# Constitutive Relations for ReactiveBond

# Babak N. Safa

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### 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
                       = 'nth_order';
kinetics.name
                       = [k,N];
kinetics.parameters
%Intrinsic hyperelasticity
IntHyper.name
                       = 'neohookean';
IntHyper.parameters
                       = C1;
%Sliding
sliding .name
                       = 'sliding_power';
sliding .parameters
                       = [c,b,r0]
% Damage
                       = 'weibull';
IntHyper.name
                       = [k, l, r0]
IntHyper.parameters
```

#### 2 Kinetics

#### 2.1 First-order

First order kinetics relation for kinetics (snytax name: first\_order)

Parameter	Physical dimension
au	[[t]]
7	$\dot{w} = -\frac{1}{\tau}w$

#### 2.2 First-order stretched

First order kinetics relation for kinetics with stretched time constant (snytax name: first\_order\_stretched)

ameter   Phys	ical dimension
$\tau$	[[t]]
β	[[-]]
$\dot{w} = -\frac{\beta}{\tau}u$	$u^{\beta-1}w$

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

#### 2.3 Second-order

Second order kinetics relation for kinetics (snytax name: second\_order)

Parameter	Physical dimension	
k	$[[t]]^{(\frac{1}{2})}$	
$\iota$	$\dot{v} = -kw^2$	(3)

#### 2.4 Nth-order

Generalized nth-order kinetics relation for kinetics (snytax name: nth\_order)

Parameter	Physical dimension
k	$[[t]]^{(\frac{1}{N})}$
$\dot{w}$	$v = -kw^N$

# 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
$C_3$	$[[N.m^{-2}]]$
$C_4$	$[[N.m^{-2}]]$
$\lambda_s$	[[-]]

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

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

Here, u is the Heaviside step function.

### 3.4 Fiber exponential simple

Exponential elastic relation for toe-region and transition to linear region (snytax name: exp\_lin\_simple)

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

$$\psi_{EFS}(\lambda) = \frac{C_1}{C_2} \left( \exp\left[ C_2(\lambda - 1) \right] - C_2 \lambda - 1 \right) u(I_4 - 1), \tag{7}$$

Here, u is the Heaviside step function.

#### 3.5 Neo-Hookean

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

Parameter	Physical dimension		
$C_1$	$[[N.m^{-2}]]$		
$\psi_{NH}(I_1)$	$(1) = C_1(I_1 - 3).$		

#### 3.6 Holmes-Mow

Holmes-Mow material for isochoric uniaxial deformation (snytax name: holmes\_mow)

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

$$\psi_{HM}(I_1, I_2, I_3) = \alpha_0 \left( I_3^{-\beta} \exp\left[\alpha_1(I_1 - 3) + \alpha_2(I_2 - 3)\right] - 1 \right). \tag{9}$$

$$\alpha_0 = C0$$
,  $\alpha_1 = \frac{E/\alpha_0}{4(1+\nu)} - \alpha_2$ , and  $\alpha_2 = \frac{(E/\alpha_0)\nu}{4(1+\nu)(1-2\nu)} = \beta - \alpha_1$ , (10)

# 4 Sliding

#### 4.1 Power-law

The power law for sliding with three model parameters (snytax name: sliding\_power)

Parameter	Physical dimension
c	[[-]]
b	[[-]]
r0	[[-]]

$$f_s(\Xi_s) = c (\Xi_s - (r_s)_0)^b$$
 (11)

#### 4.2 Modified Weibull

The modified Weibull (sliding exponential) for sliding with three model parameters (snytax name: sliding\_exp)

Parameter	Physical dimension
k	[[-]]
l	[[-]]
r0	[[-]]

$$f_s(\Xi_s) = (\Xi_s - 1) \left( 1 - \exp\left[ -\left(\frac{\Xi_s - (r_s)_0}{l - 1}\right)^k \right] \right)$$
 (12)

# 5 Damage

### 5.1 Weibull

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

Parameter	Physical dimension
k	[[-]]
l	[[-]]
r0	[[-]]

$$f_D(\Xi_D) = 1 - \exp\left[-\left(\frac{\Xi_D - (r_D)_0}{l - 1}\right)^k\right]$$
(13)