1 Variables

2 root

	var	symbol	documentation	type	units	tokens	eqs
5	$F_{N,A}$	`F`	incidence matrix of a directed graph	network		[]	
6	t	`t`	time	frame	s	[]	
7	t_o	`to`	starting time	frame	s	[]	4
8	t_e	`te`	end time	frame	s	[]	5
1	#	`value`	numerical value	constant		[]	
2	0	`zero`	numerical value zero	constant		[]	1
3	1	`one`	numerical value one	constant		[]	2
4	0.5	`onehalf`	numerical value one half	constant		[]	3

3 physical

	var	symbol	documentation	type	units	tokens	eqs
161	$P_{N,A}$	P_N_A	project node to arc for material properties	projection		[]	
9	r_{xN}	r_x	x-coordinate	frame	m	[]	
10	r_{yN}	r_y	y-coordinate	frame	m	[]	
23	r_{zN}	r_z	z-coordinate	frame	m	[]	
11	U_N	U	foundation state – internal energy	state	$kg\, m^2\, s^{-2}$	[]	
12	S_N	S	foundation state – entropy	state	$kg\, m^2\, K^{-1}\, s^{-2}$	[]	
13	V_N	V	foundation state – volume	state	m^3	[]	
18	H_N	H	enthalpy	state	$kg\, m^2\, s^{-2}$	[]	9 122 123
19	A_N	A	Helmholtz energy	state	$kg\, m^2\, s^{-2}$	[]	10
20	G_N	G	Gibbs energy	state	$kg\, m^2\, s^{-2}$	[]	11
42	n_{NS}	n	species molar mass	state	mol	[]	116
170	C	Charge	charge	state	$A\, s$	[]	
26	A^v	Avogadro	Avogadro number	constant	mol^{-1}	[]	
27	Bo_N	Boltzmann	Boltzmann constant	constant	$kg\, m^2\, K^{-1}\, s^{-2}$	[]	16
28	R_N	GasConstant	Gas constant	constant	$kg\, m^2\, mol^{-1}\, K^{-1}\, s^{-2}$	[]	17
15	p_N	p	thermodynamic pressure	effort	$kg\, m^{-1}\, s^{-2}$	[]	6 115
16	T_N	T	temperature	effort	K	[]	7 113
45	μ_{NS}	chem_pot	chemical potential	effort	$kg\, m^2\, mol^{-1}\, s^{-2}$	[]	32 114
179	Ue_N	Ue	electrical potential	effort	$kg\, m^2\, A^{-1} s^{-3}$	[]	176 181 188 195
21	v_{xN}	v_x	velocity in x-direction	secondaryState	ms^{-1}	[]	12

Continued on next page

	var	symbol	documentation	type	units	tokens	eqs
22	v_{yN}	`v_y`	velocity in y direction	secondaryState	ms^{-1}	[]	13
24	v_{zN}	`v_z`	velocity in z-direction	secondaryState	ms^{-1}	[]	14
25	v_N	`v`	velocity vector	secondaryState	ms^{-1}	[]	15

4 control

	var	symbol	documentation	type	units	tokens	eqs
139	m_A	mc	measurements	input		[]	
158	u_A	u	data link	input		[]	155
129	$I_{N,D}$	I_N_D	identity to shift from differential space integral space	network		[]	
130	$I_{A,D}$	I_A_D	identity to shift from differential space to arc	network		[]	
137	x_N	x	controller state	state		[]	112
138	$x^o{}_N$	xo	controller initial condition	state		[]	103
133	$C_{N,A}$	Cx	measurement matrix	constant		[]	144
134	$D_{N,D}$	Dx	event matrix (dimension issue)	constant		[]	145
135	$y^o{}_A$	setpoint	set point	constant		[]	146
136	D_A	D_A	event diagonal matrix (no dimension problem)	constant		[]	147
142	$A_{N,D}$	Ax	dynamic control matrix	constant	s^{-1}	[]	148
143	$B_{A,D}$	Bx	input matrix	constant	s^{-1}	[]	149
144	$\dot{x}_D$	dxdt	differential controller state	diffState	s^{-1}	[]	106
140	e_A	e	control error	algebraic		[]	104
155	y_A	y	controller output	algebraic		[]	150 153
187	I	measuredCurrent	measured current	algebraic	A	[]	190
188	U_N	measuredPotentialDiff	measured potential differences	algebraic	$kg\, m^2\, A^{-1} s^{-3}$	[]	191
189	a_N	measuredAdditive		algebraic		[]	192
190	R_N	compResistance	computed potential difference	algebraic	$kg\, m^2\, A^{-2} s^{-3}$	[]	193
191	$store$	store		algebraic		[]	194

5 reactions

	var	symbol	documentation	type	units	tokens	eqs
86	$N_{S,K}$	`N`	stoichiometric matrix	constant		[]	
87	E_{aNK}	`Ea`	Arrhenius's activation energy	constant	$kg\, m^2\, mol^{-1}\, s^{-2}$	[]	64
88	$K^o{}_K$	`Ko`	Arrhenius's frequency factor	constant	$m^{-3}\, mol\, s^{-1}$	[]	
89	K_{NK}	`K_NK`	Arrhenius reaction constant	constant	$m^{-3}\, mol\, s^{-1}$	[]	65
114	c_{KS}	`c_KS`	molar concentrations in reactive system	constant	$m^{-3}\, mol$	[]	90
115	$c^o{}_{KS}$	`co_KS`	norming molar concentrations	constant	$m^{-3}\, mol$	[]	91
116	ϕ_{KS}	`phi_KS`	probability of species to meet	constant		[]	92

6 material

	var	symbol	documentation	type	units	tokens	eqs
29	λ_S	`Mm`	species molecular masses	constant	$kg\, mol^{-1}$	[]	142
175	ξ_N	`additiveFraction`	active additive fraction	constant		[]	171
30	$C_{p\,N}$	`Cp`	total heat capacity at constant pressure	property	$kg\, m^2\, K^{-1}\, s^{-2}$	[]	18
31	$C_{v\,N}$	`Cv`	total heat capacity at constant volume	property	$kg\, m^2\, K^{-1}\, s^{-2}$	[]	19
34	$k^q_x{}_N$	`kq_x`	thermal conductivity in x-direction	property	$kg\, K^{-1}\, s^{-3}$	[]	22 131
35	$k^q_y{}_N$	`kq_y`	thermal conductivity in y-direction	property	$kg\, K^{-1}\, s^{-3}$	[]	23 132
36	$k^q_z{}_N$	`kq_z`	thermal conductivity in z-direction	property	$kg\, K^{-1}\, s^{-3}$	[]	24 133
37	$k^q{}_N$	`kq`	Carthesian thermal conductivity vector	property	$kg\, K^{-1}\, s^{-3}$	[]	25
50	$k^c_x{}_N$	`kc_x`	convective mass convectivity in x-direction	property	$m^{-1}\, s$	[]	37 134
51	$k^c_y{}_N$	`kc_y`	convective mass convectivity in y-direction	property	$m^{-1}\, s$	[]	38 135
52	$k^c_z{}_N$	`kc_z`	convective mass convectivity in z-direction	property	$m^{-1}\, s$	[]	39 136
53	$k^c{}_N$	`kc`	Cartesian convective mass convectivity vector	property	$m^{-1}\, s$	[]	40
54	$k^d_x{}_{NS}$	`kd_x`	diffusional mass conductivity in x-direction	property	$kg^{-1}\, m^{-4}\, mol^2\, s$	[]	41 137
55	$k^d_y{}_{NS}$	`kd_y`	diffusional mass conductivity in y-direction	property	$kg^{-1}\, m^{-4}\, mol^2\, s$	[]	42 138
56	$k^d_z{}_{NS}$	`kd_z`	diffusional mass conductivity in z-direction	property	$kg^{-1}\, m^{-4}\, mol^2\, s$	[]	43
57	$k^d{}_{NS}$	`kd`	Cartesian dffusional mass conductivity vector	property	$kg^{-1}\, m^{-4}\, mol^2\, s$	[]	44
58	h_{NS}	`h`	partial molar enthalpies	property	$kg\, m^2\, mol^{-1}\, s^{-2}$	[]	45 139

Continued on next page

	var	symbol	documentation	type	units	tokens	eqs
71	ρ_N	`density`	mass density	property	$kg\,m^{-3}$	[]	49 154
148	cp_N	`cp`	specific heat capacity at constant pressure	property	$m^2\,K^{-1}\,s^{-2}$	[]	120 140
149	cv_N	`cv`	specific heat capacity at constant volume	property	$m^2\,K^{-1}\,s^{-2}$	[]	121 141
154	θ	`data`	available data set	property		[]	143
181	${R^e}_N$	`elResistance`	electrical conductivity	property	$kg\,m^2\,A^{-2}s^{-3}$	[]	178 180
182	${k^{e,\xi}}_N$	`elConducC`	electrical conductivity of electrolyte simple model	property	$kg^{-1}\,m^{-2}\,A^2s^3$	[]	179
186	${k^e}_N$	`elConduc`	electrical conductivity	property	$kg^{-1}\,m^{-2}\,A^2s^3$	[]	187

7 macroscopic

	var	symbol	documentation	type	units	tokens	eqs
65	d_A	`d`	direction of convective flow	transport		[]	46
98	$\hat{V}_A$	`fV`	volumetric flow in x-direction	transport	$m^3\,s^{-1}$	[]	74
104	$\hat{n}^d{}_{AS}$	`fnd_AS`	diffusional mass transfer per arc	transport	$mol\,s^{-1}$	[]	80
105	$\hat{n}^d{}_{NS}$	`fnd`	net diffusional mass transfer	transport	$mol\,s^{-1}$	[]	81
106	$\hat{H}^d{}_A$	`fHd_A`	enthalpy flow due to mass diffusion per arc	transport	$kg\,m^2\,s^{-3}$	[]	82
107	$\hat{H}^d{}_N$	`fHd`	net enthalpy flow due to mass diffusion	transport	$kg\,m^2\,s^{-3}$	[]	83
109	c_{AS}	`c_AS`	moler concentration in convective arc	transport	$m^{-3}\,mol$	[]	85
110	$\hat{n}^c{}_{AS}$	`fnc_AS`	convective molar mass flow per arc	transport	$mol\,s^{-1}$	[]	86
111	$\hat{n}^c{}_{NS}$	`fnc`	net convective molar mass flow	transport	$mol\,s^{-1}$	[]	87
120	$\hat{H}^c{}_A$	`fHc_A`	enthalpy flow due to convective mass flow	transport	$kg\,m^2\,s^{-3}$	[]	96
121	$\hat{H}^c{}_N$	`fHc`	net enthalpy flow due to convective mass flow	transport	$kg\,m^2\,s^{-3}$	[]	97
122	$\hat{w}_A$	`fw_A`	example of work flow	transport	$kg\,m^2\,s^{-3}$	[]	98
123	$\hat{w}_N$	`fw`	net work flow	transport	$kg\,m^2\,s^{-3}$	[]	99
124	$\hat{q}_A$	`fq_A_x`	heat flow in x-direction	transport	$kg\,m^2\,s^{-3}$	[]	100
125	$\hat{q}_N$	`fq`	net heat flow	transport	$kg\,m^2\,s^{-3}$	[]	101
185	i_A	`courrentA`	current in arcs is the same in the circuit	transport	A	[]	186
95	$A_{yz\,N}$	`Ayz`	cross sectional area in x-direction	geometry	m^2	[]	71
96	$A_{xz\,N}$	`Axz`	cross sectional area in y direction	geometry	m^2	[]	72
97	$A_{xy\,N}$	`Axy`	cross sectional area in z-direction	geometry	m^2	[]	73
73	$F_{NS,AS}$	`F_NS_AS`	incidence matrix of directed graphs for for species NS x AS	network		[]	51
59	$P_{NS,AS}$	`P_NS_AS`	node species to arc species projection	projection		[]	
60	$P_{K,NK}$	`P_K_NK`	projection of conversion to node x conversion	projection		[]	

Continued on next page

	var	symbol	documentation	type	units	tokens	eqs
61	$P_{S,NS}$	P_S_NS	projection species to conversion x species	projection		[]	
62	$P_{N,NK}$	P_N_NK	projection node to node x conversion	projection		[]	
63	$P_{NK,KS}$	P_NK_KS	projection node x conversion to conversion x species	projection		[]	
64	$P_{NS,KS}$	P_NS_KS	projection node x species to conversion x species	projection		[]	
168	$P_{A,NS}$	P_NS_A	projection of node species to arc for conductivity	projection		[]	
127	$D_{N,A}$	D	difference operator	differenceOperator		[]	
128	$D_{NS,AS}$	D_NS_AS	block difference operator	differenceOperator		[]	
153	phi	phi	state for mass and energy	state		[]	130
145	$T_{ref\,N}$	T_ref	refernce temperature	constant	K	[]	117
150	${n^o}_{NS}$	no	initial condition for species mass in nodes	constant	mol	[]	124
151	${H^o}_N$	Ho	initial condition for enthalpy in nodes	constant	$kg\, m^2\, s^{-2}$	[]	125
164	1_{NS}	ones_NS	block vector of ones	constant		[]	
177	1_N	one_N	vector of ones of length N	constant		[]	
184	1_A	one_A	vector of ones with length A	constant		[]	
69	m_N	m	mass	secondaryState	kg	[]	47
108	c_{NS}	c	molar concentration	secondaryState	$m^{-3}\, mol$	[]	84 127
152	ψ	intensities	collected intensities	secondaryState		[]	126
165	$c_{norm\,N}$	cnorm	moles per node	secondaryState	$m^{-3}\, mol$	[]	161
166	ξ_{NS}	x_frac	mole fractions	secondaryState		[]	162
77	T_{NK}	T_NK	temperature in reactive systems	conversion	K	[]	55
93	$N_{NS,NK}$	N_NS_NK	extended stoichiometric matrix	conversion		[]	69
117	ξ_{NK}	xi	extend of reaction per volume	conversion	$m^{-3}\, mol\, s^{-1}$	[]	93

Continued on next page

	var	symbol	documentation	type	units	tokens	eqs
118	$\tilde{n}_{NS}$	`pn`	production term	conversion	$mol\, s^{-1}$	[]	94
119	$\dot{n}_{NS}$	`dndt`	differential molar mass balance	diffState	$mol\, s^{-1}$	[]	95 129
126	$\dot{H}_{N}$	`dHdt`	differential enthalpy balance	diffState	$kg\, m^{2}\, s^{-3}$	[]	102 128
183	$\dot{U^e}_{N}$	`dUedt`	Kirkhoff first law	diffState	$kg\, m^{2}\, A^{-1} s^{-3}$	[]	182 183
180	i	`current`	electrical current	internalTransport	A	[]	177 185 189

8 solid

	var	symbol	documentation	type	units	tokens	eqs

9 fluid

	var	symbol	documentation	type	units	tokens	eqs

10 liquid

	var	symbol	documentation	type	units	tokens	eqs

11 gas

	var	symbol	documentation	type	units	tokens	eqs

12 control–control

	var	symbol	documentation	type	units	tokens	eqs

13 gas–liquid

	var	symbol	documentation	type	units	tokens	eqs

14 gas–gas

	var	symbol	documentation	type	units	tokens	eqs

15 liquid–liquid

	var	symbol	documentation	type	units	tokens	eqs

16 gas–solid

	var	symbol	documentation	type	units	tokens	eqs

17 solid–solid

	var	symbol	documentation	type	units	tokens	eqs

18 liquid–solid

	var	symbol	documentation	type	units	tokens	eqs

19 material–material

	var	symbol	documentation	type	units	tokens	eqs

20 reactions–reactions

	var	symbol	documentation	type	units	tokens	eqs

21 Equations

22 Generic

no	equation	documentation	layer
1	$0 := \text{Instantiate}(\#, \#)$	numerical value zero	root
2	$1 := \text{Instantiate}(\#, \#)$	numerical value one	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
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 energy	physical
12	$v_{x\,N} := \frac{\partial r_{x\,N}}{\partial t}$	velocity in x-direction	physical
13	$v_{y\,N} := \frac{\partial r_{y\,N}}{\partial t}$	velocity in y direction	physical
14	$v_{z\,N} := \frac{\partial r_{z\,N}}{\partial t}$	velocity in z-direction	physical
15	$v_N := \text{Stack}\left(v_{x\,N}, v_{y\,N}, v_{z\,N}\right)$	velocity vector	physical
16	$Bo_N := \text{Instantiate}(S_N, \#)$	Boltzmann constant	physical
17	$R_N := A^v \, . \, Bo_N$	Gas constant	physical

Continued on next page

no	equation	documentation	layer
18	$C_{p\,N} := \frac{\partial H_N}{\partial T_N}$	total heat capacity	material
19	$C_{v\,N} := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	material
22	$k^q_{x\,N} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{x\,N}$	thermal conductivity in x-direction	material
23	$k^q_{y\,N} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{y\,N}$	thermal conductivity in y-direction	material
24	$k^q_{z\,N} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{z\,N}$	thermal conductivity in z-direction	material
25	$k^q{}_N := \text{Stack}\left(k^q_{x\,N}, k^q_{y\,N}, k^q_{z\,N}\right)$	Carthesian thermal conductivity vector	material
32	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	chemical potential	physical
37	$k^c_{x\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{x\,N}$	convective mass convectivity in x-direction	material
38	$k^c_{y\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{y\,N}$	convective mass convectivity in y-direction	material
39	$k^c_{z\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{z\,N}$	convective mass convectivity in z-direction	material
40	$k^c{}_N := \text{Stack}\left(k^c_{x\,N}, k^c_{y\,N}, k^c_{z\,N}\right)$	Cartesian convective mass convectivity vector	material
41	$k^d_{x\,NS} := (\mu_{NS})^{-1} \cdot \left(v_{x\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in x-direction	material
42	$k^d_{y\,NS} := (\mu_{NS})^{-1} \cdot \left(v_{y\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in y-direction	material
43	$k^d_{z\,NS} := (\mu_{NS})^{-1} \cdot \left(v_{z\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in z-direction	material

Continued on next page

no	equation	documentation	layer
44	$k^d{}_{NS} := \text{Stack}\left(k^d_{x NS}, k^d_{y NS}, k^d_{z NS}\right)$	Cartesian dffusional mass conductivity vector	material
45	$h_{NS} := H_N \odot (n_{NS})^{-1}$	partial molar enthalpies	material
46	$d_A := \text{sign}\left(F_{N,A} \overset{N}{\star} p_N\right)$	direction of convective flow	macroscopic
47	$m_N := \lambda_S \overset{S \in NS}{\star} n_{NS}$	mass	macroscopic
49	$\rho_N := m_N \,.\, (V_N)^{-1}$	mass density	material
51	$F_{NS,AS} := F_{N,A} \odot P_{NS,AS}$	incidence matrix of directed graphs for for species NS x AS	macroscopic
55	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature in reactive systems	macroscopic
64	$E_{a NK} := \text{Instantiate}(P_{N,NK} \overset{N}{\star} R_N \,.\, T_{NK}, \#)$	Arrhenius's activation energy	reactions
65	$K_{NK} := K^o{}_K \odot exp((-E_{a NK}) \,.\, \left(R_N \overset{N}{\star} P_{N,NK} \,.\, T_{NK}\right)^{-1})$	Arrhenius reaction constant	reactions
69	$N_{NS,NK} := P_{S,NS} \overset{S}{\star} \left(\left(P_{K,NK} \,.\, T_{NK} \,.\, (T_{NK})^{-1}\right) \overset{K}{\star} N_{S,K}\right)$	extended stoichiometric matrix	macroscopic
71	$A_{yz N} := r_{y N} \,.\, r_{z N}$	cross sectional area in x-direction	macroscopic
72	$A_{xz N} := r_{x N} \,.\, r_{z N}$	cross sectional area in y direction	macroscopic
73	$A_{xy N} := r_{x N} \,.\, r_{y N}$	cross sectional area in z-direction	macroscopic
74	$\hat{V}_A := (\rho_N)^{-1} \,.\, k^c_{x N} \,.\, A_{yz N} \,.\, D_{N,A} \overset{N}{\star} p_N$	volumetric flow in x-direction	macroscopic
80	$\hat{n}^d{}_{AS} := A_{yz N} \odot \left(-k^d_{x NS}\right) \,.\, D_{NS,AS} \overset{NS}{\star} \mu_{NS}$	diffusional mass transfer per arc	macroscopic
81	$\hat{n}^d{}_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^d{}_{AS}$	net diffusional mass transfer	macroscopic

Continued on next page

no	equation	documentation	layer
82	$\hat{H}^d{}_A := \left(F_{NS,AS} \overset{NS}{\star} h_{NS}\right) \overset{S\in AS}{\star} \hat{n}^d{}_{AS}$	enthalpy flow due to mass diffusion per arc	macroscopic
83	$\hat{H}^d{}_N := F_{N,A} \overset{A}{\star} \hat{H}^d{}_A$	net enthalpy flow due to mass diffusion	macroscopic
84	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar concentration	macroscopic
85	$c_{AS} := (0.5 \,.\, (F_{NS,AS} - d_A \odot \lvert F_{NS,AS}\rvert)) \overset{NS}{\star} c_{NS}$	moler concentration in convective arc	macroscopic
86	$\hat{n}^c{}_{AS} := \hat{V}_A \odot c_{AS}$	convective molar mass flow per arc	macroscopic
87	$\hat{n}^c{}_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^c{}_{AS}$	net convective molar mass flow	macroscopic
90	$c_{KS} := c_{NS} \overset{NS}{\star} P_{NS,KS}$	molar concentrations in reactive system	reactions
91	$c^o{}_{KS} := \text{Instantiate}(c_{KS}, \#)$	norming molar concentrations	reactions
92	$\phi_{KS} := \prod \left(c_{KS} \,.\, (c^o{}_{KS})^{-1}\right)$	probability of species to meet	reactions
93	$\xi_{NK} := K_{NK} \,.\, P_{NK,KS} \overset{KS}{\star} \phi_{KS}$	extend of reaction per volume	macroscopic
94	$\tilde{n}_{NS} := V_N \odot \left(N_{NS,NK} \overset{NK}{\star} \xi_{NK}\right)$	production term	macroscopic
95	$\dot{n}_{NS} := \hat{n}^c{}_{NS} + \hat{n}^d{}_{NS} + \tilde{n}_{NS}$	differential molar mass balance	macroscopic
96	$\hat{H}^c{}_A := \left(F_{NS,AS} \overset{NS}{\star} h_{NS}\right) \overset{S\in AS}{\star} \hat{n}^c{}_{AS}$	enthalpy flow due to convective mass flow	macroscopic
97	$\hat{H}^c{}_N := F_{N,A} \overset{A}{\star} \hat{H}^c{}_A$	net enthalpy flow due to convective mass flow	macroscopic
98	$\hat{w}_A := \text{Instantiate}(\hat{H}^c{}_A, \#)$	example of work flow	macroscopic
99	$\hat{w}_N := F_{N,A} \overset{A}{\star} \hat{w}_A$	net work flow	macroscopic

Continued on next page

no	equation	documentation	layer
100	$\hat{q}_A := A_{yz\,N} \,.\, k^q_{x\,N} \,.\, D_{N,A} \overset{N}{\star} T_N$	heat flow in x-direction	macroscopic
101	$\hat{q}_N := F_{N,A} \overset{A}{\star} \hat{q}_A$	net heat flow	macroscopic
102	$\dot{H}_N := \hat{H}^c{}_N + \hat{H}^d{}_N + \hat{q}_N + \hat{w}_N$	differential enthalpy balance	macroscopic
103	$x^o{}_N := \text{Instantiate}(x_N, \#)$	controller initial condition	control
104	$e_A := m_A - y^o{}_A$	control error	control
106	$\dot{x}_D := A_{N,D} \overset{N}{\star} x_N + B_{A,D} \overset{A}{\star} e_A$	differential controller state	control
112	$x_N := \int_{t_o}^{t_e} I_{N,D} \overset{D}{\star} \dot{x}_D \;\; dt$	controller state	control
113	$T_N := \text{Instantiate}(T_N, \#)$	temperature	physical
114	$\mu_{NS} := \text{Instantiate}(\mu_{NS}, \#)$	chemical potential	physical
115	$p_N := \text{Instantiate}(p_N, \#)$	thermodynamic pressure	physical
116	$n_{NS} := \int_{t_o}^{t_e} \dot{n}_{NS} \;\; dt + n^o{}_{NS}$	species molar mass	macroscopic
117	$T_{ref\,N} := \text{Instantiate}(T_N, \#)$	refernce temperature	macroscopic

Continued on next page

no	equation	documentation	layer
120	$cp_N := C_{pN} \, . \, (m_N)^{-1}$	specific heat capacity at constant pressure	material
121	$cv_N := C_{vN} \, . \, (m_N)^{-1}$	specific heat capacity at constant volume	material
122	$H_N := m_N \, . \, \int_{T_{ref\,N}}^{T_N} cp_N \; d\,T_N$	enthalpy	macroscopic
123	$H_N := \int_{t_o}^{t_e} \dot{H}_N \; d\,t + H^o{}_N$	enthalpy	macroscopic
124	$n^o{}_{NS} := \text{Instantiate}(n_{NS}, \#)$	initial condition for species mass in nodes	macroscopic
125	$H^o{}_N := \text{Instantiate}(H_N, \#)$	initial condition for enthalpy in nodes	macroscopic
126	$\psi := \text{MixedStack}\,(p_N, T_N, \mu_{NS}, c_{NS})$	collected intensities	macroscopic
127	$c_{NS} := \text{Instantiate}(c_{NS}, \#)$	molar concentration	macroscopic
128	$\dot{H}_N := \text{Instantiate}(\dot{H}_N, 0)$	differential enthalpy balance	macroscopic
129	$\dot{n}_{NS} := \text{Instantiate}(\dot{n}_{NS}, 0)$	differential molar mass balance	macroscopic
130	$phi := \text{MixedStack}\,(n_{NS}, H_N)$	state for mass and energy	macroscopic
131	$k^q_{x\,N} := \text{Instantiate}(k^q_{x\,N}, \#)$	thermal conductivity in x-direction	material

Continued on next page

no	equation	documentation	layer
132	$k^q_{y\,N} := \text{Instantiate}(k^q_{y\,N}, \#)$	thermal conductivity in y-direction	material
133	$k^q_{z\,N} := \text{Instantiate}(k^q_{z\,N}, \#)$	thermal conductivity in z-direction	material
134	$k^c_{x\,N} := \text{Instantiate}(k^c_{x\,N}, \#)$	convective mass convectivity in x-direction	material
135	$k^c_{y\,N} := \text{Instantiate}(k^c_{y\,N}, \#)$	convective mass convectivity in y-direction	material
136	$k^c_{z\,N} := \text{Instantiate}(k^c_{z\,N} \,.\, \#, -)$	convective mass convectivity in z-direction	material
137	$k^d_{x\,NS} := \text{Instantiate}(k^d_{x\,NS}, \#)$	diffusional mass conductivity in x-direction	material
138	$k^d_{y\,NS} := \text{Instantiate}(k^d_{y\,NS}, \#)$	diffusional mass conductivity in y-direction	material
139	$h_{NS} := \text{Instantiate}(h_{NS}, \#)$	partial molar enthalpies	material
140	$cp_N := \text{Instantiate}(cp_N, \#)$	specific heat capacity at constant pressure	material
141	$cv_N := \text{Instantiate}(cv_N, \#)$	specific heat capacity at constant volume	material
142	$\lambda_S := \text{Instantiate}(\lambda_S, \#)$	species molecular masses	material
143	$\theta := \text{MixedStack}\left(k^q{}_N, k^c{}_N, k^d{}_{NS}, h_{NS}, cp_N, cv_N, \lambda_S, \rho_N\right)$	available data set	material

Continued on next page

no	equation	documentation	layer
144	$C_{N,A} := \text{Instantiate}(C_{N,A}, \#)$	measurement matrix	control
145	$D_{N,D} := \text{Instantiate}(D_{N,D}, \#)$	event matrix (dimension issue)	control
146	$y^o{}_A := \text{Instantiate}(y^o{}_A, \#)$	set point	control
147	$D_A := \text{Instantiate}(D_A, \#)$	event diagonal matrix (no dimension problem)	control
148	$A_{N,D} := \text{Instantiate}(A_{N,D}, \#)$	dynamic control matrix	control
149	$B_{A,D} := \text{Instantiate}(B_{A,D}, \#)$	input matrix	control
150	$y_A := C_{N,A} \overset{N}{\star} x_N + D_A \,.\, e_A$	controller output	control
153	$y_A := D_A \,.\, e_A$	controller output	control
154	$\rho_N := \text{Instantiate}(\rho_N, \#)$	mass density	material
155	$u_A := 1 \,.\, y_A$	data link	control
161	$c_{norm\,N} := 1_{NS} \overset{S \in NS}{\star} c_{NS}$	moles per node	macroscopic
162	$\xi_{NS} := (c_{norm\,N})^{-1} \odot c_{NS}$	mole fractions	macroscopic

Continued on next page

no	equation	documentation	layer
171	$\xi_N := \text{Instantiate}(\xi_N, \#)$	active additive fraction	material
176	$Ue_N := (C)^{-1} \, . U_N$	electrical potential	physical
177	$i := \frac{dC}{dt}$	electrical current	macroscopic
178	$R^e{}_N := (i)^{-1} \, . Ue_N$	electrical conductivity	material
179	$k^{e,\xi}{}_N := (R^e{}_N)^{-1} \, . \xi_N$	electrical conductivity of electrolyte simple model	material
180	$R^e{}_N := \text{Instantiate}(R^e{}_N, \#)$	electrical conductivity	material
181	$Ue_N := \left(k^{e,\xi}{}_N\right)^{-1} \, . i$	electrical potential	macroscopic
182	$\dot{U}^e{}_N := 1_N \, . Ue_N$	Kirkhoff first law	macroscopic
183	$\dot{U}^e{}_N := \text{Instantiate}(\dot{U}^e{}_N, 0)$	Kirkhoff first law	macroscopic
185	$i := Root\left(\dot{U}^e{}_N\right)$	electrical current	macroscopic
186	$i_A := 1_A \, . i$	current in arcs is the same in the circuit	macroscopic
187	$k^e{}_N := (R^e{}_N)^{-1}$	electrical conductivity	material

Continued on next page

no	equation	documentation	layer
188	$Ue_N := {R^e}_N \,.\, i$	electrical potential	macroscopic
189	$i := Root\,(Ue_N)$	electrical current	macroscopic
190	$I := i$	measured current	control
191	$U_N := Ue_N$	measured potential differences	control
192	$a_N := \xi_N$	var doc :	control
193	$R_N := (I)^{-1} \,.\, U_N$	computed potential difference	control
194	$store := \mathrm{MixedStack}\,(I, U_N, R_N, a_N)$	var doc :	control
195	$Ue_N := \mathrm{Instantiate}(Ue_N, \#)$	electrical potential	macroscopic