1 Variables

2 root

	var	symbol	documentation	type	units	eqs
2	$F_{N,A}$	`F`	incidence matrix	network		
15	$S_{N,q,t}$	`S_Nqt`	selection matrix or splitter	network		
5	${F^{source}}_{A,I}$	`F_AI_source`	incidence matrix AI source	network		
6	${F^{sink}}_{A,I}$	`F_AI_sink`	incidence matrix AI sink	network		
3	${F^{source}}_{N,I}$	`F_NI_source`	incidence matrix NI source	network		
10	$S_{I,q}$	`S_Iq`	selection matrix interface to control output	network		
19	$A_{N,p,q}$	`A_Npq`	mapping from inputs to outputs	network		
12	$S_{A,p}$	`S_Ap`	selection matrix interface species-related measures	network		
7	${F^{source}}_{N,A}$	`F_NA_source`	incidence matrix NA source	network		
9	$S_{I,p}$	`S_Ip`	selection matrix interface to control input	network		
8	${F^{sink}}_{N,A}$	`F_NA_sink`	incidence matrix NA sink	network		
17	cz_N	`cz_N`	output from control	network		
4	${F^{sink}}_{N,I}$	`F_NI_sink`	incidence matrix NI sink	network		
11	$I_{t,u}$	`I_tu`	identity mapping from <t> to <u>	network		
14	$S_{N,p,q}$	`S_Npu`	selection matrix for stacker	network		
16	mv_I	`mv_I`	interface variable macro −> control	network		
27	$I_{N,A}$	`I_NA`	identity mapping from <N> to <A>	network		
18	cz_I	`cz_I`	interface variable macro −> control	network		
22	$y_{N,t,u}$	`y_Ntu`	output signal in control domain	network		
20	$A_{N,t,u}$	`A_Ntu`	mapping from input elements to outputs	network		
21	$u_{N,t,u}$	`u_Ntu`	input signal in control domain	network		
13	$S_{I,q}$	`S_Aq`	selection matrix arcs to outputs	network		

Continued on next page

	var	symbol	documentation	type	units	eqs
107	Δt	`t_interval`	time interval	frame	s	6
105	t^o	`to`	starting time	frame	s	4
106	t^e	`te`	end time	frame	s	5
1	t	`t`	time	frame	s	
103	1	`one`	numerical value one	constant		2
102	0	`zero`	numerical value zero	constant		1
101	#	`value`	numerical value	constant		
104	0.5	`oneHalf`	numerical value one half	constant		3

3 physical

	var	symbol	documentation	type	units	eqs
23	$r_{x\,N}$	`r_x`	x-coordinate	frame	m	
24	$r_{y\,N}$	`r_y`	y-coordinate	frame	m	
25	$r_{z\,N}$	`r_z`	z-coordinate	frame	m	
110	V_{N}	`V`	volume	state	m^{3}	7
144	C_{N}	`C`	fundamental state – charge	state	$A\,s$	
108	U_{N}	`U`	fundamental state – internal energy	state	$kg\,m^{2}\,s^{-2}$	
137	m_{N}	`m`	mass	state	kg	30
109	S_{N}	`S`	fundamental state – internal entropy	state	$kg\,m^{2}\,K^{-1}\,s^{-2}$	
111	$n_{N,S}$	`n`	fundamental state – molar mass	state	mol	93
122	k^{B}	`Boltz`	Boltzmann constant	constant	$kg\,m^{2}\,K^{-1}\,s^{-2}$	
123	R	`R`	gas constant	constant	$kg\,m^{2}\,mol^{-1}\,K^{-1}\,s^{-2}$	17
132	λ_{S}	`Mm`	molecular masses	constant	$kg\,mol^{-1}$	
121	N^{A}	`Avo`	Avogadro constant	constant	mol^{-1}	
150	$A_{yz\,N}$	`Ayz`	cross sectional area yz	secondaryState	m^{2}	42
143	ρ_{N}	`rho`	density	secondaryState	$kg\,m^{-3}$	36
149	$A_{xz\,N}$	`Axz`	cross sectional are xz	secondaryState	m^{2}	41
148	$A_{xy\,N}$	`Axy`	cross sectional area xy	secondaryState	m^{2}	40

4 macroscopic

	var	symbol	documentation	type	units	eqs
160	$\hat{n}^{c}_{x\,A,S}$	`fnc_x`	molar convective flow in x-direction	transport	$mol\, s^{-1}$	52
158	$c_{A,S}$	`c_AS`	concentration in convective event-dynamic flow	transport	$m^{-3}\, mol$	50
205	$\dot{H}^{d}_{x\,N}$	`aHnd_x`	accumulation of enthalpy due to diffusional mass flow in x-direction	transport	$kg\, m^{2}\, s^{-3}$	100
195	$\dot{n}^{d}_{x\,N,S}$	`and_x`	accumulation due to diffusion in x-direction	transport	$mol\, s^{-1}$	88
207	$\dot{H}^{d}_{z\,N}$	`aHnd_z`	accumulation of enthalpy due to diffusional mass flow in z-direction	transport	$kg\, m^{2}\, s^{-3}$	102
152	$\hat{q}_{y\,A}$	`fq_y`	heat flow in y-direction	transport	$kg\, m^{2}\, s^{-3}$	44
212	$\dot{n}^{d}_{y\,N,S}$	`and_y`	accumulation due to diffusion in y-direction	transport	$mol\, s^{-1}$	107
204	$\dot{H}^{c}_{x\,N}$	`aHnc_x`	accumulation of enthalpy due to convective mass flow in x-direction	transport	$kg\, m^{2}\, s^{-3}$	99
213	$\dot{n}^{d}_{z\,N,S}$	`and_z`	accumulation due to diffusion in z-direction	transport	$mol\, s^{-1}$	108
208	$\dot{q}_{x\,N}$	`aq_x`	accumulation due to heat flow in x-direction	transport	$kg\, m^{2}\, s^{-3}$	103
214	$\dot{w}_{N}$	`aw`	accumulation of enthalpy due to work flow	transport	$kg\, m^{2}\, s^{-3}$	109
155	$\hat{n}^{d}_{y\,A,S}$	`fnd_y`	diffusion flow in y-direction	transport	$mol\, s^{-1}$	47 90
154	$\hat{n}^{d}_{x\,A,S}$	`fnd_x`	diffusion flow in x-direction	transport	$mol\, s^{-1}$	46 89
209	$\dot{q}_{y\,N}$	`aq_y`	accumulation due to heat flow in y-direction	transport	$kg\, m^{2}\, s^{-3}$	104
210	$\dot{q}_{z\,N}$	`aq_z`	accumulation due to heat flow in z-direction	transport	$kg\, m^{2}\, s^{-3}$	105
194	$\dot{n}^{c}_{x\,N,S}$	`anc_x`	accumulation of molar mass due to convection	transport	$mol\, s^{-1}$	87
159	$\hat{V}_{A}$	`fV`	volumetric flow in x-direction	transport	$m^{3}\, s^{-1}$	51
157	d_{A}	`d`	flow direction of convective flow	transport		49
153	$\hat{q}_{z\,A}$	`fq_z`	heat flow in z-direction	transport	$kg\, m^{2}\, s^{-3}$	45
156	$\hat{n}^{d}_{z\,A,S}$	`fnd_z`	diffusion flow in z-direction	transport	$mol\, s^{-1}$	48 91

Continued on next page

	var	symbol	documentation	type	units	eqs
206	$\dot{H}^{d}_{y\,N}$	`aHnd_y`	accumulation of enthalpy due to diffusional mass flow in y-direction	transport	$kg\,m^{2}\,s^{-3}$	101
151	$\hat{q}_{x\,A}$	`fq_x`	heat flow in x-direction	transport	$kg\,m^{2}\,s^{-3}$	43
211	$\hat{w}_{A}$	`fw`	a fixed work flow to start with	transport	$kg\,m^{2}\,s^{-3}$	106
234	$fm_{N,A}$	`fm`	convective mass flow	transport	$kg\,s^{-1}$	133
189	ρ_{A}	`rhoA`	density in arc	properties	$kg\,m^{-3}$	82
191	$\hat{k}^{d,Fick}_{y}{}_{A,S}$	`kdAFick_y`	Fick diffusivity in arc and y-direction	properties	ms^{-1}	84
184	$k^{c}_{y\,A}$	`kcA_y`	convective mass conductivity in arc and y-direction	properties	$m^{-1}\,s$	77
192	$\hat{k}^{d,Fick}_{z}{}_{A,S}$	`kdAFick_z`	Fick diffusivity in arc and z-direction	properties	ms^{-1}	85
183	$k^{c}_{x\,A}$	`kcA_x`	convective mass conductivity in arc and x diretion	properties	$m^{-1}\,s$	76
186	$k^{q}_{x\,A}$	`kqA_x`	thermal conductivity in arc and x-direction	properties	$kg\,K^{-1}\,s^{-3}$	79
193	$h_{A,S}$	`hA`	partial molar enthalpiies in arc	properties	$kg\,m^{2}\,mol^{-1}\,s^{-2}$	86
188	$k^{q}_{z\,A}$	`kqA_z`	thermal conductivity in arc and z-direction	properties	$kg\,K^{-1}\,s^{-3}$	81
182	$k^{d}_{z\,A,S}$	`kdA_z`	diffusivity in arc and z-direction	properties	$kg^{-1}\,m^{-4}\,mol^{2}\,s$	75
180	$k^{d}_{x\,A,S}$	`kdA_x`	diffusivity in arc and x-direction	properties	$kg^{-1}\,m^{-4}\,mol^{2}\,s$	73
185	$k^{c}_{z\,A}$	`kcA_z`	convecive mass conductivity in arc and y-direction	properties	$m^{-1}\,s$	78
187	$k^{q}_{y\,A}$	`kqA_y`	thermal conductivity in arc and y-direction	properties	$kg\,K^{-1}\,s^{-3}$	80
190	$\hat{k}^{d,Fick}_{x}{}_{A,S}$	`kdAFick_x`	Fick's diffusivity in arc and x-direction	properties	ms^{-1}	83
219	$R^{e}{}_{N}$	`elResistant`	electrical resistant	properties	$kg\,m^{2}\,A^{-2}s^{-3}$	115
181	$k^{d}_{y\,A,S}$	`kdA_y`	diffusivity in arc and y-direction	properties	$kg^{-1}\,m^{-4}\,mol^{2}\,s$	74
116	A_{N}	`A`	Helmholtz energy	state	$kg\,m^{2}\,s^{-2}$	12
115	H_{N}	`H`	Enthalpy	state	$kg\,m^{2}\,s^{-2}$	11 112
117	G_{N}	`G`	Gibbs free energy	state	$kg\,m^{2}\,s^{-2}$	13
203	$n^{o}{}_{N,S}$	`no`	initial mass	state	mol	98

Continued on next page

	var	symbol	documentation	type	units	eqs
216	${H^o}_N$	Ho	initial enthalpy	state	$kg\,m^2\,s^{-2}$	111
161	${\mu^o}_{N,S}$	chemPotStandard	instantiating standard chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	53
217	${U^e}_N$	Ue	electrical potential – voltage	effort	$kg\,m^2\,A^{-1}s^{-3}$	113
112	p_N	p	thermodynamic pressure	effort	$kg\,m^{-1}\,s^{-2}$	8
113	T_N	T	temperature	effort	K	9 121
114	$\mu_{N,S}$	chemPot	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	10 54
140	$x_{N,S}$	x	mole fraction	secondaryState		33
120	${v_z}_N$	v_z	velocity in z-direction	secondaryState	ms^{-1}	16
125	${C_V}_N$	CV	total heat capacity at constant volume	secondaryState	$kg\,m^2\,K^{-1}\,s^{-2}$	19
136	$h_{N,S}$	h	partial molar enthalpies	secondaryState	$kg\,m^2\,mol^{-1}\,s^{-2}$	29
118	${v_x}_N$	v_x	velocity in x-direction	secondaryState	ms^{-1}	14
138	$c_{N,S}$	c	molar concentration	secondaryState	$m^{-3}\,mol$	31
142	${c_V}_N$	cV	specific heat capacity at constant volume	secondaryState	$m^2\,K^{-1}\,s^{-2}$	35
222	${T^{ref}}_N$	T_ref	reference temperature	secondaryState	K	119
119	${v_y}_N$	v_y	velocity in y-direction	secondaryState	ms^{-1}	15
124	${C_p}_N$	Cp	total heat capacity at constant pressure	secondaryState	$kg\,m^2\,K^{-1}\,s^{-2}$	18 117
141	${c_p}_N$	cp	specific heat capacity at constant pressure	secondaryState	$m^2\,K^{-1}\,s^{-2}$	34 120
224	$\bar{T}_N$	T_meas	temperature measurement	secondaryState		123
139	${n^t}_N$	nt	total number of moles	secondaryState	mol	32
223	${T^n}_N$	T_meas_norming	value to norm measurement of temperature	secondaryState	K	122
202	$\tilde{n}_{N,S}$	np	link variable np to interface macroscopic	conversion	$m^{-3}\,mol\,s^{-1}$	97
215	$\dot{H}_N$	dH	accumulation of enthalpy	diffState	$kg\,m^2\,s^{-3}$	110
220	${\dot{U}^e}_A$	dUe	Kirkhoffs first law	diffState	$kg\,m^2\,A^{-1}s^{-3}$	116

Continued on next page

	var	symbol	documentation	type	units	eqs
196	$\dot{n}_{N,S}$	`an`	differential mass balance without reaction	diffState	$mol\, s^{-1}$	92
218	${I^e}_N$	`current`	current definition	internalTransport	A	114

5 reactions

	var	symbol	documentation	type	units	eqs
197	${E^{a}}_{K}$	`Ea`	Arrhenius activation energy	constant	$kg\, m^{2}\, mol^{-1}\, s^{-2}$	
26	$N_{S,K}$	`N`	stoichiometric matrix	constant		
198	${K^{o}}_{K}$	`Ko`	Arrhenius frequency factor	constant	$m^{-3}\, mol\, s^{-1}$	
167	$T_{N,p}$	`T`	link variable T to interface reactions	effort	K	60
163	$c_{N,S,p}$	`c`	link variable c to interface reactions	secondaryState	$m^{-3}\, mol$	56
165	$x_{N,S,p}$	`x`	link variable x to interface reactions	secondaryState		58
169	$\xi_{N,K,p}$	`probability`	probability of reaction to take place	conversion		62
168	$f_{N,S,K,p}$	`factor`	factor for probability computation	conversion		61
200	$\tilde{n}_{N,S,q}$	`np`	production from reaction set	conversion	$m^{-3}\, mol\, s^{-1}$	95
199	$K_{N,K,p}$	`K`	Arrhenius reaction "constant"	conversion	$m^{-3}\, mol\, s^{-1}$	94

6 control

	var	symbol	documentation	type	units	eqs
233	$l_{N,p}$	`limit`	limit	algebraic		132
226	$\bar{T}_{N,p}$	`T_meas`	link variable T meas to interface control	algebraic		125
228	p	`p_gain`	proportional gain	algebraic		127
227	$T_{setpoint\,N,p}$	`T_setpoint`	setpoint for temperatue	algebraic		126
229	$u_{N,p}$	`u`	output of straight proportional controller direction heating	algebraic		128
230	$d^{heating}{}_{N,p}$	`d_dir`	direction of heating	algebraic		129
231	$e_{N,p}$	`control_error`	control error in normed temperature	algebraic		130

7 reactions–macroscopic

	var	symbol	documentation	type	units	eqs
201	$\_np_{I,S}$	`_np`	link variable np to interface reactions »> macroscopic with source:node	get	$m^{-3}\, mol\, s^{-1}$	96

8 macroscopic–reactions

	var	symbol	documentation	type	units	eqs
162	$\_c_{I,S}$	`_c`	link variable c to interface macroscopic »> reactions with source:node	get	$m^{-3}\,mol$	55
166	$\_T_{I}$	`_T`	link variable T to interface macroscopic »> reactions with source:node	get	K	59
164	$\_x_{I,S}$	`_x`	link variable x to interface macroscopic »> reactions with source:node	get		57

9 macroscopic–control

	var	symbol	documentation	type	units	eqs
225	$\_T\_meas_I$	`_T_meas`	link variable T meas to interface macroscopic »> control with source:node	get		124

10 Equations

11 Generic

no	equation	documentation	layer
1	$0 := \textbf{Instantiate}(\#, \#)$	numerical value zero	root
2	$1 := \textbf{Instantiate}(\#, \#)$	numerical value one	root
3	$0.5 := \textbf{Instantiate}(\#, \#)$	numerical value one half	root
4	$t^o := \textbf{Instantiate}(t, \#)$	starting time	root
5	$t^e := \textbf{Instantiate}(t, \#)$	end time	root
6	$\Delta t := \textbf{Instantiate}(t, \#)$	time interval	root
7	$V_N := r_{xN} \, . \, r_{yN} \, . \, r_{zN}$	volume	physical
8	$p_N := \frac{\partial U_N}{\partial V_N}$	thermodynamic pressure	physical
9	$T_N := \frac{\partial U_N}{\partial S_N}$	temperature	macroscopic
10	$\mu_{N,S} := \frac{\partial U_N}{\partial n_{N,S}}$	chemical potential	macroscopic
11	$H_N := U_N - p_N \, . \, V_N$	Enthalpy	macroscopic
12	$A_N := U_N - T_N \, . \, S_N$	Helmholtz energy	macroscopic
13	$G_N := U_N + p_N \, . \, V_N - T_N \, . \, S_N$	Gibbs free energy	macroscopic
14	$v_{xN} := \frac{\partial r_{xN}}{\partial t}$	velocity in x-direction	macroscopic
15	$v_{yN} := \frac{\partial r_{yN}}{\partial t}$	velocity in y-direction	macroscopic
16	$v_{zN} := \frac{\partial r_{zN}}{\partial t}$	velocity in z-direction	macroscopic

Continued on next page

no	equation	documentation	layer
17	$R := N^A \,.\, k^B$	gas constant	physical
18	$C_{p\,N} := \frac{\partial H_N}{\partial T_N}$	total heat capacity at constant pressure	macroscopic
19	$C_{V\,N} := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	macroscopic
29	$h_{N,S} := H_N \,.\, (n_{N,S})^{-1}$	partial molar enthalpies	macroscopic
30	$m_N := \lambda_S \overset{S}{\star} n_{N,S}$	mass	macroscopic
31	$c_{N,S} := (V_N)^{-1} \,.\, n_{N,S}$	molar concentration	macroscopic
32	$n^t{}_N := \mathbf{reduceSum}\,(n_{N,S}, S)$	total number of moles	macroscopic
33	$x_{N,S} := (n^t{}_N)^{-1} \,.\, n_{N,S}$	mole fraction	macroscopic
34	$c_{p\,N} := C_{p\,N} \,.\, (m_N)^{-1}$	specific heat capacity at constant pressure	physical
35	$c_{V\,N} := C_{V\,N} \,.\, (m_N)^{-1}$	specific heat capacity at constant volume	macroscopic
36	$\rho_N := (V_N)^{-1} \,.\, m_N$	density	physical
40	$A_{xy\,N} := r_{x\,N} \,.\, r_{y\,N}$	cross sectional area xy	physical
41	$A_{xz\,N} := r_{x\,N} \,.\, r_{z\,N}$	cross sectional are xz	physical
42	$A_{yz\,N} := r_{y\,N} \,.\, r_{z\,N}$	cross sectional area yz	physical
43	$\hat{q}_{x\,A} := k^q_{x\,A} \,.\, A_{yz\,N} \,.\, F_{N,A} \overset{N}{\star} T_N$	heat flow in x-direction	macroscopic
44	$\hat{q}_{y\,A} := k^q_{y\,A} \,.\, A_{xz\,N} \,.\, F_{N,A} \overset{N}{\star} T_N$	heat flow in y-direction	macroscopic
45	$\hat{q}_{z\,A} := k^q_{z\,A} \,.\, A_{xy\,N} \,.\, F_{N,A} \overset{N}{\star} T_N$	heat flow in z-direction	macroscopic

Continued on next page

no	equation	documentation	layer
46	$\hat{n}^d_{x}{}_{A,S} := \hat{k}^{d,Fick}_{x}{}_{A,S} \,.\, A_{yz}{}_N \,.\, F_{N,A} \overset{N}{\star} c_{N,S}$	Fick diffusion flow in x-direction	macroscopic
47	$\hat{n}^d_{y}{}_{A,S} := \hat{k}^{d,Fick}_{y}{}_{A,S} \,.\, A_{xz}{}_N \,.\, F_{N,A} \overset{N}{\star} c_{N,S}$	Fick diffusion flow in y-direction	macroscopic
48	$\hat{n}^d_{z}{}_{A,S} := \hat{k}^{d,Fick}_{z}{}_{A,S} \,.\, \left(A_{xy}{}_N \,.\, F_{N,A}\right) \overset{N}{\star} c_{N,S}$	Fick diffusion flow in z-direction	macroscopic
49	$d_A := \mathbf{sign}\left(F_{N,A} \overset{N}{\star} p_N\right)$	flow direction of convective flow	macroscopic
50	$c_{A,S} := \left(0.5 \,.\, \left(F_{N,A} - d_A \,.\, \lvert F_{N,A}\rvert\right)\right) \overset{N}{\star} c_{N,S}$	concentration in convective event-dynamic flow	macroscopic
51	$\hat{V}_A := \left(\rho_A\right)^{-1} \,.\, k^c_{x}{}_A \,.\, A_{yz}{}_N \,.\, F_{N,A} \overset{N}{\star} p_N$	volumetric flow in x-direction	macroscopic
52	$\hat{n}^c_{x}{}_{A,S} := \hat{V}_A \,.\, c_{A,S}$	molar convective flow in x-direction	macroscopic
53	$\mu^o{}_{N,S} := \mathbf{Instantiate}(\mu_{N,S}, \#)$	instantiating standard chemical potential	macroscopic
54	$\mu_{N,S} := \mu^o{}_{N,S} + R \,.\, T_N \,.\, \mathbf{ln}\left(x_{N,S}\right)$	chemical potential standard model with mole fraction	macroscopic
61	$f_{N,S,K,p} := x_{N,S,p}{}^{((\lvert N_{S,K}\rvert))}$	factor for probability computation	reactions
62	$\xi_{N,K,p} := \prod_S f_{N,S,K,p}$	probability of reaction to take place	reactions
73	$k^d_{x}{}_{A,S} := I_{N,A} \overset{N}{\star} \left(\left(\mu_{N,S}\right)^{-1} \,.\, \left(v_{x}{}_N \,.\, \left(\left(V_N\right)^{-1} \,.\, \frac{\partial U_N}{\partial \mu_{N,S}}\right)\right)\right)$	diffusivity in arc and x-direction	macroscopic
74	$k^d_{y}{}_{A,S} := I_{N,A} \overset{N}{\star} \left(\left(\mu_{N,S}\right)^{-1} \,.\, \left(v_{y}{}_N \,.\, \left(\left(V_N\right)^{-1} \,.\, \frac{\partial U_N}{\partial \mu_{N,S}}\right)\right)\right)$	diffusivity in arc and y-direction	macroscopic
75	$k^d_{z}{}_{A,S} := I_{N,A} \overset{N}{\star} \left(\left(\mu_{N,S}\right)^{-1} \,.\, \left(v_{z}{}_N \,.\, \left(\left(V_N\right)^{-1} \,.\, \frac{\partial U_N}{\partial \mu_{N,S}}\right)\right)\right)$	diffusivity in arc and z-direction	macroscopic
76	$k^c_{x}{}_A := I_{N,A} \overset{N}{\star} \left(\left(\lambda_S \overset{S}{\star} \left(\mu_{N,S}\right)^{-1}\right) \,.\, \left(V_N\right)^{-1} \,.\, \frac{\partial U_N}{\partial p_N} \,.\, v_{x}{}_N\right)$	convective mass conductivity in arc and x diretion	macroscopic
77	$k^c_{y}{}_A := I_{N,A} \overset{N}{\star} \left(\left(\lambda_S \overset{S}{\star} \left(\mu_{N,S}\right)^{-1}\right) \,.\, \left(V_N\right)^{-1} \,.\, \frac{\partial U_N}{\partial p_N} \,.\, v_{y}{}_N\right)$	convective mass conductivity in arc and y-direction	macroscopic

Continued on next page

no	equation	documentation	layer
78	$k^c_{zA} := I_{N,A} \overset{N}{\star} \left(\left(\lambda_S \overset{S}{\star} (\mu_{N,S})^{-1}\right) . (V_N)^{-1} . \frac{\partial U_N}{\partial p_N} . v_{zN}\right)$	convecive mass conductivity in arc and y-direction	macroscopic
79	$k^q_{xA} := I_{N,A} \overset{N}{\star} \left((V_N)^{-1} . C_{pN} . v_{xN}\right)$	thermal conductivity in arc and x-direction	macroscopic
80	$k^q_{yA} := I_{N,A} \overset{N}{\star} \left((V_N)^{-1} . C_{pN} . v_{yN}\right)$	thermal conductivity in arc and y-direction	macroscopic
81	$k^q_{zA} := I_{N,A} \overset{N}{\star} \left((V_N)^{-1} . C_{pN} . v_{zN}\right)$	thermal conductivity in arc and z-direction	macroscopic
82	$\rho_A := I_{N,A} \overset{N}{\star} \rho_N$	density in arc	macroscopic
83	$\hat{k}^{d,Fick}_{x}{}_{A,S} := I_{N,A} \overset{N}{\star} \left(v_{xN} . \frac{\partial U_N}{\partial \mu_{N,S}} . (n_{N,S})^{-1}\right)$	Fick's diffusivity in arc and x-direction	macroscopic
84	$\hat{k}^{d,Fick}_{y}{}_{A,S} := I_{N,A} \overset{N}{\star} \left(v_{yN} . \frac{\partial U_N}{\partial \mu_{N,S}} . (n_{N,S})^{-1}\right)$	Fick diffusivity in arc and y-direction	macroscopic
85	$\hat{k}^{d,Fick}_{z}{}_{A,S} := I_{N,A} \overset{N}{\star} \left(v_{zN} . \frac{\partial U_N}{\partial \mu_{N,S}} . (n_{N,S})^{-1}\right)$	Fick diffusivity in arc and z-direction	macroscopic
86	$h_{A,S} := I_{N,A} \overset{N}{\star} h_{N,S}$	partial molar enthalpiies in arc	macroscopic
87	$\dot{n}^c_{xN,S} := F_{N,A} \overset{A}{\star} \hat{n}^c_{xA,S}$	accumulation of molar mass due to convection	macroscopic
88	$\dot{n}^d_{xN,S} := F_{N,A} \overset{A}{\star} \hat{n}^d_{xA,S}$	accumulation due to diffusion in x-direction	macroscopic
89	$\hat{n}^d_{xA,S} := k^d_{xA,S} . (A_{yzN} . F_{N,A}) \overset{N}{\star} \mu_{N,S}$	Fick diffusion flow in x-direction	macroscopic
90	$\hat{n}^d_{yA,S} := k^d_{yA,S} . (A_{yzN} . F_{N,A}) \overset{N}{\star} \mu_{N,S}$	Fick diffusion flow in y-direction	macroscopic
91	$\hat{n}^d_{zA,S} := k^d_{zA,S} . (A_{xyN} . F_{N,A}) \overset{N}{\star} \mu_{N,S}$	mass diffusion flow in z-direction	macroscopic
92	$\dot{n}_{N,S} := \dot{n}^c_{xN,S} + \dot{n}^d_{xN,S} + V_N . \tilde{n}_{N,S}$	differential mass balance without reaction	macroscopic

Continued on next page

no	equation	documentation	layer
93	$n_{N,S} := \int_{t^o}^{t^e} \dot{n}_{N,S} \; dt + n^o{}_{N,S}$	fundamental state – molar mass	macroscopic
94	$K_{N,K,p} := K^o{}_K \, . \, \mathbf{exp}\left((-E^a{}_K) \, . \, (R \, . \, T_{N,p})^{-1}\right)$	Arrhenius reaction "constant"	reactions
95	$\tilde{n}_{N,S,q} := A_{N,p,q} \overset{p}{\star} \left(N_{S,K} \overset{K}{\star} (K_{N,K,p} \, . \, \xi_{N,K,p})\right)$	production from reaction set	reactions
98	$n^o{}_{N,S} := \mathbf{Instantiate}(n_{N,S}, \#)$	initial mass	macroscopic
99	$\dot{H}^c_{x N} := F_{N,A} \overset{A}{\star} \left(\hat{n}^c_{x A,S} \overset{S}{\star} h_{N,S}\right)$	enthalpy accumulation due to convective flow in x-direction	macroscopic
100	$\dot{H}^d_{x N} := F_{N,A} \overset{A}{\star} \left(\hat{n}^d_{x A,S} \overset{S}{\star} h_{N,S}\right)$	accumulation of enthalpy due to diffusional mass flow in x-direction	macroscopic
101	$\dot{H}^d_{y N} := F_{N,A} \overset{A}{\star} \left(\hat{n}^d_{y A,S} \overset{S}{\star} h_{N,S}\right)$	accumulation of enthalpy due to diffusional mass flow in y-direction	macroscopic
102	$\dot{H}^d_{z N} := F_{N,A} \overset{A}{\star} \left(\hat{n}^d_{z A,S} \overset{S}{\star} h_{N,S}\right)$	accumulation of enthalpy due to diffusional mass flow in z-direction	macroscopic
103	$\dot{q}_{x N} := F_{N,A} \overset{A}{\star} \hat{q}_{x A}$	accumulation due to heat flow in x-direction	macroscopic
104	$\dot{q}_{y N} := F_{N,A} \overset{A}{\star} \hat{q}_{y A}$	accumulation due to heat flow in y-direction	macroscopic
105	$\dot{q}_{z N} := F_{N,A} \overset{A}{\star} \hat{q}_{z A}$	accumulation due to heat flow in z-direction	macroscopic
106	$\hat{w}_A := \mathbf{Instantiate}(\hat{q}_{x A}, \#)$	a fixed work flow to start with	macroscopic
107	$\dot{n}^d_{y N,S} := F_{N,A} \overset{A}{\star} \hat{n}^d_{y A,S}$	accumulation due to diffusion in y-direction	macroscopic
108	$\dot{n}^d_{z N,S} := F_{N,A} \overset{A}{\star} \hat{n}^d_{z A,S}$	accumulation due to diffusion in z-direction	macroscopic

Continued on next page

no	equation	documentation	layer
109	$\dot{w}_N := F_{N,A} \overset{A}{\star} \hat{w}_A$	accumulation of enthalpy due to work flow	macroscopic
110	$\dot{H}_N := \dot{H}^c_{x\,N} + \dot{H}^d_{x\,N} + \dot{H}^d_{y\,N} + \dot{H}^d_{z\,N} + \dot{q}_{x\,N} + \dot{q}_{y\,N} + \dot{q}_{z\,N} + \dot{w}_N$	accumulation of enthalpy	macroscopic
111	$H^o{}_N := \mathbf{Instantiate}(H_N, \#)$	initial enthalpy	macroscopic
112	$H_N := \int_{t^o}^{t^e} \dot{H}_N \; dt + H^o{}_N$	Enthalpy	macroscopic
113	$U^e{}_N := (C_N)^{-1} \,.\, U_N$	electrical potential – voltage	macroscopic
114	$I^e{}_N := \frac{d\, C_N}{d\, t}$	current definition	macroscopic
115	$R^e{}_N := (I^e{}_N)^{-1} \,.\, U^e{}_N$	electrical resistant	macroscopic
116	$\dot{U}^e{}_A := F_{N,A} \overset{A}{\star} (R^e{}_N \,.\, I^e{}_N)$	Kirkhoffs first law	macroscopic
117	$C_{p\,N} := m_N \,.\, c_{p\,N}$	total heat capacity at constant pressure	macroscopic
119	$T^{ref}{}_N := \mathbf{Instantiate}(T_N, \#)$	reference temperature	macroscopic
120	$c_{p\,N} := \mathbf{Instantiate}(c_{p\,N}, \#)$	constant specific heat capacity at constant pressure	macroscopic
121	$T_N := H_N \,.\, (C_{p\,N})^{-1} + T^{ref}{}_N$	temperature from constant heat capacity	macroscopic
122	$T^n{}_N := \mathbf{Instantiate}(T_N, \#)$	value to norm measurement of temperature	macroscopic
123	$\bar{T}_N := T_N \,.\, (T^n{}_N)^{-1}$	temperature measurement	macroscopic
126	$T_{setpoint\,N,p} := \mathbf{Instantiate}(\bar{T}_{N,p}, \#)$	setpoint for temperatue	control
127	$p := \mathbf{Instantiate}(\#, \#)$	proportional gain	control

Continued on next page

no	equation	documentation	layer
128	$u_{N,p} := (-p)\ .\ e_{N,p}$	output of straight proportional temperature controller	control
129	$d^{heating}{}_{N,p} := \mathbf{sign}\,(u_{N,p})$	direction of heating	control
130	$e_{N,p} := T_{setpoint\,N,p} - \bar{T}_{N,p}$	control error in normed temperature	control
132	$l_{N,p} := \mathbf{Instantiate}(u_{N,p}, \#)$	maximum limit	control
133	$fm_{N,A} := \hat{V}_A\ .\ \rho_N$	convective mass flow	macroscopic

12 Interface Link Equation

no	equation	documentation	layer
55	$\_c_{I,S} := F^{source}{}_{N,I} \overset{N}{\star} c_{N,S}$	interface equation	macroscopic –> reactions
56	$c_{N,S,p} := \left(F^{sink}{}_{N,I} \cdot \_c_{I,S}\right) \overset{I}{\star} S_{I,p}$	interface equation	reactions
57	$\_x_{I,S} := F^{source}{}_{N,I} \overset{N}{\star} x_{N,S}$	interface equation	macroscopic –> reactions
58	$x_{N,S,p} := \left(F^{sink}{}_{N,I} \cdot \_x_{I,S}\right) \overset{I}{\star} S_{I,p}$	interface equation	reactions
59	$\_T_I := F^{source}{}_{N,I} \overset{N}{\star} T_N$	interface equation	macroscopic –> reactions
60	$T_{N,p} := \left(F^{sink}{}_{N,I} \cdot \_T_I\right) \overset{I}{\star} S_{I,p}$	interface equation	reactions
96	$\_np_{I,S} := \textbf{reduceSum}\left(\left(\left(F^{source}{}_{N,I} \overset{N}{\star} \tilde{n}_{N,S,q}\right) \cdot S_{I,q}\right), q\right)$	interface equation	reactions –> macroscopic
97	$\tilde{n}_{N,S} := F^{source}{}_{N,I} \overset{I}{\star} \_np_{I,S}$	interface equation	macroscopic
124	$\_T\_meas_I := F^{source}{}_{N,I} \overset{N}{\star} \bar{T}_N$	interface equation	macroscopic –> control
125	$\bar{T}_{N,p} := \left(F^{sink}{}_{N,I} \cdot \_T\_meas_I\right) \overset{I}{\star} S_{I,p}$	interface equation	control