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		
162	$P_{N,NS}$	P_N_NS	projection of nodes onto the node species	projection		
10	$r_{x\,N}$	r_x	x-coordinate	frame	m	
11	$r_{y\,N}$	r_y	y-coordinate	frame	m	
12	$r_{z\,N}$	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	86
20	H_N	H	enthalpy	state	$kg\,m^2\,s^{-2}$	9 87
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}	
17	p_N	p	thermodynamic pressure	effort	$kg\,m^{-1}\,s^{-2}$	6
18	T_N	T	temperature	effort	K	7

Continued on next page

	var	symbol	documentation	type	units	eqs
19	μ_{NS}	`chemPot`	chemical potential	effort	$kg\, m^2\, mol^{-1}\, s^{-2}$	8
27	Ue_N	`Ue`	electrical potential – voltage	effort	$kg\, m^2\, A^{-1} s^{-3}$	14 95
28	$v_{x\,N}$	`v_x`	velocitiy in x-direction	secondaryState	ms^{-1}	15
29	$v_{y\,N}$	`v_y`	velocity in y-direction	secondaryState	ms^{-1}	16
30	$v_{z\,N}$	`v_z`	velocity in z-direction	secondaryState	ms^{-1}	17

4 control

	var	symbol	documentation	type	units	eqs
136	x_N	`x`	state	state		111
137	xo_N	`xo`	initial state	state		109
129	$A_{N,D}$	`A`	dynamic matrix	constant	s^{-1}	
130	$B_{A,D}$	`B`	input matrix	constant	s^{-1}	
131	$C_{N,A}$	`C`	measurement matrix	constant		
132	D_A	`D`	diagonal event matrix (no dimensional problems)	constant		
133	${y^o}_A$	`setPoint`	set point	constant		119
134	m_A	`meas`	measurements	constant		
135	e_A	`e`	control error	constant		108
139	$1_{N,D}$	`I_N_D`	space transformation D to N	constant		
138	$\dot{x}_D$	`dxdt`	differential state (ABCD) model	diffState	s^{-1}	110
141	$\check{I}_N$	`Imeasured`	measured current	algebraic	A	113
143	${\check{U}^e}_N$	`UeMeasured`	measured electrical potential	algebraic	$kg\, m^2\, A^{-1} s^{-3}$	115
144	$\check{\xi}$	`addMeasured`	measured additive fraction	algebraic		116
145	R_N	`RComputed`	measured resistance	algebraic	$kg\, m^2\, A^{-2} s^{-3}$	117
146	S	`store`	quantities to be stored	algebraic		118
154	y_A	`y`	output equation	algebraic		126

5 reactions

	var	symbol	documentation	type	units	eqs
147	P_{NK}	P_NK	reactions per node	projection		
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
155	B	Boltzmann	Boltzmann constant	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	
157	R	GasConstant	gas constant	constant	$kg\,m^2\,mol^{-1}\,K^{-1}\,s^{-2}$	127
158	$N_{K,KS}$	N_K_KS	stoichiometry	constant		
159	$N_{NK,KS}$	N_NK_KS	extended stoichiometrix matrix	constant		128
60	T_{NK}	T_NK	temperature of the reactive system	effort	K	39
151	$c_{NK,KS}$	c	concentration matrix reaction per node and species per reaction	secondaryState	$m^{-3}\,mol$	123
152	${c^o}_{NK,KS}$	co	norming concentration	secondaryState	$m^{-3}\,mol$	124
153	$x_{NK,KS}$	x	matrix of normed, dimensionless mole fractions	secondaryState		125
160	ϕ_{NK}	phi	probability function for reactions	secondaryState		129
163	$\tilde{n}_{NS}$	nProd	the species production term	secondaryState	$mol\,s^{-1}$	130

6 material

	var	symbol	documentation	type	units	eqs
40	λ_S	`Mm`	species molecular mass	constant	$kg\,mol^{-1}$	
112	ξ	`additive`	fraction of additives	constant		88
42	$C_{p\,N}$	`Cp`	total heat capacity at constant pressure	property	$kg\,m^2\,K^{-1}\,s^{-2}$	21
43	$C_{V\,N}$	`Cv`	total heat capacity at constant volume	property	$kg\,m^2\,K^{-1}\,s^{-2}$	22
44	$k^q_x{}_N$	`kq_x`	thermal conductivity in x-direction	property	$kg\,K^{-1}\,s^{-3}$	23
45	$k^q_y{}_N$	`kq_y`	thermal conductivity in y-direction	property	$kg\,K^{-1}\,s^{-3}$	24
46	$k^q_z{}_N$	`kq_z`	thermal conductivity in z-direction'	property	$kg\,K^{-1}\,s^{-3}$	25
47	$k^q{}_N$	`kq`	thermal conductivity	property	$kg\,K^{-1}\,s^{-3}$	26
48	$k^c_x{}_N$	`kc_x`	convecitve mass conductivity in x-direction	property	$m^{-1}\,s$	27
49	$k^c_y{}_N$	`kc_y`	convecitve mass conductivity in y-direction	property	$m^{-1}\,s$	28
50	$k^c_z{}_N$	`kc_z`	convecitve mass conductivity in z-direction	property	$m^{-1}\,s$	29
51	$k^c{}_N$	`kc`	convective mass conductivity	property	$m^{-1}\,s$	30
52	$k^d_x{}_{NS}$	`kd_x`	diffusional mass conductivity in x-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	31
53	$k^d_y{}_{NS}$	`kd_y`	diffusional mass conductivity in y-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	32
54	$k^d_z{}_{NS}$	`kd_z`	diffusional mass conductivity in z-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	33
55	$k^d{}_{NS}$	`kd`	diffusional mass condctivity	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	ρ_N	`density`	density	property	$kg\,m^{-3}$	38
115	$R^e{}_N$	`elResist`	electrical resistant	property	$kg\,m^2\,A^{-2}s^{-3}$	91 92
116	$k^{e,\xi}{}_N$	`elConductC`	simple model for the electrical conductivity as a function of the additive	property	$kg^{-1}\,m^{-2}\,A^2s^3$	93

7 macroscopic

	var	symbol	documentation	type	units	eqs
92	$\hat{V}_A$	fV	volumetric flow	transport	$m^3\,s^{-1}$	67
93	$\hat{n}^d{}_{AS}$	fnd_AS	diffusional mass flow in a given stream	transport	$mol\,s^{-1}$	68
94	$\hat{n}^d{}_{NS}$	fnd	net diffusional mass flow	transport	$mol\,s^{-1}$	69
95	$\hat{H}^d{}_A$	fHd_A	enthalpy flow per diffusional mass stream	transport	$kg\,m^2\,s^{-3}$	70
96	$\hat{H}^d{}_N$	fHd	net enthaply stream due to diffusion	transport	$kg\,m^2\,s^{-3}$	71
97	d_A	d	flow direction of convectional flow	transport		72
102	$\hat{H}^c{}_A$	fHc_A	convective enthalpy flow for given stream	transport	$kg\,m^2\,s^{-3}$	77
103	$\hat{H}^c{}_N$	fHc	net convectional enthalpy stream	transport	$kg\,m^2\,s^{-3}$	78
104	$\hat{w}_A$	fw_A	sample work stream	transport	$kg\,m^2\,s^{-3}$	79
105	$\hat{w}_N$	fw	net work stream	transport	$kg\,m^2\,s^{-3}$	80
106	$\hat{q}_{x\,A}$	fq_A_x	heat flow in x-direction for given stream	transport	$kg\,m^2\,s^{-3}$	81
107	$\hat{q}_N$	fq	net heat flow	transport	$kg\,m^2\,s^{-3}$	82
71	$A_{yz\,N}$	Ayz	cross sectional area yz	geometry	m^2	48
72	$A_{xz\,N}$	Axz	cross sectional area xz	geometry	m^2	49
73	$A_{xy\,N}$	Axy	cross sectional area xy	geometry	m^2	50
70	$F_{NS,AS}$	F_NS_AS	species related incidence matrix	network		
90	$D_{N,A}$	D	difference operator	differenceOperator		
91	$D_{NS,AS}$	D_NS_AS	difference operator for species topology	differenceOperator		
109	$H^o{}_N$	Ho	initial enthalpy	state	$kg\,m^2\,s^{-2}$	84
110	$n^o{}_{NS}$	no	initial species	state	mol	85
127	1_S	one_S	a vector of ones with the length of the ordinal number of S	constant		
57	m_N	m	total mass	secondaryState	kg	36

Continued on next page

	var	symbol	documentation	type	units	eqs
66	c_{NS}	`c`	molar composition	secondaryState	$m^{-3}\,mol$	44
98	c_{AS}	`c_AS`	concentration in convectional flow	secondaryState	$m^{-3}\,mol$	73
99	$\hat{n}^c{}_{AS}$	`fnc_AS`	molar convetional mass flow in the given stream	secondaryState	$mol\,s^{-1}$	74
100	$\hat{n}^c{}_{NS}$	`fnc`	net molar convectional mass flow	secondaryState	$mol\,s^{-1}$	75
126	ϕ	`intensities`	collected intensities	secondaryState		106
128	$n^t{}_N$	`nTotal`	total number of moles	secondaryState	mol	107
101	$\dot{n}_{NS}$	`dndt`	differential species balance	diffState	$mol\,s^{-1}$	76
108	$\dot{H}_N$	`dHdt`	differential enthalpy balance	diffState	$kg\,m^2\,s^{-3}$	83
118	$\dot{U}^e{}_N$	`dUedt`	Kirkhoff first law	diffState	$kg\,m^2\,A^{-1}s^{-3}$	96 97 98
113	I_N	`i`	electrical current definition	internalTransport	A	89

8 solid

	var	symbol	documentation	type	units	eqs

9 fluid

	var	symbol	documentation	type	units	eqs

10 liquid

	var	symbol	documentation	type	units	eqs

11 gas

	var	symbol	documentation	type	units	eqs

12 control–control

	var	symbol	documentation	type	units	eqs

13 gas–liquid

	var	symbol	documentation	type	units	eqs

14 gas–gas

	var	symbol	documentation	type	units	eqs

15 liquid–liquid

	var	symbol	documentation	type	units	eqs

16 gas–solid

	var	symbol	documentation	type	units	eqs

17 solid–solid

	var	symbol	documentation	type	units	eqs

18 liquid–solid

	var	symbol	documentation	type	units	eqs

19 material–material

	var	symbol	documentation	type	units	eqs

20 reactions–reactions

	var	symbol	documentation	type	units	eqs

21 control–reactions

	var	symbol	documentation	type	units	eqs

22 reactions–control

	var	symbol	documentation	type	units	eqs

23 control–material

	var	symbol	documentation	type	units	eqs

24 material–control

	var	symbol	documentation	type	units	eqs
124	$\mathring{\xi}$	`_additive`	link variable additive to interface material »> control	get		104

25 control–macroscopic

	var	symbol	documentation	type	units	eqs

26 macroscopic–control

	var	symbol	documentation	type	units	eqs
119	$\mathring{I}_N$	`_i`	link variable i to interface macroscopic »> control	get	A	99
125	$\mathring{T}_N$	`_T`	link variable T to interface macroscopic »> control	get	K	105
142	$\mathring{U}e_N$	`_Ue`	link variable Ue to interface macroscopic »> control	get	$kg\, m^2\, A^{-1} s^{-3}$	114

27 reactions–material

	var	symbol	documentation	type	units	eqs

28 material–reactions

	var	symbol	documentation	type	units	eqs

29 reactions–macroscopic

	var	symbol	documentation	type	units	eqs
164	$\mathring{\tilde{n}}_{NS}$	`_nProd`	link variable nProd to interface reactions »> macroscopic	get	$mol\ s^{-1}$	131

30 macroscopic–reactions

	var	symbol	documentation	type	units	eqs
67	$\mathring{c}_{NS}$	`_c`	link variable c to interface macroscopic »> reactions	get	$m^{-3}\,mol$	45

31 material–macroscopic

	var	symbol	documentation	type	units	eqs
41	$\mathring{\lambda}_{S}$	_Mm	link variable Mm to interface material »> macroscopic	get	$kg\,mol^{-1}$	20
74	$\mathring{\rho}_{N}$	_density	link variable density to interface material »> macroscopic	get	$kg\,m^{-3}$	51
75	$\mathring{h}_{NS}$	_h	link variable h to interface material »> macroscopic	get	$kg\,m^{2}\,mol^{-1}\,s^{-2}$	52
76	$\mathring{k}^{q}_{x\,N}$	_kq_x	link variable kq x to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	53
77	$\mathring{C}_{v\,N}$	_Cv	link variable Cv to interface material »> macroscopic	get	$kg\,m^{2}\,K^{-1}\,s^{-2}$	54
78	$\mathring{k}^{q}_{y\,N}$	_kq_y	link variable kq y to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	55
79	$\mathring{k}^{q}_{z\,N}$	_kq_z	link variable kq z to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	56
80	$\mathring{k}^{q}{}_{N}$	_kq	link variable kq to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	57
81	$\mathring{k}^{c}_{x\,N}$	_kc_x	link variable kc x to interface material »> macroscopic	get	$m^{-1}\,s$	58
82	$\mathring{C}_{p\,N}$	_Cp	link variable Cp to interface material »> macroscopic	get	$kg\,m^{2}\,K^{-1}\,s^{-2}$	59
83	$\mathring{k}^{c}_{y\,N}$	_kc_y	link variable kc y to interface material »> macroscopic	get	$m^{-1}\,s$	60
84	$\mathring{k}^{c}_{z\,N}$	_kc_z	link variable kc z to interface material »> macroscopic	get	$m^{-1}\,s$	61
85	$\mathring{k}^{c}{}_{N}$	_kc	link variable kc to interface material »> macroscopic	get	$m^{-1}\,s$	62
86	$\mathring{k}^{d}_{x\,NS}$	_kd_x	link variable kd x to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^{2}\,s$	63
87	$\mathring{k}^{d}_{y\,NS}$	_kd_y	link variable kd y to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^{2}\,s$	64
88	$\mathring{k}^{d}_{z\,NS}$	_kd_z	link variable kd z to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^{2}\,s$	65

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	var	symbol	documentation	type	units	eqs
89	$\mathring{k}^{d}{}_{NS}$	`_kd`	link variable kd to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^{2}\,s$	66
117	$\mathring{R}^{e}{}_{N}$	`_elConductC`	link variable elConductC to interface material »> macroscopic	get	$kg^{-1}\,m^{-2}\,A^{2}s^{3}$	94
140	$\mathring{\xi}$	`_additive`	link variable additive to interface material »> macroscopic	get		112

32 macroscopic–material

	var	symbol	documentation	type	units	eqs
58	$\mathring{m}_N$	`_m`	link variable m to interface macroscopic »> material	get	kg	37
114	$\mathring{I}_N$	`_i`	link variable i to interface macroscopic »> material	get	A	90

33 Equations

34 Generic

no	equation	documentation	layer
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	$H_N := U_N - p_N \,.\, V_N$	enthalpy	physical
10	$A_N := U_N - T_N \,.\, S_N$	Helmholtz energy	physical
11	$G_N := U_N + p_N \,.\, V_N - T_N \,.\, S_N$	Gibbs free energy	physical
14	$Ue_N := (C_N)^{-1} \,.\, U_N$	electrical potential – voltage	physical
15	$v_{xN} := \frac{\partial r_{xN}}{\partial t}$	velocitiy in x-direction	physical
16	$v_{yN} := \frac{\partial r_{yN}}{\partial t}$	velocity in y direction	physical
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	$k^q_{xN} := (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial T_N} \,.\, v_{xN}$	thermal conductivity in x-direction	material
24	$k^q_{yN} := (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial T_N} \,.\, v_{yN}$	thermal conductivity in y-direction	material
25	$k^q_{zN} := (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial T_N} \,.\, v_{zN}$	thermal conductivity in z-direction'	material
26	$k^q{}_N := \mathrm{Stack}\left(k^q_{xN}, k^q_{yN}, k^q_{zN}\right)$	thermal conductivity	material

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no	equation	documentation	layer
27	$k^c_{xN} := \left(\lambda_S \overset{S\in NS}{\star} (\mu_{NS})^{-1}\right) . (V_N)^{-1} . \frac{\partial U_N}{\partial p_N} . v_{xN}$	convecitve mass conductivity in x-direction	material
28	$k^c_{yN} := \left(\lambda_S \overset{S\in NS}{\star} (\mu_{NS})^{-1}\right) . (V_N)^{-1} . \frac{\partial U_N}{\partial p_N} . v_{yN}$	convecitve mass conductivity in y-direction	material
29	$k^c_{zN} := \left(\lambda_S \overset{S\in NS}{\star} (\mu_{NS})^{-1}\right) . (V_N)^{-1} . \frac{\partial U_N}{\partial p_N} . v_{zN}$	convecitve mass conductivity in z-direction	material
30	$k^c{}_N := \text{Stack}\left(k^c_{xN}, k^c_{yN}, k^c_{zN}\right)$	convective mass conductivity	material
31	$k^d_{xNS} := (\mu_{NS})^{-1} . \left(v_{xN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in x-direction	material
32	$k^d_{yNS} := (\mu_{NS})^{-1} . \left(v_{yN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in y-direction	material
33	$k^d_{zNS} := (\mu_{NS})^{-1} . \left(v_{zN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in z-direction	material
34	$k^d{}_{NS} := \text{Stack}\left(k^d_{xNS}, k^d_{yNS}, k^d_{zNS}\right)$	diffusional mass condctivity	material
35	$h_{NS} := H_N \odot (n_{NS})^{-1}$	partial molar enthalpies	material
36	$m_N := \mathring{\lambda}_S \overset{S\in NS}{\star} n_{NS}$	total mass	macroscopic
38	$\rho_N := \mathring{m}_N . (V_N)^{-1}$	density	material
39	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature of the reactive system	reactions
42	$K_{NK} := K^o{}_K \odot exp((-E^a{}_{NK}) . (R . T_{NK})^{-1})$	Arrhenius reaction 'constant'	reactions
44	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar composition	macroscopic
48	$A_{yzN} := r_{yN} . r_{zN}$	cross sectional area yz	macroscopic

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no	equation	documentation	layer
49	$A_{xz\,N} := r_{x\,N} \,.\, r_{z\,N}$	cross sectional area xz	macroscopic
50	$A_{xy\,N} := r_{x\,N} \,.\, r_{y\,N}$	cross sectional area xy	macroscopic
67	$\hat{V}_A := \left(\mathring{\rho}_N\right)^{-1} \,.\, \mathring{k}^c_{x\,N} \,.\, A_{yz\,N} \,.\, D_{N,A} \overset{N}{\star} p_N$	volumetric flow	macroscopic
68	$\hat{n}^d{}_{AS} := A_{yz\,N} \odot \left(-\mathring{k}^d_{x\,NS}\right) \,.\, D_{NS,AS} \overset{NS}{\star} \mu_{NS}$	diffusional mass flow in a given stream	macroscopic
69	$\hat{n}^d{}_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^d{}_{AS}$	net diffusional mass flow	macroscopic
70	$\hat{H}^d{}_A := \left(F_{NS,AS} \overset{NS}{\star} \mathring{h}_{NS}\right) \overset{S\in AS}{\star} \hat{n}^d{}_{AS}$	enthalpy flow per diffusional mass stream	macroscopic
71	$\hat{H}^d{}_N := F_{N,A} \overset{A}{\star} \hat{H}^d{}_A$	net enthaply stream due to diffusion	macroscopic
72	$d_A := \mathrm{sign}\left(F_{N,A} \overset{N}{\star} p_N\right)$	flow direction of convectional flow	macroscopic
73	$c_{AS} := \left(0.5 \,.\, \left(F_{NS,AS} - d_A \odot \lvert F_{NS,AS}\rvert\right)\right) \overset{NS}{\star} c_{NS}$	concentration in convectional flow	macroscopic
74	$\hat{n}^c{}_{AS} := \hat{V}_A \odot c_{AS}$	molar convetional mass flow in the given stream	macroscopic
75	$\hat{n}^c{}_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^c{}_{AS}$	net molar convectional mass flow	macroscopic
76	$\dot{n}_{NS} := \hat{n}^c{}_{NS} + \hat{n}^d{}_{NS} + \mathring{\tilde{n}}_{NS}$	differential species balance	macroscopic
77	$\hat{H}^c{}_A := \left(F_{NS,AS} \overset{NS}{\star} \mathring{h}_{NS}\right) \overset{S\in AS}{\star} \hat{n}^c{}_{AS}$	convective enthalpy flow for given stream	macroscopic
78	$\hat{H}^c{}_N := F_{N,A} \overset{A}{\star} \hat{H}^c{}_A$	net convectional enthalpy stream	macroscopic
80	$\hat{w}_N := F_{N,A} \overset{A}{\star} \hat{w}_A$	net work stream	macroscopic
81	$\hat{q}_{x\,A} := A_{yz\,N} \,.\, \mathring{k}^q_{x\,N} \,.\, D_{N,A} \overset{N}{\star} T_N$	heat flow in x-direction for given stream	macroscopic
82	$\hat{q}_N := F_{N,A} \overset{A}{\star} \hat{q}_{x\,A}$	net heat flow	macroscopic

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no	equation	documentation	layer
83	$\dot{H}_N := \hat{H}^c{}_N + \hat{H}^d{}_N + \hat{q}_N + \hat{w}_N$	differential enthalpy balance	macroscopic
86	$n_{NS} := \int_{t^o}^{t^e} \dot{n}_{NS} \; dt$	fundamental state – molar mass	macroscopic
87	$H_N := \int_{t^o}^{t^e} \dot{H}_N \; dt$	enthalpy	macroscopic
89	$I_N := \frac{d C_N}{d t}$	electrical current definition	macroscopic
93	$k^{e,\xi}{}_N := (R^e{}_N)^{-1} . \xi$	simple model for the electrical conductivity as a function of the additive	material
95	$Ue_N := \left(\mathring{R}^e{}_N\right)^{-1} . I_N$	electrical potential – voltage	macroscopic
96	$\dot{U}^e{}_N := 1 . Ue_N$	Kirkhoff first law	macroscopic
97	$\dot{U}^e{}_N := Root\,(Ue_N)$	Kirkhoff first law	macroscopic
106	$\phi := \mathrm{MixedStack}\,(p_N, T_N, \mu_{NS}, c_{NS}, Ue_N)$	collected intensities	macroscopic
107	$n^t{}_N := 1_S \overset{S \in NS}{\star} n_{NS}$	total number of moles	macroscopic
108	$e_A := m_A - y^o{}_A$	control error	control
110	$\dot{x}_D := A_{N,D} \overset{N}{\star} x_N + B_{A,D} \overset{A}{\star} e_A$	differential state (ABCD) model	control
111	$x_N := \int_{t^o}^{t^e} 1_{N,D} \overset{D}{\star} \dot{x}_D \; dt$	state	control
113	$\check{I}_N := \mathring{I}_N$	measured current	control

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no	equation	documentation	layer
115	$\check{U^e}_N := \mathring{U}e_N$	measured electrical potential	control
116	$\check{\xi} := \mathring{\xi}$	measured additive fraction	control
117	$R_N := \left(\check{I}_N\right)^{-1} . \check{U^e}_N$	measured resistance	control
118	$S := \text{MixedStack}\left(\check{I}_N, \check{U^e}_N, R_N, \check{\xi}\right)$	quantities to be stored	control
123	$c_{NK,KS} := P_{NK} . \left(P_{NS,KS} \overset{NS}{\star} \mathring{c}_{NS}\right)$	var doc :	reactions
125	$x_{NK,KS} := \left({c^o}_{NK,KS}\right)^{-1} . c_{NK,KS}$	matrix of normed, dimensionless mole fractions	reactions
126	$y_A := C_{N,A} \overset{N}{\star} x_N + D_A . e_A$	output equation	control
127	$R := A^v . B$	gas constant	reactions
128	$N_{NK,KS} := P_{K,NK} \overset{K}{\star} N_{K,KS}$	extended stoichiometrix matrix	reactions
129	$\phi_{NK} := \prod_{KS} {x_{NK,KS}}^{N_{NK,KS}}$	probability function for reactions	reactions
130	$\tilde{n}_{NS} := V_N \overset{N}{\star} \left(P_{N,NK} \overset{NK}{\star} \left(\left(K_{NK} . \phi_{NK}\right) . \left(P_{NS,KS} \overset{KS}{\star} N_{NK,KS}\right)\right)\right)$	the species production term	reactions

35 Instantiate

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
41	$E^a{}_{NK} := \text{Instantiate}(R \,.\, T_{NK}, \#)$	Arrhenius activation energy	reactions
79	$\hat{w}_A := \text{Instantiate}(\hat{H}^c{}_A, \#)$	sample work stream	macroscopic
84	$H^o{}_N := \text{Instantiate}(H_N, \#)$	initial enthalpy	macroscopic
85	$n^o{}_{NS} := \text{Instantiate}(n_{NS}, \#)$	initial species	macroscopic
88	$\xi := \text{Instantiate}(\xi, \#)$	fraction of additives	material
91	$R^e{}_N := \left(\mathring{I}_N\right)^{-1} . Ue_N$	electrical resistant	material
92	$R^e{}_N := \text{Instantiate}(R^e{}_N, \#)$	electrical resistant	material
98	$\dot{U}^e{}_N := \text{Instantiate}(\dot{U}^e{}_N, 0)$	Kirkhoff first law	macroscopic
109	$xo_N := \text{Instantiate}(x_N, \#)$	initial state	control
119	$y^o{}_A := \text{Instantiate}(y^o{}_A, \#)$	set point	control

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no	equation	documentation	layer
124	${c^o}_{NK,KS} := \mathrm{Instantiate}(c_{NK,KS}, \#)$	norming concentration	reactions

36 Interface Link Equation

no	equation	documentation	layer
20	$\mathring{\lambda}_S := \lambda_S$	interface equation	material –> macroscopic
37	$\mathring{m}_N := m_N$	interface equation	macroscopic –> material
45	$\mathring{c}_{NS} := c_{NS}$	interface equation	macroscopic –> reactions
51	$\mathring{\rho}_N := \rho_N$	interface equation	material –> macroscopic
52	$\mathring{h}_{NS} := h_{NS}$	interface equation	material –> macroscopic
53	$\mathring{k}^q_{x\,N} := k^q_{x\,N}$	interface equation	material –> macroscopic
54	$\mathring{C}_{v\,N} := C_{V\,N}$	interface equation	material –> macroscopic
55	$\mathring{k}^q_{y\,N} := k^q_{y\,N}$	interface equation	material –> macroscopic
56	$\mathring{k}^q_{z\,N} := k^q_{z\,N}$	interface equation	material –> macroscopic
57	$\mathring{k}^q{}_N := k^q{}_N$	interface equation	material –> macroscopic
58	$\mathring{k}^c_{x\,N} := k^c_{x\,N}$	interface equation	material –> macroscopic

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no	equation	documentation	layer
59	$\mathring{C}_{pN} := C_{pN}$	interface equation	material –> macro-scopic
60	$\mathring{k}^c_{yN} := k^c_{yN}$	interface equation	material –> macro-scopic
61	$\mathring{k}^c_{zN} := k^c_{zN}$	interface equation	material –> macro-scopic
62	$\mathring{k}^c{}_N := k^c{}_N$	interface equation	material –> macro-scopic
63	$\mathring{k}^d_{xNS} := k^d_{xNS}$	interface equation	material –> macro-scopic
64	$\mathring{k}^d_{yNS} := k^d_{yNS}$	interface equation	material –> macro-scopic
65	$\mathring{k}^d_{zNS} := k^d_{zNS}$	interface equation	material –> macro-scopic
66	$\mathring{k}^d{}_{NS} := k^d{}_{NS}$	interface equation	material –> macro-scopic
90	$\mathring{I}_N := I_N$	interface equation	macroscopic –> material
94	$\mathring{R}^e{}_N := k^{e,\xi}{}_N$	interface equation	material –> macro-scopic
99	$\mathring{I}_N := I_N$	interface equation	macroscopic –> control
104	$\mathring{\xi} := \xi$	interface equation	material –> control

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no	equation	documentation	layer
105	$\mathring{T}_N := T_N$	interface equation	macroscopic –> control
112	$\mathring{\xi} := \xi$	interface equation	material –> macroscopic
114	$\mathring{U}e_N := Ue_N$	interface equation	macroscopic –> control
131	$\mathring{\tilde{n}}_{NS} := \tilde{n}_{NS}$	interface equation	reactions –> macroscopic