1 Variables

2 root

	var	symbol	documentation	type	units	eqs
10	$F_{N,A}$	`F`	basic directed graph incidence matrix	network		
96	I_N	`I_N`	vector of ones of length nodes	projection		
48	$I_{N,A}$	`I_N_A`	project node on arc	projection		
97	I_A	`I_A`	vector of ones of length arcs	projection		
4	t	`t`	time	frame	s	
7	Δt	`t_interval`	time interval	frame	s	5
6	t^e	`te`	time end	frame	s	4
5	t^o	`to`	time zero	frame	s	3
9	Δ	`pulse`	pulse of length time interval	frame		7
3	0	`zero`	numerical value zero	constant		2
8	0.5	`onehalf`	numerical one half	constant		6
2	1	`one`	numerical one	constant		1
1	$\#$	`value`	numerical value	constant		

3 physical

	var	symbol	documentation	type	units	eqs
170	S_S	S_S	species selection	projection		
98	I_S	I_S	vector of ones of length sepecies	projection		
11	ℓ_N	l	length	frame	m	
13	r_{yN}	r_y	y-direction	frame	m	9
12	r_{xN}	r_x	x-direction	frame	m	8
14	r_{zN}	r_z	z-direction	frame	m	10
18	$n_{N,S}$	n	fundamental state - molar mass	state	mol	129
15	V_N	V	fundamental state - volume	state	m^3	11
23	A_N	A	Helmholts energy	state	$kg\,m^2\,s^{-2}$	17
24	G_N	G	Gibbs free energy	state	$kg\,m^2\,s^{-2}$	18
22	H_N	H	Enthalpy	state	$kg\,m^2\,s^{-2}$	15 128 161
16	U_N	U	fundamental state - internal energy	state	$kg\,m^2\,s^{-2}$	
17	S_N	S	fundamental state - entropy	state	$kg\,m^2\,K^{-1}\,s^{-2}$	
25	C_N	C	fundamental state - charge	state	$A\,s$	
34	R_N	R	Gas constant	constant	$kg\,m^2\,mol^{-1}\,K^{-1}\,s^{-2}$	25
32	A^v	Av	Avogadro number	constant	mol^{-1}	
33	B_N	Boltz	Boltzmann constant	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	24
20	p_N	p	pressure	effort	$kg\,m^{-1}\,s^{-2}$	13
21	$\mu_{N,S}$	chemPot	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	14 88
19	T_N	T	temperature	effort	K	16 162
35	${U^e}_N$	Ue	electrical potential – voltage	effort	$kg\,m^2\,A^{-1}s^{-3}$	26

Continued on next page

	var	symbol	documentation	type	units	eqs
28	$v_{y\,N}$	`v_y`	velocity in y-direction	secondaryState	ms^{-1}	20
29	$v_{z\,N}$	`v_z`	velocity in z-direction	secondaryState	ms^{-1}	21
27	$v_{x\,N}$	`v_x`	velocity in x-direction	secondaryState	ms^{-1}	19

4 reactions

	var	symbol	documentation	type	units	eqs
113	$P_{N,K}$	P_N_K	what node has what reaction	projection		
114	$T_{N,K}$	T_K	temparature of the nodes with reactions	effort	K	99
129	$\bar{n}_{N,S,K}$	cn_NK	normed concentration – context node and conversion	secondaryState		113
128	$\bar{n}_{N,S}$	cn	normed concentration	secondaryState		112
131	$\phi_{N,K}$	interactionProbability	probability for the species to meet to undergo reaction	properties		115
135	$K_{N,K}$	K	reaction"constant	properties	$m^{-3}\,mol\,s^{-1}$	119
126	${c^n}_{N,S}$	c_norming	norming concentration used in the definition of the species interaction probability	properties	$m^{-3}\,mol$	110
118	$N_{S,K}$	N	stoichiometric matrix	properties		
115	${E_a}_{N,K}$	Ea	Arrhenius activation energy	properties	$kg\,m^2\,mol^{-1}\,s^{-2}$	100
134	${K^o}_K$	Ko	Arrhenius frequency factor – a strange construction	properties	$m^{-3}\,mol\,s^{-1}$	118
136	$\tilde{n}_{N,S}$	nProd	production term for differential component mass balance	conversion	$mol\,s^{-1}$	120

5 material

	var	symbol	documentation	type	units	eqs
63	${k_z^{d,Fick}}_{A,S}$	kd_z_Fick	Fick's diffusivity in arc and z-direction	property	$m s^{-1}$	53
55	${k_x^q}_A$	kq_x_A	thermal conductivity in x-direction in arc	property	$kg\, K^{-1}\, s^{-3}$	45
46	${k_z^c}_N$	kc_z	convective mass conductivity in z-direction	property	$m^{-1}\, s$	37
168	${R^e}_N$	Re	electrical resistance	property	$kg\, m^2\, A^{-2} s^{-3}$	154
49	${k_x^c}_A$	kc_x_A	convective mass conductivity in x-direction in arc	property	$m^{-1}\, s$	39
45	${k_y^c}_N$	kc_y	convective mass conductivity in y-direction	property	$m^{-1}\, s$	36
59	ρ_N	density	density	property	$kg\, m^{-3}$	49
89	ρ_A	density_A	density of arc material	property	$kg\, m^{-3}$	78
42	${k_y^d}_{N,S}$	kd_y	diffusional mass conductivity in z-direction	property	$kg^{-1}\, m^{-4}\, mol^2\, s$	33
51	${k_z^c}_A$	kc_z_A	convective mass conductivity in z-direction in arc	property	$m^{-1}\, s$	41
57	${k_z^q}_A$	kq_z_A	thermal conductivity in z-direction in arc	property	$kg\, K^{-1}\, s^{-3}$	47
56	${k_y^q}_A$	kq_y_A	thermal conductivity in y-direction in arc	property	$kg\, K^{-1}\, s^{-3}$	46
171	${k^{e,x}}_N$	kex	electrical conductivity – a simple model being a function of a selected set of species	property	$kg^{-1}\, m^{-2}\, A^2 s^3$	155
52	${k_x^d}_{A,S}$	kd_x_A	diffusional mass conductivity in x-direction in arc	property	$kg^{-1}\, m^{-4}\, mol^2\, s$	42
61	${k_x^{d,Fick}}_{A,S}$	kd_x_Fick	Fick's diffusivity in arc and x-direction	property	$m s^{-1}$	51
38	${k_x^q}_N$	kq_x	thermal conductivity in x-direction	property	$kg\, K^{-1}\, s^{-3}$	29
54	${k_z^d}_{A,S}$	kd_z_A	diffusional mass conductivity in z-direction in arc	property	$kg^{-1}\, m^{-4}\, mol^2\, s$	44
47	$h_{N,S}$	h	partial molar enthalpies	property	$kg\, m^2\, mol^{-1}\, s^{-2}$	38
39	${k_y^q}_N$	kq_y	thermal conductivity in y-direction	property	$kg\, K^{-1}\, s^{-3}$	30
58	m_N	m	mass	property	kg	48
53	${k_y^d}_{A,S}$	kd_y_A	diffusional mass conductivity in y-direction in arc	property	$kg^{-1}\, m^{-4}\, mol^2\, s$	43
41	${k_x^d}_{N,S}$	kd_x	diffusional mass conductivity in x-direction	property	$kg^{-1}\, m^{-4}\, mol^2\, s$	32
107	$h_{A,S}$	h_A	partial molar enthalpies of transport system	property	$kg\, m^2\, mol^{-1}\, s^{-2}$	93

Continued on next page

	var	symbol	documentation	type	units	eqs
62	${k_y^{d,Fick}}_{A,S}$	kd_y_Fick	Fick's diffusivity in arc and y-direction	property	ms^{-1}	52
50	${k_y^c}_A$	kc_y_A	convective mass conductivity in y-direction in arc	property	$m^{-1}\,s$	40
36	${C_p}_N$	Cp	total heat capacity at constant pressure	property	$kg\,m^2\,K^{-1}\,s^{-2}$	27
43	${k_z^d}_{N,S}$	kd_z	diffusional mass conductivity in z-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	34
60	v_S	v	molar volume of species	property	$m^3\,mol^{-1}$	50
37	${C_v}_N$	Cv	total heat capacity at constant volume	property	$kg\,m^2\,K^{-1}\,s^{-2}$	28
40	${k_z^q}_N$	kq_z	thermal conductivity in z-direction	property	$kg\,K^{-1}\,s^{-3}$	31
26	λ_S	Mm	species' molecular mass	property	$kg\,mol^{-1}$	
172	cp_N	cp	specific heat capacity at constant pressure	property	$m^2\,K^{-1}\,s^{-2}$	156
44	${k_x^c}_N$	kc_x	convective mass conductivity in x-direction	property	$m^{-1}\,s$	35
102	${\mu^o}_{N,S}$	chemPot_o	standard chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	86

6 macroscopic

	var	symbol	documentation	type	units	eqs
87	$c_{A,S}$	`c_A`	concentration in convective mass flow	transport	$m^{-3}\,mol$	76
104	$\dot{n}^d{}_{N,S}$	`and`	accumulation due to diffusional mass transfer	transport	$mol\,s^{-1}$	90
111	$\dot{H}^c{}_N$	`aHc`	enthalpy accumulation due to convective mass flow	transport	$kg\,m^2\,s^{-3}$	97
91	$\dot{V}_A$	`fV`	volumetric flow	transport	$m^3\,s^{-1}$	80
112	$\dot{H}^d{}_N$	`aHd`	enthalpy accumulation due to diffusive mass flow	transport	$kg\,m^2\,s^{-3}$	98
86	d_A	`d`	fow direction of convective flow	transport		75
110	$\hat{H}^d{}_A$	`fHd`	enthalpy flow due to diffusive mass flow	transport	$kg\,m^2\,s^{-3}$	96
101	$\hat{n}^d{}_{A,S}$	`fnd`	diffusional mass flow in arc	transport	$mol\,s^{-1}$	85 89
109	$\hat{H}^c{}_A$	`fHc`	enthalpy flow due to convective mass flow	transport	$kg\,m^2\,s^{-3}$	95
141	$\hat{w}_A$	`fw`	just an numerical work flow term – as a starter	transport	$kg\,m^2\,s^{-3}$	125
142	$\dot{w}_N$	`aw`	enthalpy accumulation due to work flows	transport	$kg\,m^2\,s^{-3}$	126
166	I_N	`I`	electric current definition	transport	A	152
83	$\hat{q}_{x\,A}$	`fq_x`	heat flow in arc and x-direction	transport	$kg\,m^2\,s^{-3}$	72
93	$\dot{n}^c{}_{N,S}$	`anc`	accumulation due to convective mass flow	transport	$mol\,s^{-1}$	82
92	$\hat{n}^c{}_{A,S}$	`fnc`	convective mass flow in an arc	transport	$mol\,s^{-1}$	81
84	$\dot{q}_N$	`aq`	accumulation due to conductive heat flow	transport	$kg\,m^2\,s^{-3}$	73
69	$A_{xz\,A}$	`A_xz_A`	cross sectional area xz of arc	geometry	m^2	58
65	$A_{xy\,N}$	`A_xy`	cross sectional area xy	geometry	m^2	54
66	$A_{xz\,N}$	`A_xz`	cross sectional area xz	geometry	m^2	55
68	$A_{xy\,A}$	`A_xy_A`	cross sectional area yz of arc	geometry	m^2	57
70	$A_{yz\,A}$	`A_yz_A`	cross sectional area yz of arc	geometry	m^2	59
67	$A_{yz\,N}$	`A_yz`	cross sectional area yz	geometry	m^2	56
64	$D_{N,A}$	`D`	difference operator	differenceOperator		

Continued on next page

	var	symbol	documentation	type	units	eqs
144	${H^o}_N$	Ho	initial enthalpy	state	$kg\, m^2\, s^{-2}$	130
145	${n^o}_{N,S}$	no	initial species masses	state	mol	131
148	${c^o}_{N,S}$	c_norming	norming concentration	secondaryState	$m^{-3}\, mol$	134
85	$c_{N,S}$	c	molar concentration	secondaryState	$m^{-3}\, mol$	74
174	m_N	m	mass	secondaryState	kg	158
176	${T^{ref}}_N$	T_ref	reference temperature	secondaryState	K	160
99	${n^t}_N$	nt	total amount	secondaryState	mol	83
150	${\bar{p}^o}_N$	p_normed	normed pressure	secondaryState		136
151	${\bar{c}^o}_{N,S}$	c_normed	normed concentration	secondaryState		137
149	${\bar{T}^o}_N$	T_normed	normed temperature	secondaryState		135
147	${p^o}_N$	p_norming	normed pressure	secondaryState	$kg\, m^{-1}\, s^{-2}$	133
100	$x_{N,S}$	x	concentration mole fraction	secondaryState		84
175	${C_p}_N$	Cp	total heat capacity	secondaryState	$kg\, m^2\, K^{-1}\, s^{-2}$	159
146	${T^o}_N$	T_norming	norming temperature	secondaryState	K	132
138	${\dot{n}^p}_{N,S}$	anProduction	production term	conversion	$mol\, s^{-1}$	122
143	$\dot{H}_N$	aH	differential enthalpy balance	diffState	$kg\, m^2\, s^{-3}$	127
139	$\dot{n}_{N,S}$	an	differentional species balance	diffState	$mol\, s^{-1}$	123

7 control

	var	symbol	documentation	type	units	eqs
184	t^s	t_switch	switching time	frame	s	167
179	x_N	x	controller state	state		165
183	${x^o}_N$	xo	initial controller state	state		166
177	$A_{N,D}$	A	LTIS A-matrix	constant	s^{-1}	
157	${m^{v\star}}_A$	setpoint_vector	setpoint for measurement vector	constant		144
159	P	P	gain	constant		
158	${m^{m\star}}_{A,S}$	setpoint_matrix	setpoiint for measurment matrix	constant		145
181	$I_{N,D}$	I_N_D	map differential space to node space	constant		
178	$B_{A,D}$	B	LTIS B-matrix	constant	s^{-1}	
182	$\dot{x}_D$	dxdt	differential controller state	diffState	s^{-1}	164
155	m_A	measurement_vector	normed measurements of temparatures	algebraic		141 142
160	${e^v}_A$	error_vector	output error vector	algebraic		146
163	${u^m}_{A,S}$	u_matrix	control output matrix	algebraic		149
156	$m_{A,S}$	measurement_matrix	normed measurment of concentration	algebraic		143
162	${u^v}_A$	u_vector	control ouput vector	algebraic		148 168
161	${e^m}_{A,S}$	error_matrix	output error matrix	algebraic		147

8 macroscopic–control

	var	symbol	documentation	type	units	eqs
152	_$\bar{p}_N$	`_p_normed`	link variable p normed to interface macroscopic »> control	get		138
153	_$\bar{T}_N$	`_T_normed`	link variable T normed to interface macroscopic »> control	get		139
154	_$\bar{c}_{N,S}$	`_c_normed`	link variable c normed to interface macroscopic »> control	get		140

9 macroscopic–material

	var	symbol	documentation	type	units	eqs
167	$_{I\,N}$	`_I`	link variable I to interface macroscopic »> material	get	A	153
103	$\_x_{N,S}$	`_x`	link variable x to interface macroscopic »> material	get		87

10 control–macroscopic

	var	symbol	documentation	type	units	eqs
164	$\_m^{m}{}_{A,S}$	`_setpoint_matrix`	link variable setpoint matrix to interface control »> macroscopic	get		150
165	$\_m^{v}{}_{A}$	`_setpoint_vector`	link variable setpoint vector to interface control »> macroscopic	get		151

11 reactions–macroscopic

	var	symbol	documentation	type	units	eqs
123	$\_T_{N,K}$	`_T_K`	link variable T K to interface reactions »> macroscopic	get	K	107
137	$\_\tilde{n}_{N,S}$	`_nProd`	link variable nProd to interface reactions »> macroscopic	get	$mol\, s^{-1}$	121
119	$\_E^{a}{}_{N,K}$	`_Ea`	link variable Ea to interface reactions »> macroscopic	get	$kg\, m^{2}\, mol^{-1}\, s^{-2}$	103
122	${}_{N\,S,K}$	`_N`	link variable N to interface reactions »> macroscopic	get		106

12 material–macroscopic

	var	symbol	documentation	type	units	eqs
76	$\_k_{y}^{d,Fick}{}_{A,S}$	`_kd_y_Fick`	link variable kd y Fick to interface material »> macroscopic	get	ms^{-1}	65
71	$\_k_{x}^{c}{}_{A}$	`_kc_x_A`	link variable kc x A to interface material »> macroscopic	get	$m^{-1}\,s$	60
90	$\_\rho_{A}$	`_density_A`	link variable density A to interface material »> macroscopic	get	$kg\,m^{-3}$	79
108	$\_h_{A,S}$	`_h_A`	link variable h A to interface material »> macroscopic	get	$kg\,m^{2}\,mol^{-1}\,s^{-2}$	94
74	$\_k_{x}^{d}{}_{A,S}$	`_kd_x_A`	link variable kd x A to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^{2}\,s$	63
30	$\_\lambda_{S}$	`_Mm`	link variable Mm to interface material »> macroscopic	get	$kg\,mol^{-1}$	22
75	$\_k_{x}^{d,Fick}{}_{A,S}$	`_kd_x_Fick`	link variable kd x Fick to interface material »> macroscopic	get	ms^{-1}	64
72	$\_k_{y}^{c}{}_{A}$	`_kc_y_A`	link variable kc y A to interface material »> macroscopic	get	$m^{-1}\,s$	61
77	$\_k_{y}^{d}{}_{A,S}$	`_kd_y_A`	link variable kd y A to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^{2}\,s$	66
88	$\_\rho_{N}$	`_density`	link variable density to interface material »> macroscopic	get	$kg\,m^{-3}$	77
80	$\_k_{x}^{q}{}_{A}$	`_kq_x_A`	link variable kq x A to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	69
81	$\_k_{y}^{q}{}_{A}$	`_kq_y_A`	link variable kq y A to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	70
73	$\_k_{z}^{c}{}_{A}$	`_kc_z_A`	link variable kc z A to interface material »> macroscopic	get	$m^{-1}\,s$	62
79	$\_k_{z}^{d,Fick}{}_{A,S}$	`_kd_z_Fick`	link variable kd z Fick to interface material »> macroscopic	get	ms^{-1}	68

Continued on next page

	var	symbol	documentation	type	units	eqs
106	$\_h_{N,S}$	`_h`	link variable h to interface material »> macroscopic	get	$kg\, m^2\, mol^{-1}\, s^{-2}$	92
173	$\_c_{p\,N}$	`_cp`	link variable cp to interface material »> macroscopic	get	$m^2\, K^{-1}\, s^{-2}$	157
82	$\_k^q_{z\,A}$	`_kq_z_A`	link variable kq z A to interface material »> macroscopic	get	$kg\, K^{-1}\, s^{-3}$	71
78	$\_k^d_{z\,A,S}$	`_kd_z_A`	link variable kd z A to interface material »> macroscopic	get	$kg^{-1}\, m^{-4}\, mol^2\, s$	67

13 macroscopic–reactions

	var	symbol	documentation	type	units	eqs
125	$\_c_{N,S}$	`_c`	link variable c to interface macroscopic »> reactions	get	$m^{-3}\,mol$	109

14 Equations

15 Generic

no	equation	documentation	layer
1	$1 := \text{Instantiate}(\#, \#)$	numerical one	root
2	$0 := \text{Instantiate}(\#, \#)$	numerical value zero	root
3	$t^o := \text{Instantiate}(t, 0)$	time zero	root
4	$t^e := \text{Instantiate}(t, \#)$	time end	root
5	$\Delta t := \text{Instantiate}(t, \#)$	time interval	root
6	$0.5 := \text{Instantiate}(\#, \#)$	numerical one half	root
7	$\Delta := \text{sign}\left(t - t^o\right) - \text{sign}\left(t - \left(t^o - \Delta t\right)\right)$	pulse of length time interval	root
8	$r_{x\,N} := \text{Instantiate}(\ell_N, \#)$	x-direction	physical
9	$r_{y\,N} := \text{Instantiate}(\ell_N, \#)$	y-direction	physical
10	$r_{z\,N} := \text{Instantiate}(\ell_N, \#)$	z-direction	physical
11	$V_N := r_{x\,N} \,.\, r_{y\,N} \,.\, r_{z\,N}$	volume	physical
13	$p_N := \frac{\partial U_N}{\partial V_N}$	pressure	physical
14	$\mu_{N,S} := \frac{\partial U_N}{\partial n_{N,S}}$	chemical potential	physical
15	$H_N := U_N - p_N \,.\, V_N$	Enthalpy	physical
16	$T_N := \frac{\partial U_N}{\partial S_N}$	temperature	physical
17	$A_N := U_N - T_N \,.\, S_N$	Helmholts energy	physical

Continued on next page

no	equation	documentation	layer
18	$G_N := U_N + p_N \,.\, V_N - T_N \,.\, S_N$	Gibbs free energy	physical
19	$v_{x\,N} := (t)^{-1} \,.\, r_{x\,N}$	velocity in x-direction	physical
20	$v_{y\,N} := (t)^{-1} \,.\, r_{y\,N}$	velocity in y-direction	physical
21	$v_{z\,N} := (t)^{-1} \,.\, r_{z\,N}$	velocity in z-direction	physical
24	$B_N := \text{Instantiate}(S_N, \#)$	Boltzmann constant	physical
25	$R_N := A^v \,.\, B_N$	Gas constant	physical
26	$U^e{}_N := (C_N)^{-1} \,.\, U_N$	electrical potential – voltage	physical
27	$C_{p\,N} := \frac{\partial H_N}{\partial T_N}$	total heat capacity at constant pressure	material
28	$C_{v\,N} := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	material
29	$k^q_{x\,N} := (V_N)^{-1} \,.\, C_{p\,N} \,.\, v_{x\,N}$	thermal conductivity in x-direction	material
30	$k^q_{y\,N} := (V_N)^{-1} \,.\, C_{p\,N} \,.\, v_{y\,N}$	thermal conductivity in y-direction	material
31	$k^q_{z\,N} := (V_N)^{-1} \,.\, C_{p\,N} \,.\, v_{z\,N}$	thermal conductivity in z-direction	material
32	$k^d_{x\,N,S} := (\mu_{N,S})^{-1} \,.\, \left(v_{x\,N} \,.\, \left((V_N)^{-1} \,.\, \frac{\partial U_N}{\partial \mu_{N,S}}\right)\right)$	diffusional mass conductivity in x-direction	material
33	$k^d_{y\,N,S} := (\mu_{N,S})^{-1} \,.\, \left(v_{y\,N} \,.\, \left((V_N)^{-1} \,.\, \frac{\partial U_N}{\partial \mu_{N,S}}\right)\right)$	diffusional mass conductivity in y-direction	material
34	$k^d_{z\,N,S} := (\mu_{N,S})^{-1} \,.\, \left(v_{z\,N} \,.\, \left((V_N)^{-1} \,.\, \frac{\partial U_N}{\partial \mu_{N,S}}\right)\right)$	diffusional mass conductivity in z-direction	material
35	$k^c_{x\,N} := \left(\lambda_S \star (\mu_{N,S})^{-1}\right) \,.\, (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial p_N} \,.\, v_{x\,N}$	convective mass conductivity in x-direction	material

Continued on next page

no	equation	documentation	layer
36	$k^c_{y\,N} := \left(\lambda_S \star \left(\mu_{N,S}\right)^{-1}\right) \,.\, \left(V_N\right)^{-1} \,.\, \frac{\partial U_N}{\partial p_N} \,.\, v_{y\,N}$	convective mass conductivity in y-direction	material
37	$k^c_{z\,N} := \left(\lambda_S \star \left(\mu_{N,S}\right)^{-1}\right) \,.\, \left(V_N\right)^{-1} \,.\, \frac{\partial U_N}{\partial p_N} \,.\, v_{z\,N}$	convective mass conductivity in z-direction	material
38	$h_{N,S} := H_N \,.\, \left(n_{N,S}\right)^{-1}$	partial molar enthalpies	material
39	$k^c_{x\,A} := I_{N,A} \star k^c_{x\,N}$	convective mass conductivity in x-direction in arc	material
40	$k^c_{y\,A} := I_{N,A} \star k^c_{y\,N}$	convective mass conductivity in y-direction in arc	material
41	$k^c_{z\,A} := I_{N,A} \star k^c_{z\,N}$	convective mass conductivity in z-direction in arc	material
42	$k^d_{x\,A,S} := I_{N,A} \star k^d_{x\,N,S}$	diffusional mass conductivity in x-direction in arc	material
43	$k^d_{y\,A,S} := I_{N,A} \star k^d_{y\,N,S}$	diffusional mass conductivity in z-direction in arc	material
44	$k^d_{z\,A,S} := I_{N,A} \star k^d_{z\,N,S}$	diffusional mass conductivity in z-direction in arc	material
45	$k^q_{x\,A} := I_{N,A} \star k^q_{x\,N}$	thermal conductivity in x-direction in arc	material
46	$k^q_{y\,A} := I_{N,A} \star k^q_{y\,N}$	thermal conductivity in y-direction in arc	material
47	$k^q_{z\,A} := I_{N,A} \star k^q_{z\,N}$	thermal conductivity in z-direction in arc	material
48	$m_N := \lambda_S \star n_{N,S}$	mass	material

Continued on next page

no	equation	documentation	layer
49	$\rho_N := (V_N)^{-1} . m_N$	density	material
50	$v_S := V_N \star (n_{N,S})^{-1}$	molar volume of species	material
51	$k_x^{d,Fick}{}_{A,S} := I_{N,A} \star \left(v_{x\,N} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1}\right)$	Fick's diffusivity in arc and x-direction	material
52	$k_y^{d,Fick}{}_{A,S} := I_{N,A} \star \left(v_{y\,N} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1}\right)$	Fick's diffusivity in arc and y-direction	material
53	$k_z^{d,Fick}{}_{A,S} := I_{N,A} \star \left(v_{z\,N} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1}\right)$	Fick's diffusivity in arc and z-direction	material
54	$A_{xy\,N} := r_{x\,N} . r_{y\,N}$	cross sectional area xy	macroscopic
55	$A_{xz\,N} := r_{x\,N} . r_{z\,N}$	cross sectional area xz	macroscopic
56	$A_{yz\,N} := r_{y\,N} . r_{z\,N}$	cross sectional area yz	macroscopic
57	$A_{xy\,A} := I_{N,A} \star A_{xy\,N}$	cross sectional area yz of arc	macroscopic
58	$A_{xz\,A} := I_{N,A} \star A_{xz\,N}$	cross sectional area xz of arc	macroscopic
59	$A_{yz\,A} := I_{N,A} \star A_{yz\,N}$	cross sectional area yz of arc	macroscopic
72	$\hat{q}_{x\,A} := A_{yz\,A} . \_k^q_{x\,A} . (D_{N,A} \star T_N)$	heat flow in arc and x-direction	macroscopic
73	$\dot{q}_N := F_{N,A} \star \hat{q}_{x\,A}$	accumulation due to conductive heat flow	macroscopic
74	$c_{N,S} := (V_N)^{-1} . n_{N,S}$	molar concentration	macroscopic
75	$d_A := \mathrm{sign}\,(D_{N,A} \star p_N)$	fow direction of convective flow	macroscopic
76	$c_{A,S} := (0.5 . (D_{N,A} - d_A . \lvert D_{N,A} \rvert)) \star c_{N,S}$	concentration in convective mass flow	macroscopic
78	$\rho_A := I_{N,A} \star \rho_N$	density of arc material	material
80	$\dot{V}_A := (\_\rho_A)^{-1} . \_k^c_{x\,A} . A_{yz\,A} . (D_{N,A} \star p_N)$	volumetric flow	macroscopic

Continued on next page

no	equation	documentation	layer
81	$\hat{n}^c{}_{A,S} := \dot{V}_A \,.\, c_{A,S}$	convective mass flow in an arc	macroscopic
82	$\dot{n}^c{}_{N,S} := F_{N,A} \star \hat{n}^c{}_{A,S}$	accumulation due to convective mass flow	macroscopic
83	$n^t{}_N := I_S \star n_{N,S}$	total amount	macroscopic
84	$x_{N,S} := \left(n^t{}_N\right)^{-1} \,.\, n_{N,S}$	concentration mole fraction	macroscopic
85	$\hat{n}^d{}_{A,S} := A_{yz\,A} \,.\, \left(-\_k_x^{d,Fick}{}_{A,S}\right) \,.\, \left(D_{N,A} \star c_{N,S}\right)$	diffusional mass flow in arc	macroscopic
86	$\mu^o{}_{N,S} := \mathrm{Instantiate}(\mu_{N,S}, \#)$	standard chemical potential	material
88	$\mu_{N,S} := \mu^o{}_{N,S} + R_N \,.\, T_N \,.\, ln(\_x_{N,S})$	chemical potential standard model with mole fraction	material
89	$\hat{n}^d{}_{A,S} := A_{yz\,A} \,.\, \left(-\_k_x^d{}_{A,S}\right) \,.\, \left(D_{N,A} \star \mu_{N,S}\right)$	diffusional mass flow in arc	macroscopic
90	$\dot{n}^d{}_{N,S} := F_{N,A} \star \hat{n}^d{}_{A,S}$	accumulation due to diffusional mass transfer	macroscopic
93	$h_{A,S} := I_{N,A} \star h_{N,S}$	partial molar enthalpies of transport system	material
95	$\hat{H}^c{}_A := I_S \star (\_h_{A,S} \,.\, \hat{n}^c{}_{A,S})$	enthalpy flow due to convective mass flow	macroscopic
96	$\hat{H}^d{}_A := I_S \star \left(\_h_{A,S} \,.\, \hat{n}^d{}_{A,S}\right)$	enthalpy flow due to diffusive mass flow	macroscopic
97	$\dot{H}^c{}_N := F_{N,A} \star \hat{H}^c{}_A$	enthalpy accumulation due to convective mass flow	macroscopic
98	$\dot{H}^d{}_N := F_{N,A} \star \hat{H}^d{}_A$	enthalpy accumulation due to diffusive mass flow	macroscopic
99	$T_{N,K} := T_N \,.\, P_{N,K}$	temparature of the nodes with reactions	reactions

Continued on next page

no	equation	documentation	layer
100	$E_{a\,N,K} :=$ Instantiate$(R_N \,.\, T_{N,K}, \#)$	Arrhenius activation energy	reactions
110	$c^n{}_{N,S} :=$ Instantiate$(_c_{N,S}, \#)$	norming concentration used in the definition of the species interaction probability	reactions
112	$\bar{n}_{N,S} := (c^n{}_{N,S})^{-1} \,.\, \_c_{N,S}$	normed concentration	reactions
113	$\bar{n}_{N,S,K} := P_{N,K} \,.\, \bar{n}_{N,S}$	normed concentration – context node and conversion	reactions
115	$\phi_{N,K} := \prod_S \bar{n}_{N,S,K}{}^{(N_{S,K})}$	probability for the species to meet to undergo reaction	reactions
118	$K^o{}_K :=$ Instantiate$(I_S \star \left(P_{N,K} \star \left((t)^{-1} \,.\, (V_N)^{-1} \,.\, n_{N,S}\right)\right), \#)$	Arrhenius frequency factor – a strange construction	reactions
119	$K_{N,K} := K^o{}_K \,.\, exp((-E_{a\,N,K}) \,.\, (R_N \,.\, T_{N,K})^{-1})$	reaction"constant	reactions
120	$\tilde{n}_{N,S} := V_N \,.\, (N_{S,K} \star (K_{N,K} \,.\, \phi_{N,K}))$	production term for differential component mass balance	reactions
122	$\dot{n}^p{}_{N,S} := \_\tilde{n}_{N,S}$	production term	macroscopic
123	$\dot{n}_{N,S} := \dot{n}^c{}_{N,S} + \dot{n}^d{}_{N,S} + \dot{n}^p{}_{N,S}$	differentional species balance	macroscopic
125	$\hat{w}_A :=$ Instantiate$(\hat{H}^c{}_A, \#)$	just an numerical work flow term – as a starter	macroscopic
126	$\dot{w}_N := F_{N,A} \star \hat{w}_A$	enthalpy accumulation due to work flows	macroscopic
127	$\dot{H}_N := \dot{H}^c{}_N + \dot{H}^d{}_N + \dot{q}_N + \dot{w}_N$	differential enthalpy balance	macroscopic
128	$H_N := \int_{t^o}^{t^e} \dot{H}_N \; dt + H^o{}_N$	Enthalpy	macroscopic

Continued on next page

no	equation	documentation	layer
129	$n_{N,S} := \int_{t^o}^{t^e} \dot{n}_{N,S} \;\; dt + {n^o}_{N,S}$	fundamental state - molar mass	macroscopic
130	${H^o}_N :=$ Instantiate$(H_N, \#)$	initial enthalpy	macroscopic
131	${n^o}_{N,S} :=$ Instantiate$(n_{N,S}, \#)$	initial species masses	macroscopic
132	${T^o}_N :=$ Instantiate$(T_N, \#)$	norming temperature	macroscopic
133	${p^o}_N :=$ Instantiate$(p_N, \#)$	normed pressure	macroscopic
134	${c^o}_{N,S} :=$ Instantiate$(c_{N,S}, \#)$	norming concentration	macroscopic
135	${\bar{T}^o}_N := T_N \, . \, ({T^o}_N)^{-1}$	normed temperature	macroscopic
136	${\bar{p}^o}_N := (p_N)^{-1} \, . \, p_N$	normed pressure	macroscopic
137	${\bar{c}^o}_{N,S} := ({c^o}_{N,S})^{-1} \, . \, c_{N,S}$	normed concentration	macroscopic
141	$m_A := F_{N,A} \star \_\bar{T}_N$	normed measurements of temparatures	control
142	$m_A := F_{N,A} \star \_\bar{p}_N$	normed measurements of pressures	control
143	$m_{A,S} := F_{N,A} \star \_\bar{c}_{N,S}$	normed measurment of concentration	control
144	${m^{v\star}}_A :=$ Instantiate$(m_A, \#)$	setpoint for measurement vector	control
145	${m^{m\star}}_{A,S} :=$ Instantiate$(m_{A,S}, \#)$	setpoiint for measurment matrix	control
146	${e^v}_A := {m^{v\star}}_A - m_A$	output error vector	control
147	${e^m}_{A,S} := {m^{m\star}}_{A,S} - m_{A,S}$	output error matrix	control
148	${u^v}_A := P \, . \, {e^v}_A$	control ouput vector	control
149	${u^m}_{A,S} := P \, . \, {e^m}_{A,S}$	control output matrix	control

Continued on next page

no	equation	documentation	layer
152	$I_N := \frac{d\,C_N}{d\,t}$	electric current definition	macroscopic
154	$R^e{}_N := ({}_{I\,N})^{-1} \,.\, U^e{}_N$	electrical resistance	material
155	$k^{e,x}{}_N := (R^e{}_N)^{-1} \,.\, (S_S \star \_x_{N,S})$	electrical conductivity – a simple model being a function of a selected set of species	material
156	$cp_N := C_{p\,N} \,.\, (m_N)^{-1}$	specific heat capacity at constant pressure	material
158	$m_N := \_\lambda_S \star n_{N,S}$	mass	macroscopic
159	$C_{p\,N} := m_N \,.\, \_c_{p\,N}$	total heat capacity	macroscopic
160	$T^{ref}{}_N := \text{Instantiate}(T_N, \#)$	reference temperature	macroscopic
161	$H_N := C_{p\,N} \,.\, \left(T_N - T^{ref}{}_N\right)$	Enthalpy	macroscopic
162	$T_N := Root\,(H_N)$	temperature	macroscopic
164	$\dot{x}_D := A_{N,D} \star x_N + B_{A,D} \star m_A$	differential controller state	control
165	$x_N := \int_{t^o}^{t^e} I_{N,D} \star \dot{x}_D \;\, d\,t + x^o{}_N$	controller state	control
166	$x^o{}_N := \text{Instantiate}(x_N, \#)$	initial controller state	control
167	$t^s := \text{Instantiate}(t, \#)$	switching time	control
168	$u^v{}_A := I_A \,.\, 0.5 \,.\, (1 + \text{sign}\,(t^s))$	control ouput vector – switch	control

16 Interface Link Equation

no	equation	documentation	layer
22	$\_\lambda_S := \lambda_S$	interface equation	material –> macro-scopic
60	$\_k^c_x{}_A := k^c_x{}_A$	interface equation	material –> macro-scopic
61	$\_k^c_y{}_A := k^c_y{}_A$	interface equation	material –> macro-scopic
62	$\_k^c_z{}_A := k^c_z{}_A$	interface equation	material –> macro-scopic
63	$\_k^d_x{}_{A,S} := k^d_x{}_{A,S}$	interface equation	material –> macro-scopic
64	$\_k_x^{d,Fick}{}_{A,S} := k_x^{d,Fick}{}_{A,S}$	interface equation	material –> macro-scopic
65	$\_k_y^{d,Fick}{}_{A,S} := k_y^{d,Fick}{}_{A,S}$	interface equation	material –> macro-scopic
66	$\_k^d_y{}_{A,S} := k^d_y{}_{A,S}$	interface equation	material –> macro-scopic
67	$\_k^d_z{}_{A,S} := k^d_z{}_{A,S}$	interface equation	material –> macro-scopic
68	$\_k_z^{d,Fick}{}_{A,S} := k_z^{d,Fick}{}_{A,S}$	interface equation	material –> macro-scopic
69	$\_k^q_x{}_A := k^q_x{}_A$	interface equation	material –> macro-scopic

Continued on next page

no	equation	documentation	layer
70	$\_k^q_{y}{}_A := k^q_{y}{}_A$	interface equation	material -> macroscopic
71	$\_k^q_{z}{}_A := k^q_{z}{}_A$	interface equation	material -> macroscopic
77	$\_\rho_N := \rho_N$	interface equation	material -> macroscopic
79	$\_\rho_A := \rho_A$	interface equation	material -> macroscopic
87	$\_x_{N,S} := x_{N,S}$	interface equation	macroscopic -> material
92	$\_h_{N,S} := h_{N,S}$	interface equation	material -> macroscopic
94	$\_h_{A,S} := h_{A,S}$	interface equation	material -> macroscopic
103	$\_E^a{}_{N,K} := E_{a\,N,K}$	interface equation	reactions -> macroscopic
106	${}_{N\,S,K} := N_{S,K}$	interface equation	reactions -> macroscopic
107	$\_T_{N,K} := T_{N,K}$	interface equation	reactions -> macroscopic
109	$\_c_{N,S} := c_{N,S}$	interface equation	macroscopic -> reactions
121	$\_\tilde{n}_{N,S} := \tilde{n}_{N,S}$	interface equation	reactions -> macroscopic

Continued on next page

no	equation	documentation	layer
138	$\_\bar{p}_N := \bar{p}^o{}_N$	interface equation	macroscopic –> control
139	$\_\bar{T}_N := \bar{T}^o{}_N$	interface equation	macroscopic –> control
140	$\_\bar{c}_{N,S} := \bar{c}^o{}_{N,S}$	interface equation	macroscopic –> control
150	$\_m^m{}_{A,S} := m^{m\star}{}_{A,S}$	interface equation	control –> macroscopic
151	$\_m^v{}_A := m^{v\star}{}_A$	interface equation	control –> macroscopic
153	${}_{IN} := I_N$	interface equation	macroscopic –> material
157	$\_c_{pN} := cp_N$	interface equation	material –> macroscopic