

Constitutive Relations for ReactiveBond

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ReactiveBond_v1.1

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Contents

1	Introduction	2
2	Kinetics	2
2.1	First-order	2
2.2	First-order stretched	2
2.3	Second-order	3
2.4	Nth-order	3
3	Intrinsic Hyperelasticity	3
3.1	Linear elastic	3
3.2	Exponential linear	3
3.3	Fiber exponential	4
3.4	Fiber exponential- Jacobs	4
3.5	Fiber exponential simple	4
3.6	Neo-Hookean	4
3.7	Holmes-Mow	5
4	Sliding	5
4.1	Power-law	5
4.2	Modified Weibull	5
5	Damage	5
5.1	Weibull	5

1 Introduction

The following includes the specific constitutive relations for **ReactiveBond** software. The Constitutive relations should be passed to the function as structures, and the parameters should be passed in vectors, with the order presented in the following tables. As an example,

```
%Kinetics equation of bonds
kinetics.name      = 'nth_order';
kinetics.parameters = [k,N];

%Intrinsic hyperelasticity
IntHyper.name      = 'neohookean';
IntHyper.parameters = C1;

%Sliding
sliding.name       = 'sliding_power';
sliding.parameters = [c,b,r0]

%Damage
damage.name        = 'weibull';
damage.parameters  = [k,l,r0]
```

2 Kinetics

2.1 First-order

First order kinetics relation for kinetics (syntax name: **first_order**)

Parameter	Physical dimension
τ	$[[t]]$

$$\dot{w} = -\frac{1}{\tau}w \quad (1)$$

2.2 First-order stretched

First order kinetics relation for kinetics with stretched time constant (syntax name: **first_order_stretched**)

Parameter	Physical dimension
τ	$[[t]]^{-\beta}$
β	$[[-]]$

$$\dot{w} = -\frac{\beta}{\tau}u^{\beta-1}w \quad (2)$$

in this equation, u is the time passed from the time the generation was initiated.

2.3 Second-order

Second order kinetics relation for kinetics (snytax name: **second_order**)

Parameter	Physical dimension
k	$[[t]]^{-1}$

$$\dot{w} = -kw^2 \quad (3)$$

2.4 Nth-order

Generalized nth-order kinetics relation for kinetics (snytax name: **nth_order**)

Parameter	Physical dimension
k	$[[t]]^{-1}$

$$\dot{w} = -kw^N \quad (4)$$

3 Intrinsic Hyperelasticity

3.1 Linear elastic

Linear elastic relation. Not recommended for large deformations (snytax name: **linear_elastic**)

Parameter	Physical dimension
E	$[[N.m^{-2}]]$

3.2 Exponential linear

Exponential-Linear elastic relation for toe-region and transition to linear region. Not recommended for large deformations (snytax name: **exp_lin**)

Parameter	Physical dimension
C_3	$[[N.m^{-2}]]$
C_4	$[[N.m^{-2}]]$
λ_s	$[[-]]$

$$\psi(\lambda) = \begin{cases} \frac{C_1}{C_2} [\exp(C_2(\lambda - 1)) - C_2\lambda - 1], & \lambda \leq \lambda_s \\ \left[\left(\frac{C_3}{2} \lambda^2 \right) + C_4 \lambda \right] + C_6, & \lambda_s < \lambda \end{cases} \quad (5)$$

In the above relation C_1, C_4, C_5 , and C_6 are determined by the conditions of smoothness.

3.3 Fiber exponential

Exponential elastic relation with (snytax name: **fiber_exp**)

Parameter	Physical dimension
C_3	$[[N.m^{-2}]]$
C_2	$[[-]]$

$$\psi_{EF}(I_4) = C_2 \left(\exp [C_3(I_4 - 1)^2] - 1 \right) u(I_4 - 1), \quad (6)$$

Here, u is the Heaviside step function.

3.4 Fiber exponential- Jacobs

Exponential elastic relation with (snytax name: **fiber_exp_Jacobs**) From Jacobs 2013 JBME

Parameter	Physical dimension
C_5	$[[N.m^{-2}]]$
C_4	$[[-]]$

$$\psi_{EF}(I_4) = \frac{C_5}{2C_4} \left(\exp [C_4(I_4 - 1)^2] - 1 \right) u(I_4 - 1), \quad (7)$$

Here, u is the Heaviside step function.

3.5 Fiber exponential simple

Exponential elastic relation (snytax name: **fiber_exp_simple**)

Parameter	Physical dimension
C_1	$[[N.m^{-2}]]$
C_2	$[[-]]$

$$\psi_{EFS}(\lambda) = (C_1 \exp(-C_2) Ei(C_2 \lambda) - C_1 \log \lambda + C_3) u(\lambda - 1), \quad (8)$$

Here, u is the Heaviside step function and C_3 is:

$$C_3 = -C_1 \exp(-C_2) Ei(C_2) \quad (9)$$

This relation results in the simple stress response for toe-region as

$$T_{EFS} = \lambda \frac{\partial \psi_{EFS}}{\partial \lambda} = C_1 \left(\exp [C_2(\lambda - 1)] - 1 \right) u(\lambda - 1) \quad (10)$$

3.6 Neo-Hookean

Neo-Hookean relation for isochoric uniaxial deformation (snytax name: **neohookean**)

Parameter	Physical dimension
C_1	$[[N.m^{-2}]]$

$$\psi_{NH}(I_1) = C_1(I_1 - 3). \quad (11)$$

3.7 Holmes-Mow

Holmes-Mow material for isochoric uniaxial deformation (snytax name: **holmes_mow**)

Parameter	Physical dimension
E	$[[N.m^{-2}]]$
ν	$[[-]]$
C_0	$[[N.m^{-2}]]$

$$\psi_{HM}(I_1, I_2, I_3) = \alpha_0 \left(I_3^{-\beta} \exp [\alpha_1(I_1 - 3) + \alpha_2(I_2 - 3)] - 1 \right) . \quad (12)$$

$$\alpha_0 = C_0, \quad \alpha_1 = \frac{E/\alpha_0}{4(1+\nu)} - \alpha_2, \text{ and } \alpha_2 = \frac{(E/\alpha_0)\nu}{4(1+\nu)(1-2\nu)} = \beta - \alpha_1, \quad (13)$$

4 Sliding

4.1 Power-law

The power law for sliding with three model parameters (snytax name: **sliding_power**)

Parameter	Physical dimension
c	$[[-]]$
b	$[[-]]$
r_0	$[[-]]$

$$f_s(\Xi_s) = c (\Xi_s - (r_s)_0)^b \quad (14)$$

4.2 Modified Weibull

The modified Weibull (sliding exponential) for sliding with three model parameters (snytax name: **sliding_exp**)

Parameter	Physical dimension
k	$[[-]]$
l	$[[-]]$
r_0	$[[-]]$

$$f_s(\Xi_s) = (\Xi_s - 1) \left(1 - \exp \left[- \left(\frac{\Xi_s - (r_s)_0}{l - 1} \right)^k \right] \right) \quad (15)$$

5 Damage

5.1 Weibull

The Weibull CDF function with three model parameters for damage rule (snytax name: **weibull**)

Parameter	Physical dimension
k	$[[-]]$
l	$[[-]]$
r_0	$[[-]]$

$$f_D(\Xi_D) = 1 - \exp \left[- \left(\frac{\Xi_D - (r_D)_0}{l - 1} \right)^k \right] \quad (16)$$