

## 1 Variables

### 2 root

	var	symbol	documentation	type	units	eqs
8	$F_{N,A}$	F_N_A	fudamental incidence matrix	network		
5	$t$	t	time	frame	$s$	
6	$t^o$	to	starting time	frame	$s$	4
7	$t^e$	te	end time	frame	$s$	5
1	#	value	numerical value	constant		
2	1	one	numerical value one	constant		1
3	0	zero	numerical value zero	constant		2
4	0.5	onehalf	numerical value one half	constant		3

### 3 physical

	var	symbol	documentation	type	units	eqs
9	$P_{N,A}$	P_N_A	projection from node to arc for arc properties	projection		
32	$P_{NS,AS}$	P_NS_AS	projection node species to arc species	projection		
33	$P_{K,NK}$	P_K_NK	projection of conversion to node conversion	projection		
34	$P_{S,NS}$	P_S_NS	projection species to node species	projection		
35	$P_{N,NK}$	P_N_NK	projection node to node conversion	projection		
36	$P_{NS,KS}$	P_NS_KS	projection node species to conversion species	projection		
37	$P_{A,NS}$	P_A_NS	projection arc to node species for conductivity	projection		
65	$P_{NK,KS}$	P_NK_KS	projection node conversion to conversion species	projection		
10	$r_{xN}$	r_x	x-coordinate	frame	$m$	
11	$r_{yN}$	r_y	y-coordinate	frame	$m$	
12	$r_{zN}$	r_z	z coordinate	frame	$m$	
13	$U_N$	U	fundamental state – internal energy	state	$kg\,m^2\,s^{-2}$	
14	$S_N$	S	fundamental state – entropy	state	$kg\,m^2\,K^{-1}\,s^{-2}$	
15	$V_N$	V	fundamental state – volume	state	$m^3$	
16	$n_{NS}$	n	fundamental state – molar mass	state	$mol$	
20	$H_N$	H	enthalpy	state	$kg\,m^2\,s^{-2}$	9
21	$A_N$	A	Helmholtz energy	state	$kg\,m^2\,s^{-2}$	10
22	$G_N$	G	Gibbs free energy	state	$kg\,m^2\,s^{-2}$	11
23	$C_N$	charge	fundamental state – charge	state	$A\,s$	
24	$A^v$	Avogadro	Avogadro number	constant	$mol^{-1}$	
25	$k^B_N$	Boltzmann	Boltzmann constant	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	12
26	$R_N$	GasConstant	gas constant	constant	$kg\,m^2\,mol^{-1}\,K^{-1}\,s^{-2}$	13
17	$p_N$	p	thermodynamic pressure	effort	$kg\,m^{-1}\,s^{-2}$	6

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	var	symbol	documentation	type	units	eqs
18	$T_N$	<b>T</b>	temperature	effort	$K$	<b>7</b>
19	$\mu_{NS}$	<b>chemPot</b>	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	<b>8</b>
27	$U_N^C$	<b>UC</b>	electrical potential – voltage	effort	$kg\,m^2\,A^{-1}\,s^{-3}$	<b>14</b>
28	$v_{xN}$	<b>v_x</b>	velocity in x-direction	secondaryState	$ms^{-1}$	<b>15</b>
29	$v_{yN}$	<b>v_y</b>	velocity in y-direction	secondaryState	$ms^{-1}$	<b>16</b>
30	$v_{zN}$	<b>v_z</b>	velocity in z-direction	secondaryState	$ms^{-1}$	<b>17</b>

## 4 control

	var	symbol	documentation	type	units	eqs
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## 5 reactions

	var	symbol	documentation	type	units	eqs
31	$N_{S,K}$	N	stoichiometric matrix	constant		
38	$K^o_K$	Ko	Arrhenius frequency factor	constant	$m^{-3} mol s^{-1}$	
62	$E^a_{NK}$	Ea	Arrhenius activation energy	constant	$kg m^2 mol^{-1} s^{-2}$	41
63	$K_{NK}$	K_NK	Arrhenius reaction 'constant'	constant	$m^{-3} mol s^{-1}$	42
64	$N_{NS,NK}$	N_NS_NK	stoichiometric block matrix node species and node reaction	constant		43
60	$T_{NK}$	T_NK	temperature of the reactive system	effort	$K$	39

## 6 material

	var	symbol	documentation	type	units	eqs
40	$\lambda_S$	Mm	species molecular mass	constant	$kg\ mol^{-1}$	
42	$C_{pN}$	Cp	total heat capacity at constant pressure	property	$kg\ m^2\ K^{-1}\ s^{-2}$	21
43	$C_{VN}$	Cv	total heat capacity at constant volume	property	$kg\ m^2\ K^{-1}\ s^{-2}$	22
44	$k_{xN}^q$	kq_x	thermal conductivity in x-direction	property	$kg\ K^{-1}\ s^{-3}$	23
45	$k_{yN}^q$	kq_y	thermal conductivity in y-direction	property	$kg\ K^{-1}\ s^{-3}$	24
46	$k_{zN}^q$	kq_z	thermal conductivity in z-direction'	property	$kg\ K^{-1}\ s^{-3}$	25
47	$k_{qN}$	kq	thermal conductivity	property	$kg\ K^{-1}\ s^{-3}$	26
48	$k_{xN}^c$	kc_x	convective mass conductivity in x-direction	property	$m^{-1}\ s$	27
49	$k_{yN}^c$	kc_y	convective mass conductivity in y-direction	property	$m^{-1}\ s$	28
50	$k_{zN}^c$	kc_z	convective mass conductivity in z-direction	property	$m^{-1}\ s$	29
51	$k_{cN}^c$	kc	convective mass conductivity	property	$m^{-1}\ s$	30
52	$k_{xNS}^d$	kd_x	diffusional mass conductivity in x-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	31
53	$k_{yNS}^d$	kd_y	diffusional mass conductivity in y-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	32
54	$k_{zNS}^d$	kd_z	diffusional mass conductivity in z-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	33
55	$k_{dNS}^d$	kd	diffusional mass conductivity	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	34
56	$h_{NS}$	h	partial molar enthalpies	property	$kg\ m^2\ mol^{-1}\ s^{-2}$	35
59	$density_N$	density	density	property	$kg\ m^{-3}$	38

## 7 macroscopic

	var	symbol	documentation	type	units	eqs
57	$m_N$	<b>m</b>	total mass	secondaryState	$kg$	<b>36</b>
66	$c_{NS}$	<b>c</b>	molar composition	secondaryState	$m^{-3} mol$	<b>44</b>

## 8 solid

	var	symbol	documentation	type	units	eqs
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## 9 fluid

	var	symbol	documentation	type	units	eqs
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## 10 liquid

	var	symbol	documentation	type	units	eqs
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## 11 gas

	var	symbol	documentation	type	units	eqs
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## 12 control-control

	var	symbol	documentation	type	units	eqs
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## 13 gas–liquid

	var	symbol	documentation	type	units	eqs
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## 14 gas–gas

	var	symbol	documentation	type	units	eqs
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## 15 liquid–liquid

	var	symbol	documentation	type	units	eqs
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## 16 gas–solid

	var	symbol	documentation	type	units	eqs
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## 17 solid-solid

	var	symbol	documentation	type	units	eqs
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## 18 liquid–solid

	var	symbol	documentation	type	units	eqs
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## 19 material–material

	var	symbol	documentation	type	units	eqs
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## 20 reactions-reactions

	var	symbol	documentation	type	units	eqs
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## 21 control-reactions

	var	symbol	documentation	type	units	eqs
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## 22 reactions-control

	var	symbol	documentation	type	units	eqs
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## 23 control-material

	var	symbol	documentation	type	units	eqs
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## 24 material-control

	var	symbol	documentation	type	units	eqs
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## 25 control-macroscopic

	var	symbol	documentation	type	units	eqs
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## 26    macroscopic-control

	var	symbol	documentation	type	units	eqs
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## 27 reactions-material

	var	symbol	documentation	type	units	eqs
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## 28 material-reactions

	var	symbol	documentation	type	units	eqs
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## 29 reactions–macroscopic

	var	symbol	documentation	type	units	eqs
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## 30 macroscopic-reactions

	var	symbol	documentation	type	units	eqs
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## 31 material–macroscopic

	var	symbol	documentation	type	units	eqs
41	$Mm_S$	Mm	link variable Mm to interface material »> macroscopic	get	$kg\,mol^{-1}$	20

## 32 macroscopic-material

	var	symbol	documentation	type	units	eqs
58	$m_N$	m	link variable m to interface macroscopic » > material	get	<i>kg</i>	37



### 33 Equations

### 34 Generic

no	equation	documentation	layer
1	$1 := \text{Instantiate}(\#, \#)$	numerical value 1	root
2	$0 := \text{Instantiate}(\#, \#)$	numerical value zero	root
3	$0.5 := \text{Instantiate}(\#, \#)$	numerical value one half	root
4	$t^o := \text{Instantiate}(t, \#)$	starting time	root
5	$t^e := \text{Instantiate}(t, \#)$	end time	root
6	$p_N := \left(-\frac{\partial U_N}{\partial V_N}\right)$	thermodynamic pressure	physical
7	$T_N := \frac{\partial U_N}{\partial S_N}$	temperature	physical
8	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	chemical potential	physical
9	$H_N := U_N - p_N \cdot V_N$	enthalpy	physical
10	$A_N := U_N - T_N \cdot S_N$	Helmholtz energy	physical
11	$G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$	Gibbs free energy	physical
12	$k^B_N := \text{Instantiate}(S_N, \#)$	Boltzmann constant	physical
13	$R_N := A^v \cdot k^B_N$	gas constant	physical
14	$U^C_N := (C_N)^{-1} \cdot U_N$	electrical potential – voltage	physical
15	$v_{xN} := \frac{\partial r_{xN}}{\partial t}$	velocity in x-direction	physical
16	$v_{yN} := \frac{\partial r_{yN}}{\partial t}$	velocity in y direction	physical

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no	equation	documentation	layer
17	$v_{zN} := \frac{\partial r_{zN}}{\partial t}$	velocity in z-direction	physical
21	$C_{pN} := \frac{\partial H_N}{\partial T_N}$	total heat capacity at constant pressure	material
22	$C_{VN} := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	material
23	$k_{xN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}$	thermal conductivity in x-direction	material
24	$k_{yN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{yN}$	thermal conductivity in y-direction	material
25	$k_{zN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{zN}$	thermal conductivity in z-direction'	material
26	$kq_N := \text{Stack}(k_{xN}^q, k_{yN}^q, k_{zN}^q)$	thermal conductivity	material
27	$k_{xN}^c := \left( \lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass conductivity in x-direction	material
28	$k_{yN}^c := \left( \lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$	convective mass conductivity in y-direction	material
29	$k_{zN}^c := \left( \lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convective mass conductivity in z-direction	material
30	$k_N^c := \text{Stack}(k_{xN}^c, k_{yN}^c, k_{zN}^c)$	convective mass conductivity	material
31	$k_{xNS}^d := (\mu_{NS})^{-1} \cdot \left( v_{xN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in x-direction	material
32	$k_{yNS}^d := (\mu_{NS})^{-1} \cdot \left( v_{yN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in y-direction	material
33	$k_{zNS}^d := (\mu_{NS})^{-1} \cdot \left( v_{zN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in z-direction	material
34	$k_{NS}^d := \text{Stack}(k_{xNS}^d, k_{yNS}^d, k_{zNS}^d)$	diffusional mass conductivity	material

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no	equation	documentation	layer
35	$h_{NS} := H_N \odot (n_{NS})^{-1}$	partial molar enthalpies	material
36	$m_N := M m_S \overset{S \in NS}{\star} n_{NS}$	total mass	macroscopic
38	$density_N := m_N \cdot (V_N)^{-1}$	density	material
39	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature of the reactive system	reactions
41	$E^a_{NK} := \text{Instantiate}(P_{N,NK} \overset{N}{\star} R_N \cdot T_{NK}, \#)$	Arrhenius activation energy	reactions
42	$K_{NK} := K^o_K \odot \exp((-E^a_{NK}) \cdot (R_N \overset{N}{\star} P_{N,NK} \cdot T_{NK})^{-1})$	Arrhenius reaction 'constant'	reactions
43	$N_{NS,NK} := P_{S,NS} \overset{S}{\star} (P_{K,NK} \overset{K}{\star} N_{S,K})$	soichiometric block matrix node species and node reaction	reactions
44	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar composition	macroscopic

## 35 Interface Link Equation

no	equation	documentation	layer
20	$Mm_S := Mm_S$	interface equation	material $\rightarrow$ macroscopic
37	$m_N := m_N$	interface equation	macroscopic $\rightarrow$ material