1 Variables

2 root

	var	symbol	documentation	type	units	eqs
8	$F_{N,A}$	`F_N_A`	fundamental 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
162	$P_{N,NS}$	P_N_NS	projection of nodes onto the node species	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		
9	$P_{N,A}$	P_N_A	projection from node to arc for arc properties	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	$A\,s$	
165	B_N	boz	Boltzmann constant	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	132
166	R_N	R	gas constant	constant	$kg\,m^2\,mol^{-1}\,K^{-1}\,s^{-2}$	133
24	A^v	Avogadro	Avogadro number	constant	mol^{-1}	

Continued on next page

	var	symbol	documentation	type	units	eqs
17	p_N	`p`	thermodynamic pressure	effort	$kg\, m^{-1}\, s^{-2}$	6
18	T_N	`T`	temperature	effort	K	7
19	μ_{NS}	`chemPot`	chemical potential	effort	$kg\, m^2\, mol^{-1}\, s^{-2}$	8 136
27	Ue_N	`Ue`	electrical potential – voltage	effort	$kg\, m^2\, A^{-1} s^{-3}$	14 95
28	$v_{x\,N}$	`v_x`	velocity 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	x_{oN}	`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
171	s	`switch`	switches at to	algebraic		138

5 reactions

	var	symbol	documentation	type	units	eqs
147	P_{NK}	P_NK	reactions per node	projection		
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 stoichiometric matrix	constant		128
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
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
112	ξ	additive	fraction of additives	constant		88
40	λ_S	Mm	species molecular mass	constant	$kg\,mol^{-1}$	
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
183	$k_{dFick}{}_{NS}$	k_d_Fick	Fick's diffusivity	property	ms^{-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	$k^q_{x}{}_N$	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	convective mass conductivity in x-direction	property	$m^{-1}\,s$	27
49	$k^c_{y}{}_N$	kc_y	convective mass conductivity in y-direction	property	$m^{-1}\,s$	28
50	$k^c_{z}{}_N$	kc_z	convective 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 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	ρ_N	density	density	property	$kg\,m^{-3}$	38

7 macroscopic

	var	symbol	documentation	type	units	eqs
100	$\hat{n}^c{}_{NS}$	`fnc`	net molar convectional mass flow	transport	$mol\, s^{-1}$	75
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
173	$\hat{n}^{c,controlled}{}_{AS}$	`fnc_AS_controlled`	switched flow	transport	$mol\, s^{-1}$	141
92	$\hat{V}_A$	`fV`	volumetric flow	transport	$m^3\, s^{-1}$	67 140
93	$\hat{n}^d{}_{AS}$	`fnd_AS`	diffusional mass flow in a given stream	transport	$mol\, s^{-1}$	68 152
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 enthalpy stream due to diffusion	transport	$kg\, m^2\, s^{-3}$	71
97	d_A	`d`	flow direction of convectional flow	transport		72
99	$\hat{n}^c{}_{AS}$	`fnc_AS`	molar convectional mass flow in the given stream	transport	$mol\, s^{-1}$	74
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

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	var	symbol	documentation	type	units	eqs
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		
126	ϕ	`intensities`	collected intensities	secondaryState		106
128	${n^t}_N$	`nTotal`	total number of moles	secondaryState	mol	107
168	n_{tN}	`nt`	total number of species in a node	secondaryState	mol	134
169	ξ_{NS}	`xi`	mole fraction	secondaryState		135
176	g_{NS}	`g`		secondaryState	mol	145
57	m_N	`m`	total mass	secondaryState	kg	36
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
170	$\tilde{n}_{NS}$	`nProd`	production term	conversion	$mol\,s^{-1}$	137
101	$\dot{n}_{NS}$	`dndt`	differential species balance	diffState	$mol\,s^{-1}$	76 142
108	$\dot{H}_N$	`dHdt`	differential enthalpy balance	diffState	$kg\,m^2\,s^{-3}$	83
118	${\dot{U}^e}_N$	`dUedt`	Kirkhoffs 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	$\mapsto \xi$	`_additive`	link variable additive to interface material »> control	get		104

25 control–macroscopic

	var	symbol	documentation	type	units	eqs
172	s	`_switch`	switches at to	get		139

26 macroscopic–control

	var	symbol	documentation	type	units	eqs
119	I_N	`_i`	link variable i to interface macroscopic »> control	get	A	99
125	T_N	`_T`	link variable T to interface macroscopic »> control	get	K	105
142	Ue_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	$\tilde{n}_{NS}$	`_nProd`	link variable nProd to interface reactions »> macroscopic	get	$mol\ s^{-1}$	131

30 macroscopic–reactions

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

31 material–macroscopic

	var	symbol	documentation	type	units	eqs
117	$\_{R^e}_N$	`_elConductC`	link variable elConductC to interface material »> macroscopic	get	$kg^{-1}\,m^{-2}\,A^2 s^3$	94
140	$\_\xi$	`_additive`	link variable additive to interface material »> macroscopic	get		112
184	$\_{k^{d,Fick}}_{NS}$	`_k_d_Fick`	link variable k d Fick to interface material »> macroscopic	get	ms^{-1}	151
41	$\_\lambda_S$	`_Mm`	link variable Mm to interface material »> macroscopic	get	$kg\,mol^{-1}$	20
74	$\_\rho_N$	`_density`	link variable density to interface material »> macroscopic	get	$kg\,m^{-3}$	51
75	$\_h_{NS}$	`_h`	link variable h to interface material »> macroscopic	get	$kg\,m^2\,mol^{-1}\,s^{-2}$	52
76	$\_{k^q_x}_N$	`_kq_x`	link variable kq x to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	53
77	$\_Cv_N$	`_Cv`	link variable Cv to interface material »> macroscopic	get	$kg\,m^2\,K^{-1}\,s^{-2}$	54
78	$\_{k^q_y}_N$	`_kq_y`	link variable kq y to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	55
79	$\_{k^q_z}_N$	`_kq_z`	link variable kq z to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	56
80	$\_{k^q}_N$	`_kq`	link variable kq to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	57
81	$\_{k^c_x}_N$	`_kc_x`	link variable kc x to interface material »> macroscopic	get	$m^{-1}\,s$	58
82	$\_Cp_N$	`_Cp`	link variable Cp to interface material »> macroscopic	get	$kg\,m^2\,K^{-1}\,s^{-2}$	59
83	$\_{k^c_y}_N$	`_kc_y`	link variable kc y to interface material »> macroscopic	get	$m^{-1}\,s$	60
84	$\_{k^c_z}_N$	`_kc_z`	link variable kc z to interface material »> macroscopic	get	$m^{-1}\,s$	61
85	$\_{k^c}_N$	`_kc`	link variable kc to interface material »> macroscopic	get	$m^{-1}\,s$	62

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	var	symbol	documentation	type	units	eqs
86	$\_k^d_x{}_{NS}$	`_kd_x`	link variable kd x to interface material »> macroscopic	get	$kg^{-1}\, m^{-4}\, mol^2\, s$	63
87	$\_k^d_y{}_{NS}$	`_kd_y`	link variable kd y to interface material »> macroscopic	get	$kg^{-1}\, m^{-4}\, mol^2\, s$	64
88	$\_k^d_z{}_{NS}$	`_kd_z`	link variable kd z to interface material »> macroscopic	get	$kg^{-1}\, m^{-4}\, mol^2\, s$	65
89	$\_k^d{}_{NS}$	`_kd`	link variable kd to interface material »> macroscopic	get	$kg^{-1}\, m^{-4}\, mol^2\, s$	66

32 macroscopic–material

	var	symbol	documentation	type	units	eqs
114	I_N	`_i`	link variable i to interface macroscopic »> material	get	A	90
58	m_N	`_m`	link variable m to interface macroscopic »> material	get	kg	37

33 Equations

34 Generic

no	equation	documentation	layer
10	$A_N := U_N - T_N \,.\, S_N$	Helmholtz energy	physical
106	$\phi := \text{MixedStack}\left(p_N, T_N, \mu_{NS}, c_{NS}, Ue_N\right)$	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
11	$G_N := U_N + p_N \,.\, V_N - T_N \,.\, S_N$	Gibbs free energy	physical
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	$\check{I}_N := I_N$	measured current	control
115	$\check{U}^e{}_N := Ue_N$	measured electrical potential	control
116	$\check{\xi} := \mapsto \xi$	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	$c_{NK,KS} := P_{NK} \,.\, \left(P_{NS,KS} \overset{NS}{\star} c_{NS}\right)$	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

Continued on next page

no	equation	documentation	layer
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	$\tilde{n}_{NS} := V_N \overset{N}{\star} \left(P_{N,NK} \overset{NK}{\star} \left((K_{NK} \, . \, \phi_{NK}) \, . \, \left(P_{NS,KS} \overset{KS}{\star} N_{NK,KS}\right)\right)\right)$	the species production term	reactions
132	$B_N := \text{Instantiate}(S_N, \#)$	Boltzmann constant	physical
133	$R_N := A^v \, . \, B_N$	gas constant	physical
134	$n_{tN} := 1_S \overset{S \in NS}{\star} n_{NS}$	total number of species in a node	macroscopic
135	$\xi_{NS} := (n_{tN})^{-1} \odot n_{NS}$	mole fraction	macroscopic
136	$\mu_{NS} := (R_N \, . \, T_N) \odot ln(\xi_{NS})$	chemical potential	macroscopic
137	$\tilde{n}_{NS} := \tilde{n}_{NS}$	production term	macroscopic
138	$s := 0.5 \, . \, (1 + \text{sign}\,(t^o))$	switches at to	control
139	$s := s$	switches at to	control –> macroscopic
14	$Ue_N := (C_N)^{-1} \, . U_N$	electrical potential – voltage	physical
141	$\hat{n}^{c,controlled}{}_{AS} := s \, . \, \hat{n}^c{}_{AS}$	switched flow	macroscopic
142	$\dot{n}_{NS} := F_{NS,AS} \overset{AS}{\star} \text{Stack}\left(\hat{n}^c{}_{AS}, \hat{n}^{c,controlled}{}_{AS}\right)$	differential species balance switched	macroscopic
145	$g_{NS} := n_{NS} + n_{NS}$		macroscopic
15	$v_{xN} := \frac{\partial \, r_{xN}}{\partial \, t}$	velocitiy in x-direction	physical
152	$\hat{n}^d{}_{AS} := A_{yzN} \odot \left(-\_k^{d,Fick}{}_{NS}\right) \, . \, D_{NS,AS} \overset{NS}{\star} c_{NS}$	diffusional mass flow in a given stream	macroscopic

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no	equation	documentation	layer
16	$v_{y\,N} := \frac{\partial\, r_{y\,N}}{\partial\, t}$	velocity in y direction	physical
17	$v_{z\,N} := \frac{\partial\, r_{z\,N}}{\partial\, t}$	velocity in z-direction	macroscopic
21	$C_{p\,N} := \frac{\partial\, H_N}{\partial\, T_N}$	total heat capacity at constant pressure	material
22	$C_{V\,N} := \frac{\partial\, U_N}{\partial\, T_N}$	total heat capacity at constant volume	material
23	$k^q_{x\,N} := (V_N)^{-1} \cdot \frac{\partial\, U_N}{\partial\, T_N} \cdot v_{x\,N}$	thermal conductivity in x-direction	material
24	$k^q_{y\,N} := (V_N)^{-1} \cdot \frac{\partial\, U_N}{\partial\, T_N} \cdot v_{y\,N}$	thermal conductivity in y-direction	material
25	$k^q_{z\,N} := (V_N)^{-1} \cdot \frac{\partial\, U_N}{\partial\, T_N} \cdot v_{z\,N}$	thermal conductivity in z-direction'	material
26	$k^q{}_N := \text{Stack}\left(k^q_{x\,N}, k^q_{y\,N}, k^q_{z\,N}\right)$	thermal conductivity	material
27	$k^c_{x\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial\, U_N}{\partial\, p_N} \cdot v_{x\,N}$	convecitve mass conductivity in x-direction	material
28	$k^c_{y\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial\, U_N}{\partial\, p_N} \cdot v_{y\,N}$	convecitve mass conductivity in y-direction	material
29	$k^c_{z\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial\, U_N}{\partial\, p_N} \cdot v_{z\,N}$	convecitve mass conductivity in z-direction	material
30	$k^c{}_N := \text{Stack}\left(k^c_{x\,N}, k^c_{y\,N}, k^c_{z\,N}\right)$	convective mass conductivity	material
31	$k^d_{x\,NS} := (\mu_{NS})^{-1} \cdot \left(v_{x\,N} \odot \left((V_N)^{-1} \odot \frac{\partial\, U_N}{\partial\, \mu_{NS}}\right)\right)$	diffusional mass conductivity in x-direction	material
32	$k^d_{y\,NS} := (\mu_{NS})^{-1} \cdot \left(v_{y\,N} \odot \left((V_N)^{-1} \odot \frac{\partial\, U_N}{\partial\, \mu_{NS}}\right)\right)$	diffusional mass conductivity in y-direction	material
33	$k^d_{z\,NS} := (\mu_{NS})^{-1} \cdot \left(v_{z\,N} \odot \left((V_N)^{-1} \odot \frac{\partial\, U_N}{\partial\, \mu_{NS}}\right)\right)$	diffusional mass conductivity in z-direction	material

Continued on next page

no	equation	documentation	layer
34	$k^d{}_{NS} := \text{Stack}\left(k^d_{x}{}_{NS}, k^d_{y}{}_{NS}, k^d_{z}{}_{NS}\right)$	diffusional mass condctivity	material
35	$h_{NS} := H_N \odot \left(n_{NS}\right)^{-1}$	partial molar enthalpies	material
36	$m_N := \_\lambda_S \overset{S \in NS}{\star} n_{NS}$	total mass	macroscopic
38	$\rho_N := m_N \,.\, \left(V_N\right)^{-1}$	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	$c_{NS} := \left(V_N\right)^{-1} \odot n_{NS}$	molar composition	macroscopic
48	$A_{yzN} := r_{yN} \,.\, r_{zN}$	cross sectional area yz	macroscopic
49	$A_{xzN} := r_{xN} \,.\, r_{zN}$	cross sectional area xz	macroscopic
50	$A_{xyN} := r_{xN} \,.\, r_{yN}$	cross sectional area xy	macroscopic
6	$p_N := \left(-\frac{\partial U_N}{\partial V_N}\right)$	thermodynamic pressure	physical
67	$\hat{V}_A := \left(\_\rho_N\right)^{-1} \,.\, \_k^c_{x}{}_N \,.\, A_{yzN} \,.\, D_{N,A} \overset{N}{\star} p_N$	volumetric flow	macroscopic
68	$\hat{n}^d{}_{AS} := A_{yzN} \odot \left(-\_k^d_{x}{}_{NS}\right) \,.\, D_{NS,AS} \overset{NS}{\star} \mu_{NS}$	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
7	$T_N := \frac{\partial U_N}{\partial S_N}$	temperature	physical
70	$\hat{H}^d{}_A := \left(F_{NS,AS} \overset{NS}{\star} \_h_{NS}\right) \overset{S \in AS}{\star} \hat{n}^d{}_{AS}$	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	$d_A := \text{sign}\left(F_{N,A} \overset{N}{\star} p_N\right)$	flow direction of convectional flow	macroscopic

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no	equation	documentation	layer
73	$c_{AS} := (0.5\,.\,(F_{NS,AS} - d_A \odot \lvert F_{NS,AS}\rvert)) \overset{NS}{\star} c_{NS}$	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	$\dot{n}_{NS} := \hat{n}^c{}_{NS} + \hat{n}^d{}_{NS} + \tilde{n}_{NS}$	differential species balance	macroscopic
77	$\hat{H}^c{}_A := \left(F_{NS,AS} \overset{NS}{\star} \_h_{NS}\right) \overset{S \in AS}{\star} \hat{n}^c{}_{AS}$	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
8	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	chemical potential	physical
80	$\hat{w}_N := F_{N,A} \overset{A}{\star} \hat{w}_A$	net work stream	macroscopic
81	$\hat{q}_{x\,A} := A_{yz\,N}\,.\,\_k^q_{x\,N}\,.\,D_{N,A} \overset{N}{\star} T_N$	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
83	$\dot{H}_N := \hat{H}^c{}_N + \hat{H}^d{}_N + \hat{q}_N + \hat{w}_N$	differential enthalpy balance	macroscopic
86	$n_{NS} := \int_{t^o}^{t^e} \dot{n}_{NS}\ dt + n^o{}_{NS}$	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
9	$H_N := U_N - p_N\,.\,V_N$	enthalpy	physical
93	$k^{e,\xi}{}_N := (R^e{}_N)^{-1}\,.\,\xi$	simple model for the electrical conductivity as a function of the additive	material
95	$Ue_N := (\_R^e{}_N)^{-1}\,.\,I_N$	electrical potential – voltage	macroscopic

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no	equation	documentation	layer
96	$\dot{U}^{e}{}_{N} := 1 \, . \, Ue_{N}$	Kirkhoff first law	macroscopic
97	$\dot{U}^{e}{}_{N} := Root \, (Ue_{N})$	Kirkhoff first law	macroscopic

35 Instantiate

no	equation	documentation	layer
1	$1 := \text{Instantiate}(\#, \#)$	numerical value 1	root
109	$x_{oN} := \text{Instantiate}(x_N, \#)$	initial state	control
119	$y^o{}_A := \text{Instantiate}(y^o{}_A, \#)$	set point	control
124	$c^o{}_{NK,KS} := \text{Instantiate}(c_{NK,KS}, \#)$	norming concentration	reactions
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
41	$E^a{}_{NK} := \text{Instantiate}(R \,.\, T_{NK}, \#)$	Arrhenius activation energy	reactions
5	$t^e := \text{Instantiate}(t, \#)$	end time	root
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	$R^e{}_N := (I_N)^{-1} \,.\, Ue_N$	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

36 Instantiation Equation

no	equation	documentation	layer
140	$\hat{V}_A := \text{Instantiate}(\hat{V}_A, \#)$	instantiation equation	macroscopic

37 Interface Link Equation

no	equation	documentation	layer
104	$\mapsto \xi := \xi$	interface equation	material –> control
105	$T_N := T_N$	interface equation	macroscopic –> control
112	$\_\xi := \xi$	interface equation	material –> macroscopic
114	$Ue_N := Ue_N$	interface equation	macroscopic –> control
131	$\tilde{n}_{NS} := \tilde{n}_{NS}$	interface equation	reactions –> macroscopic
151	$\_k^{d,Fick}{}_{NS} := k_{dF}ick_{NS}$	interface equation	material –> macroscopic
20	$\_\lambda_S := \lambda_S$	interface equation	material –> macroscopic
37	$m_N := m_N$	interface equation	macroscopic –> material
45	$c_{NS} := c_{NS}$	interface equation	macroscopic –> reactions
51	$\_\rho_N := \rho_N$	interface equation	material –> macroscopic
52	$\_h_{NS} := h_{NS}$	interface equation	material –> macroscopic

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no	equation	documentation	layer
53	$\_k^q_x{}_N := k^q_x{}_N$	interface equation	material –> macroscopic
54	$\_Cv_N := C_{V\,N}$	interface equation	material –> macroscopic
55	$\_k^q_y{}_N := k^q_y{}_N$	interface equation	material –> macroscopic
56	$\_k^q_z{}_N := k^q_z{}_N$	interface equation	material –> macroscopic
57	$\_k^q{}_N := k^q{}_N$	interface equation	material –> macroscopic
58	$\_k^c_x{}_N := k^c_x{}_N$	interface equation	material –> macroscopic
59	$\_Cp_N := C_{p\,N}$	interface equation	material –> macroscopic
60	$\_k^c_y{}_N := k^c_y{}_N$	interface equation	material –> macroscopic
61	$\_k^c_z{}_N := k^c_z{}_N$	interface equation	material –> macroscopic
62	$\_k^c{}_N := k^c{}_N$	interface equation	material –> macroscopic
63	$\_k^d_x{}_{NS} := k^d_x{}_{NS}$	interface equation	material –> macroscopic
64	$\_k^d_y{}_{NS} := k^d_y{}_{NS}$	interface equation	material –> macroscopic

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no	equation	documentation	layer
65	$\_k^{d}_{z}{}_{NS} := k^{d}_{z}{}_{NS}$	interface equation	material −> macroscopic
66	$\_k^{d}{}_{NS} := k^{d}{}_{NS}$	interface equation	material −> macroscopic
90	$I_{N} := I_{N}$	interface equation	macroscopic −> material
94	$\_R^{e}{}_{N} := k^{e,\xi}{}_{N}$	interface equation	material −> macroscopic
99	$I_{N} := I_{N}$	interface equation	macroscopic −> control