model with two species
MF	ODE solver method: EQ.0: Default EQ.1: An alternative ODE solver

Material axis definition. This card sets the material axes for the orthotropic heat conduction properties.

Card 2	1	2	3	4	5	6	7	8
Variable	AOPT	XP	YP	ZP	A1	A2	A3	
Type	I	F	F	F	F	F	F	

Card 3	1	2	3	4	5	6	7	8
Variable	D1	D2	D3					
Type	F	F	F					

VARIABLE	DESCRIPTION
AOPT	Material axes definition (see *MAT_*OPTION*TROPIC_ELASTIC for a more complete description): EQ.0.0: Locally orthotropic with material axes by element nodes N1, N2 and N4 EQ.1.0: Locally orthotropic with material axes determined by a point in space and global location of element center EQ.2.0: Globally orthotropic with material axes determined by vectors EQ.3.0: Locally orthotropic with first material axis orthogonal to element normal (defined by element nodes N1, N2 and N4) and to a vector **d**- Third material direction corresponds to element normal. EQ.4.0: Local orthogonal in cylindrical coordinates with the material axes determined by a vector **d**, and an originating point, *P*, which define the centerline axis.
XP, YP, ZP	Coordinates of point *p* for AOPT = 1 and 4
A1, A2, A3	Components of vector **a** for AOPT = 2
D1, D2, D3	Components of vector **d** for AOPT = 2, 3 and 4

Filler Material Properties. This card sets the material properties for the filler material, such as carbon fiber. This card must be included, but all parameters can be set to 0 if no filler material is present.

Card 4	1	2	3	4	5	6	7	8
Variable	RHOf	LCCf	LCK1f	LCK2f	LCK3f	VFf		
Type	F	I	I	I	I	F		

VARIABLE	DESCRIPTION
RHOf	Density of the filler material
LCCf	Load curve ID specifying the specific heat as a function of temperature for the filler material
LCK1f	Load curve ID specifying thermal conductivity K_1, in the local x-direction, as a function of temperature for the filler material
LCK2f	Load curve ID specifying thermal conductivity K_2, in the local y-direction, as a function of temperature for the filler material
LCK3f	Load curve ID specifying thermal conductivity K_3, in the local z-direction, as a function of temperature for the filler material
VFf	Volume fraction of the filler material. The remaining volume is occupied by the reacting chemicals.

Chemical Species Cards. Include one card for each of the NCHSP species. These cards set properties for each species. The dummy index *i* is the species number and is equal to 1 for the first species card, 2 for the second, and so on.

Card 5	1	2	3	4	5	6	7	8
Variable	RHO*i*	LCC*i*	LCK1*i*	LCK2*i*	LCK3*i*	VF*i*	MW*i*	
Type	F	I	I	I	I	F	F	

Reaction Cards. Include one card for each of the NCHSP species. Each field contains the species' coefficient for one of the NCHRX chemical reactions. See Card 5 for explanation of the species index *i*.

Card 6	1	2	3	4	5	6	7	8
Variable	RC*i*1	RC*i*2	RC*i*3	RC*i*4	RC*i*5	RC*i*6	RC*i*7	RC*i*8
Type	F	F	F	F	F	F	F	F

Reaction Rate Exponent Cards. Include one card for each of the NCHSP species. Each field contains the species' rate exponent for one of the NCHRX chemical reactions. See Card 5 for explanation of the species index *i*.

Card 7	1	2	3	4	5	6	7	8
Variable	RX*i*1	RX*i*2	RX*i*3	RX*i*4	RX*i*5	RX*i*6	RX*i*7	RX*i*8
Type	F	F	F	F	F	F	F	F

VARIABLE	DESCRIPTION
RHO*i*	Density of the i^{th} species
LCC*i*	Load curve ID specifying the specific heat as a function of temperature for the i^{th} species
LCK1*i*	Load curve ID specifying thermal conductivity K_1, in the local x-direction, as a function of temperature for the i^{th} species
LCK2*i*	Load curve ID specifying thermal conductivity K_2, in the local y-direction, as a function of temperature for the i^{th} species
LCK3*i*	Load curve ID specifying thermal conductivity K_3, in the local z-direction, as a function of temperature for the i^{th} species
VF*i*	Initial fraction of the i^{th} species relative to the other reacting chemicals. Note that $\sum_i \mathrm{VF}_i = 1$.
MW*i*	Molecular weight of the i^{th} species
RC*ij*	Reaction coefficient for species *i* in reaction *j*. Leave blank for undefined reactions.

VARIABLE	DESCRIPTION
RX*ij*	Rate exponent for species *i* in reaction *j*. Leave blank for undefined reactions.

Pre-exponential Factor Card. Each field contains the natural logarithm of its corresponding reaction's pre-exponential factor.

Card 8	1	2	3	4	5	6	7	8
Variable	LCZ1	LCZ2	LCZ3	LCZ4	LCZ5	LCZ6	LCZ7	LCZ8
Type	I	I	I	I	I	I	I	I

VARIABLE	DESCRIPTION
LCZ*j*	Load curve defining data pairs of $(\text{temperature}, \ln Z_j)$ where Z_j is the pre-exponential factor for reaction *j*. Leave blank for undefined reactions.

Activation Energy Card. Each field contains the activation energy value for its corresponding reaction.

Card 9	1	2	3	4	5	6	7	8
Variable	E1	E2	E3	E4	E5	E6	E7	E8
Type	F	F	F	F	F	F	F	F

VARIABLE	DESCRIPTION
E*j*	Activation energy for reaction *j*. Leave blank for undefined reactions.

Heat of Reaction Card. Each field contains the heat of reaction value for its corresponding reaction.

Card 10	1	2	3	4	5	6	7	8
Variable	Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8
Type	F	F	F	F	F	F	F	F

VARIABLE	DESCRIPTION
Q*j*	Heat of reaction for reaction *j*. Leave blank for undefined reactions.

Remarks:

See the remarks for *MAT_T06.

*MAT_THERMAL_ISPG

This is Thermal Material Type 18. It is only available for ISPG elements. With this material, isotropic thermal properties can be defined.

> **NOTE:** This thermal material only works for ISPG element formulations set on *SECTION_ISPG. It may only be in the ISPG input deck included in the LS-DYNA input deck with *INCLUDE_ISPG.

Card 1	1	2	3	4	5	6	7	8
Variable	TMID	TRO						
Type	I	F						

Card 2	1	2	3	4	5	6	7	8
Variable	HC	TC						
Type	F	F						

VARIABLE	DESCRIPTION
TMID	Thermal material identification. A unique number or label must be specified. (see *PART)
TRO	Thermal density: EQ.0.0: Default to fluid density
TH	Specific heat
TC	Thermal conductivity