

1 Variables

2 root

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

3 physical

	var	symbol	documentation	type	units	eqs
98	I_S	I_S	vector of ones of length sepecies	projection		
170	S_S	S_S	species selection	projection		
14	r_{zN}	r_z	z-direction	frame	m	10
13	r_{yN}	r_y	y-direction	frame	m	9
11	ℓ_N	l	length	frame	m	
12	r_{xN}	r_x	x-direction	frame	m	8
189	h_N	height	height	frame	m	176
25	C_N	C	fundamental state - charge	state	$A s$	
16	U_N	U	fundamental state - internal energy	state	$kg m^2 s^{-2}$	
18	$n_{N,S}$	n	fundamental state - molar mass	state	mol	129
24	G_N	G	Gibbs free energy	state	$kg m^2 s^{-2}$	18
17	S_N	S	fundamental state - entropy	state	$kg m^2 K^{-1} s^{-2}$	
15	V_N	V	fundamental state - volume	state	m^3	11
22	H_N	H	Enthalpy	state	$kg m^2 s^{-2}$	15 128 161
23	A_N	A	Helmholts energy	state	$kg m^2 s^{-2}$	17
190	g	g	gravitational constant	constant	ms^{-2}	
33	B_N	Boltz	Boltzmann constant	constant	$kg m^2 K^{-1} s^{-2}$	24
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}	
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

Continued on next page

	var	symbol	documentation	type	units	eqs
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
29	v_{zN}	v_z	velocity in z-direction	secondaryState	ms^{-1}	21
28	v_{yN}	v_y	velocity in y-direction	secondaryState	ms^{-1}	20
27	v_{xN}	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
135	$K_{N,K}$	K	reaction"constant	properties	$m^{-3} mol s^{-1}$	119
131	$\phi_{N,K}$	interactionProbability	probability for the species to meet to undergo reaction	properties		115
115	$E_{a,N,K}$	Ea	Arrhenius activation energy	properties	$kg m^2 mol^{-1} s^{-2}$	100
118	$N_{S,K}$	N	stoichiometric matrix	properties		
134	K^o_K	Ko	Arrhenius frequency factor – a strange construction	properties	$m^{-3} mol s^{-1}$	118
126	$c^n_{N,S}$	c_norming	norming concentration used in the definition of the species interaction probability	properties	$m^{-3} mol$	110
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
172	cp_N	cp	specific heat capacity at constant pressure	property	$m^2 K^{-1} s^{-2}$	156
47	$h_{N,S}$	h	partial molar enthalpies	property	$kg m^2 mol^{-1} s^{-2}$	38
61	$k_x^{d,Fick}{}_{A,S}$	kd_x_Fick	Fick's diffusivity in arc and x-direction	property	ms^{-1}	51
58	m_N	m	mass	property	kg	48
50	k_{yA}^c	kc_y_A	convective mass conductivity in y-direction in arc	property	$m^{-1} s$	40
54	$k_{zA,S}^d$	kd_z_A	diffusional mass conductivity in z-direction in arc	property	$kg^{-1} m^{-4} mol^2 s$	44
45	k_{yN}^c	kc_y	convective mass conductivity in y-direction	property	$m^{-1} s$	36
42	$k_{yN,S}^d$	kd_y	diffusional mass conductivity in z-direction	property	$kg^{-1} m^{-4} mol^2 s$	33
26	λ_S	Mm	species' molecular mass	property	$kg mol^{-1}$	
52	$k_{xA,S}^d$	kd_x_A	diffusional mass conductivity in x-direction in arc	property	$kg^{-1} m^{-4} mol^2 s$	42
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
89	ρ_A	density_A	density of arc material	property	$kg m^{-3}$	78
49	k_{xA}^c	kc_x_A	convective mass conductivity in x-direction in arc	property	$m^{-1} s$	39
59	ρ_N	density	density	property	$kg m^{-3}$	49
60	v_S	v	molar volume of species	property	$m^3 mol^{-1}$	50
63	$k_z^{d,Fick}{}_{A,S}$	kd_z_Fick	Fick's diffusivity in arc and z-direction	property	ms^{-1}	53
56	k_{yA}^q	kq_y_A	thermal conductivity in y-direction in arc	property	$kg K^{-1} s^{-3}$	46
46	k_{zN}^c	kc_z	convective mass conductivity in z-direction	property	$m^{-1} s$	37
168	R_N^e	Re	electrical resistance	property	$kg m^2 A^{-2} s^{-3}$	154
53	$k_{yA,S}^d$	kd_y_A	diffusional mass conductivity in y-direction in arc	property	$kg^{-1} m^{-4} mol^2 s$	43
107	$h_{A,S}$	h_A	partial molar enthalpies of transport system	property	$kg m^2 mol^{-1} s^{-2}$	93
44	k_{xN}^c	kc_x	convective mass conductivity in x-direction	property	$m^{-1} s$	35

Continued on next page

	var	symbol	documentation	type	units	eqs
36	C_{pN}	Cp	total heat capacity at constant pressure	property	$kg\,m^2\,K^{-1}\,s^{-2}$	27
43	$k_{zN,S}^d$	kd_z	diffusional mass conductivity in z-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	34
39	k_{yN}^q	kq_y	thermal conductivity in y-direction	property	$kg\,K^{-1}\,s^{-3}$	30
55	k_{xA}^q	kq_x_A	thermal conductivity in x-direction in arc	property	$kg\,K^{-1}\,s^{-3}$	45
38	k_{xN}^q	kq_x	thermal conductivity in x-direction	property	$kg\,K^{-1}\,s^{-3}$	29
57	k_{zA}^q	kq_z_A	thermal conductivity in z-direction in arc	property	$kg\,K^{-1}\,s^{-3}$	47
51	k_{zA}^c	kc_z_A	convective mass conductivity in z-direction in arc	property	$m^{-1}\,s$	41
37	C_{vN}	Cv	total heat capacity at constant volume	property	$kg\,m^2\,K^{-1}\,s^{-2}$	28
41	$k_{xN,S}^d$	kd_x	diffusional mass conductivity in x-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	32
62	$k_{yA,S}^{d,Fick}$	kd_y_Fick	Fick's diffusivity in arc and y-direction	property	ms^{-1}	52
40	k_{zN}^q	kq_z	thermal conductivity in z-direction	property	$kg\,K^{-1}\,s^{-3}$	31
102	$\mu_{N,S}^o$	chemPot_o	standard chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	86

6 macroscopic

	var	symbol	documentation	type	units	eqs
196	$length_{pipe_A}$	length_pipe	length of pipe	transport	m	181
93	$\dot{n}_{N,S}^c$	anc	accumulation due to convective mass flow	transport	$mol\ s^{-1}$	82
101	$\hat{n}_{A,S}^d$	fnd	diffusional mass flow in arc	transport	$mol\ s^{-1}$	85 89
87	$c_{A,S}$	c_A	concentration in convective mass flow	transport	$m^{-3}\ mol$	76
112	\dot{H}_N^d	aHd	enthalpy accumulation due to diffusive mass flow	transport	$kg\ m^2\ s^{-3}$	98
91	\dot{V}_A	fV	volumetric flow	transport	$m^3\ s^{-1}$	80 172 175
188	\hat{m}_A	fm	mass flow rate	transport	$kg\ s^{-1}$	174
197	$friction_{coeff_{linear}}$	friction_coeff_linear	friction factor for linear friction model	transport	$kg\ ms^{-3}$	182
194	$height_{AA}$	height_A	height in arc node	transport	m	179
198	$fw_{friction}$	fw_friction	flow of energy loss due to friction – linear model	transport	$kg\ m^2\ s^{-3}$	183
110	\hat{H}_A^d	fHd	enthalpy flow due to diffusive mass flow	transport	$kg\ m^2\ s^{-3}$	96
141	\hat{w}_A	fw	just an numerical work flow term – as a starter	transport	$kg\ m^2\ s^{-3}$	125
109	\hat{H}_A^c	fHc	enthalpy flow due to convective mass flow	transport	$kg\ m^2\ s^{-3}$	95
84	\dot{q}_N	aq	accumulation due to conductive heat flow	transport	$kg\ m^2\ s^{-3}$	73
83	\hat{q}_{xA}	fq_x	heat flow in arc and x-direction	transport	$kg\ m^2\ s^{-3}$	72
199	\hat{E}_A^k	fE_kinetic	flow of kinetic energy	transport	$kg\ m^2\ s^{-3}$	184
166	I_N	I	electric current definition	transport	A	152
111	\dot{H}_N^c	aHc	enthalpy accumulation due to convective mass flow	transport	$kg\ m^2\ s^{-3}$	97
142	\dot{w}_N	aw	enthalpy accumulation due to work flows	transport	$kg\ m^2\ s^{-3}$	126
195	$fE_{potential_A}$	fE_potential	flow of potential energy	transport	$kg\ m^2\ s^{-3}$	180
86	d_A	d	fow direction of convective flow	transport		75

Continued on next page

	var	symbol	documentation	type	units	eqs
92	$\hat{n}_{A,S}^c$	fnc	convective mass flow in an arc	transport	$mol\ s^{-1}$	81
104	$\hat{n}_{N,S}^d$	and	accumulation due to diffusional mass transfer	transport	$mol\ s^{-1}$	90
66	A_{xzN}	A_xz	cross sectional area xz	geometry	m^2	55
70	A_{yzA}	A_yz_A	cross sectional area yz of arc	geometry	m^2	59
69	A_{xzA}	A_xz_A	cross sectional area xz of arc	geometry	m^2	58
67	A_{yzN}	A_yz	cross sectional area yz	geometry	m^2	56
68	A_{xyA}	A_xy_A	cross sectional area yz of arc	geometry	m^2	57
65	A_{xyN}	A_xy	cross sectional area xy	geometry	m^2	54
191	f	f	friction factor	properties		
186	k_A^{valve}	valveConstant	valve constant – pressure difference must be dimensionless	properties	$m^3\ s^{-1}$	171
64	$D_{N,A}$	D	difference operator	differenceOperator		
145	$n_{N,S}^o$	no	initial species masses	state	mol	131
144	H_N^o	Ho	initial enthalpy	state	$kg\ m^2\ s^{-2}$	130
174	m_N	m	mass	secondaryState	kg	158
85	$c_{N,S}$	c	molar concentration	secondaryState	$m^{-3}\ mol$	74
100	$x_{N,S}$	x	concentration mole fraction	secondaryState		84
150	\bar{p}_N^o	p_normed	normed pressure	secondaryState		136
146	T_N^o	T_norming	norming temperature	secondaryState	K	132
151	$\bar{c}_{N,S}^o$	c_normed	normed concentration	secondaryState		137
192	v_{xA}	v_x_A	velocity in arc	secondaryState	ms^{-1}	177
147	p_N^o	p_norming	normed pressure	secondaryState	$kg\ m^{-1}\ s^{-2}$	133
99	n_N^t	nt	total amount	secondaryState	mol	83
175	C_{pN}	Cp	total heat capacity	secondaryState	$kg\ m^2\ K^{-1}\ s^{-2}$	159
148	$c_{N,S}^o$	c_norming	norming concentration	secondaryState	$m^{-3}\ mol$	134

Continued on next page

	var	symbol	documentation	type	units	eqs
176	T^{ref}_N	T_ref	reference temperature	secondaryState	K	160
149	\bar{T}^o_N	T_normed	normed temperature	secondaryState		135
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	differential species balance	diffState	$mol\ s^{-1}$	123

7 control

	var	symbol	documentation	type	units	eqs
185	t_{sA}	<code>t_switch_A</code>	switching times	frame	s	169
183	x_N^o	<code>xo</code>	initial controller state	state		166
179	x_N	<code>x</code>	controller state	state		165
159	P	<code>P</code>	gain	constant		
157	m^{v*}_A	<code>setpoint_vector</code>	setpoint for measurement vector	constant		144
181	$I_{N,D}$	<code>I_N_D</code>	map differential space to node space	constant		
177	$A_{N,D}$	<code>A</code>	LTIS A-matrix	constant	s^{-1}	
158	$m^{m*}_{A,S}$	<code>setpoint_matrix</code>	setpoint for measurement matrix	constant		145
178	$B_{A,D}$	<code>B</code>	LTIS B-matrix	constant	s^{-1}	
182	\dot{x}_D	<code>dxdt</code>	differential controller state	diffState	s^{-1}	164
155	m_A	<code>measurement_vector</code>	normed measurements of temperatures	algebraic		141 142
156	$m_{A,S}$	<code>measurement_matrix</code>	normed measurement of concentration	algebraic		143
162	u^v_A	<code>u_vector</code>	control output vector	algebraic		148 170
160	e^v_A	<code>error_vector</code>	output error vector	algebraic		146
161	$e^m_{A,S}$	<code>error_matrix</code>	output error matrix	algebraic		147
163	$u^m_{A,S}$	<code>u_matrix</code>	control output matrix	algebraic		149

8 macroscopic-reactions

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

9 control-macroscopic

	var	symbol	documentation	type	units	eqs
164	$_{m^m_{A,S}}$	<code>_setpoint_matrix</code>	link variable setpoint matrix to interface control »> macroscopic	get		150
187	$_{u^v_A}$	<code>_u_vector</code>	link variable u vector to interface control »> macroscopic	get		173
165	$_{m^v_A}$	<code>_setpoint_vector</code>	link variable setpoint vector to interface control »> macroscopic	get		151

10 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
122	$_N_{S,K}$	$_N$	link variable N to interface reactions »> macroscopic	get		106
119	$_E^a_{N,K}$	$_Ea$	link variable Ea to interface reactions »> macroscopic	get	$kg\,m^2\,mol^{-1}\,s^{-2}$	103
137	$_n_{N,S}$	$_nProd$	link variable nProd to interface reactions »> macroscopic	get	$mol\,s^{-1}$	121

11 material–macroscopic

	var	symbol	documentation	type	units	eqs
76	$_{k_y^{d,Fick}}{}_{A,S}$	<code>_kd_y_Fick</code>	link variable kd y Fick to interface material »> macroscopic	get	ms^{-1}	65
78	$_{k_z^d}{}_{A,S}$	<code>_kd_z_A</code>	link variable kd z A to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	67
72	$_{k_y^c}{}_A$	<code>_kc_y_A</code>	link variable kc y A to interface material »> macroscopic	get	$m^{-1} s$	61
81	$_{k_y^q}{}_A$	<code>_kq_y_A</code>	link variable kq y A to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	70
30	$_{\lambda_S}$	<code>_Mm</code>	link variable Mm to interface material »> macroscopic	get	$kg mol^{-1}$	22
74	$_{k_x^d}{}_{A,S}$	<code>_kd_x_A</code>	link variable kd x A to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	63
79	$_{k_z^{d,Fick}}{}_{A,S}$	<code>_kd_z_Fick</code>	link variable kd z Fick to interface material »> macroscopic	get	ms^{-1}	68
90	$_{\rho_A}$	<code>_density_A</code>	link variable density A to interface material »> macroscopic	get	$kg m^{-3}$	79
106	$_{h_{N,S}}$	<code>_h</code>	link variable h to interface material »> macroscopic	get	$kg m^2 mol^{-1} s^{-2}$	92
77	$_{k_y^d}{}_{A,S}$	<code>_kd_y_A</code>	link variable kd y A to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	66
108	$_{h_{A,S}}$	<code>_h_A</code>	link variable h A to interface material »> macroscopic	get	$kg m^2 mol^{-1} s^{-2}$	94
80	$_{k_x^q}{}_A$	<code>_kq_x_A</code>	link variable kq x A to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	69
82	$_{k_z^q}{}_A$	<code>_kq_z_A</code>	link variable kq z A to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	71
75	$_{k_x^{d,Fick}}{}_{A,S}$	<code>_kd_x_Fick</code>	link variable kd x Fick to interface material »> macroscopic	get	ms^{-1}	64

Continued on next page

	var	symbol	documentation	type	units	eqs
88	$_{\rho N}$	_density	link variable density to interface material »> macroscopic	get	$kg\,m^{-3}$	77
173	$_{c_{pN}}$	_cp	link variable cp to interface material »> macroscopic	get	$m^2\,K^{-1}\,s^{-2}$	157
73	$_{k_{zA}^c}$	_kc_z_A	link variable kc z A to interface material »> macroscopic	get	$m^{-1}\,s$	62
71	$_{k_{xA}^c}$	_kc_x_A	link variable kc x A to interface material »> macroscopic	get	$m^{-1}\,s$	60

12 macroscopic-material

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

13 macroscopic-control

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

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	$\Delta := \text{sign}(t - t^o) - \text{sign}(t - (t^o - \Delta t))$	pulse of length time interval	root
8	$r_{xN} := \text{Instantiate}(\ell_N, \#)$	x-direction	physical
9	$r_{yN} := \text{Instantiate}(\ell_N, \#)$	y-direction	physical
10	$r_{zN} := \text{Instantiate}(\ell_N, \#)$	z-direction	physical
11	$V_N := r_{xN} \cdot r_{yN} \cdot r_{zN}$	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	$H_N := U_N - p_N \cdot V_N$	Enthalpy	physical
16	$T_N := \frac{\partial U_N}{\partial S_N}$	temperature	physical
17	$A_N := U_N - T_N \cdot S_N$	Helmholts energy	physical

Continued on next page

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

Continued on next page

no	equation	documentation	layer
36	$k_{yN}^c := \left(\lambda_S \star (\mu_{N,S})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$	convective mass conductivity in y-direction	material
37	$k_{zN}^c := \left(\lambda_S \star (\mu_{N,S})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convective mass conductivity in z-direction	material
38	$h_{N,S} := H_N \cdot (n_{N,S})^{-1}$	partial molar enthalpies	material
39	$k_{xA}^c := I_{N,A} \star k_{xN}^c$	convective mass conductivity in x-direction in arc	material
40	$k_{yA}^c := I_{N,A} \star k_{yN}^c$	convective mass conductivity in y-direction in arc	material
41	$k_{zA}^c := I_{N,A} \star k_{zN}^c$	convective mass conductivity in z-direction in arc	material
42	$k_{xA,S}^d := I_{N,A} \star k_{xN,S}^d$	diffusional mass conductivity in x-direction in arc	material
43	$k_{yA,S}^d := I_{N,A} \star k_{yN,S}^d$	diffusional mass conductivity in z-direction in arc	material
44	$k_{zA,S}^d := I_{N,A} \star k_{zN,S}^d$	diffusional mass conductivity in z-direction in arc	material
45	$k_{xA}^q := I_{N,A} \star k_{xN}^q$	thermal conductivity in x-direction in arc	material
46	$k_{yA}^q := I_{N,A} \star k_{yN}^q$	thermal conductivity in y-direction in arc	material
47	$k_{zA}^q := I_{N,A} \star k_{zN}^q$	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	$\rho_N := (V_N)^{-1} \cdot m_N$	density	material
50	$v_S := V_N \star (n_{N,S})^{-1}$	molar volume of species	material
51	$k_{x,A,S}^{d,Fick} := I_{N,A} \star \left(v_{xN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$	Fick's diffusivity in arc and x-direction	material
52	$k_{y,A,S}^{d,Fick} := I_{N,A} \star \left(v_{yN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$	Fick's diffusivity in arc and y-direction	material
53	$k_{z,A,S}^{d,Fick} := I_{N,A} \star \left(v_{zN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$	Fick's diffusivity in arc and z-direction	material
54	$A_{xyN} := r_{xN} \cdot r_{yN}$	cross sectional area xy	macroscopic
55	$A_{xzN} := r_{xN} \cdot r_{zN}$	cross sectional area xz	macroscopic
56	$A_{yzN} := r_{yN} \cdot r_{zN}$	cross sectional area yz	macroscopic
57	$A_{xyA} := I_{N,A} \star A_{xyN}$	cross sectional area yz of arc	macroscopic
58	$A_{xzA} := I_{N,A} \star A_{xzN}$	cross sectional area xz of arc	macroscopic
59	$A_{yzA} := I_{N,A} \star A_{yzN}$	cross sectional area yz of arc	macroscopic
72	$\hat{q}_{xA} := A_{yzA} \cdot _k_{xA}^q \cdot (D_{N,A} \star T_N)$	heat flow in arc and x-direction	macroscopic
73	$\dot{q}_N := F_{N,A} \star \hat{q}_{xA}$	accumulation due to conductive heat flow	macroscopic
74	$c_{N,S} := (V_N)^{-1} \cdot n_{N,S}$	molar concentration	macroscopic
75	$d_A := \mathbf{sign}(D_{N,A} \star p_N)$	flow direction of convective flow	macroscopic
76	$c_{A,S} := (0.5 \cdot (D_{N,A} - d_A \cdot D_{N,A})) \star c_{N,S}$	concentration in convective mass flow	macroscopic
78	$\rho_A := I_{N,A} \star \rho_N$	density of arc material	material
80	$\dot{V}_A := (_ \rho_A)^{-1} \cdot _k_{xA}^c \cdot A_{yzA} \cdot (D_{N,A} \star p_N)$	volumetric flow	macroscopic

Continued on next page

no	equation	documentation	layer
81	$\hat{n}_{A,S}^c := \dot{V}_A \cdot c_{A,S}$	convective mass flow in an arc	macroscopic
82	$\dot{n}_{N,S}^c := F_{N,A} \star \hat{n}_{A,S}^c$	accumulation due to convective mass flow	macroscopic
83	$n_N^t := I_S \star n_{N,S}$	total amount	macroscopic
84	$x_{N,S} := (n_N^t)^{-1} \cdot n_{N,S}$	concentration mole fraction	macroscopic
85	$\hat{n}_{A,S}^d := A_{yzA} \cdot (-_x k_{A,S}^{d,Fick}) \cdot (D_{N,A} \star c_{N,S})$	diffusional mass flow in arc	macroscopic
86	$\mu_{N,S}^o := \text{Instantiate}(\mu_{N,S}, \#)$	standard chemical potential	material
88	$\mu_{N,S} := \mu_{N,S}^o + R_N \cdot T_N \cdot \ln(_x x_{N,S})$	chemical potential standard model with mole fraction	material
89	$\hat{n}_{A,S}^d := A_{yzA} \cdot (-_x k_{A,S}^d) \cdot (D_{N,A} \star \mu_{N,S})$	diffusional mass flow in arc	macroscopic
90	$\dot{n}_{N,S}^d := F_{N,A} \star \hat{n}_{A,S}^d$	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	$\hat{H}_A^c := I_S \star (_h h_{A,S} \cdot \hat{n}_{A,S}^c)$	enthalpy flow due to convective mass flow	macroscopic
96	$\hat{H}_A^d := I_S \star (_h h_{A,S} \cdot \hat{n}_{A,S}^d)$	enthalpy flow due to diffusive mass flow	macroscopic
97	$\dot{H}_N^c := F_{N,A} \star \hat{H}_A^c$	enthalpy accumulation due to convective mass flow	macroscopic
98	$\dot{H}_N^d := F_{N,A} \star \hat{H}_A^d$	enthalpy accumulation due to diffusive mass flow	macroscopic
99	$T_{N,K} := T_N \cdot P_{N,K}$	temparature of the nodes with reactions	reactions

Continued on next page

no	equation	documentation	layer
100	$E_{aN,K} := \mathbf{Instantiate}(R_N . T_{N,K}, \#)$	Arrhenius activation energy	reactions
110	$c^n_{N,S} := \mathbf{Instantiate}(_c c_{N,S}, \#)$	norming concentration used in the definition of the species interaction probability	reactions
112	$\bar{n}_{N,S} := (c^n_{N,S})^{-1} . _c c_{N,S}$	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	$K^o_K := \mathbf{Instantiate}(I_S \star (P_{N,K} \star ((t)^{-1} . (V_N)^{-1} . n_{N,S})), \#)$	Arrhenius frequency factor – a strange construction	reactions
119	$K_{N,K} := K^o_K . \mathbf{exp}((-E_{aN,K}) . (R_N . T_{N,K})^{-1})$	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	$\dot{n}^p_{N,S} := _n \tilde{n}_{N,S}$	production term	macroscopic
123	$\dot{n}_{N,S} := \dot{n}^c_{N,S} + \dot{n}^d_{N,S} + \dot{n}^p_{N,S}$	differential species balance	macroscopic
125	$\hat{w}_A := \mathbf{Instantiate}(\hat{H}^c_A, \#)$	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	$n_{N,S} := \int_{t^o}^{t^e} \dot{n}_{N,S} dt + n_{N,S}^o$	fundamental state - molar mass	macroscopic
130	$H_N^o := \text{Instantiate}(H_N, \#)$	initial enthalpy	macroscopic
131	$n_{N,S}^o := \text{Instantiate}(n_{N,S}, \#)$	initial species masses	macroscopic
132	$T_N^o := \text{Instantiate}(T_N, \#)$	norming temperature	macroscopic
133	$p_N^o := \text{Instantiate}(p_N, \#)$	normed pressure	macroscopic
134	$c_{N,S}^o := \text{Instantiate}(c_{N,S}, \#)$	norming concentration	macroscopic
135	$\bar{T}_N^o := T_N \cdot (T_N^o)^{-1}$	normed temperature	macroscopic
136	$\bar{p}_N^o := (p_N)^{-1} \cdot p_N$	normed pressure	macroscopic
137	$\bar{c}_{N,S}^o := (c_{N,S}^o)^{-1} \cdot c_{N,S}$	normed concentration	macroscopic
141	$m_A := F_{N,A} \star \bar{T}_N$	normed measurements of temperatures	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	$m^{v\star}_A := \text{Instantiate}(m_A, \#)$	setpoint for measurement vector	control
145	$m^{m\star}_{A,S} := \text{Instantiate}(m_{A,S}, \#)$	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	$u^v_A := P \cdot e^v_A$	control ouput vector	control
149	$u^m_{A,S} := P \cdot e^m_{A,S}$	control output matrix	control

Continued on next page

no	equation	documentation	layer
152	$I_N := \frac{dC_N}{dt}$	electric current definition	macroscopic
154	$R_N^e := (I_N)^{-1} \cdot U_N^e$	electrical resistance	material
155	$k^{e,x}_N := (R_N^e)^{-1} \cdot (S_S \star _x_{N,S})$	electrical conductivity – a simple model being a function of a selected set of species	material
156	$cp_N := C_{pN} \cdot (m_N)^{-1}$	specific heat capacity at constant pressure	material
158	$m_N := _ \lambda_S \star n_{N,S}$	mass	macroscopic
159	$C_{pN} := m_N \cdot _ c_{pN}$	total heat capacity	macroscopic
160	$T_N^{ref} := \mathbf{Instantiate}(T_N, \#)$	reference temperature	macroscopic
161	$H_N := C_{pN} \cdot (T_N - T_N^{ref})$	Enthalpy	macroscopic
162	$T_N := \mathbf{Root}(H_N)$	temperature	macroscopic
164	$\dot{x}_D := A_{N,D} \star x_N + B_{A,D} \star m_A$	differential controller state	control
165	$x_N := \int_{t^o}^{t^e} I_{N,D} \star \dot{x}_D \, dt + x_N^o$	controller state	control
166	$x_N^o := \mathbf{Instantiate}(x_N, \#)$	initial controller state	control
169	$t_{sA} := \mathbf{Instantiate}(I_A \cdot t, \#)$	switching times	control
170	$u_A^v := 0.5 \cdot (I_A \cdot 1 - \mathbf{sign}((I_A \cdot t) - t_{sA}))$	control output vector – switches	control
171	$k^{valve}_A := \mathbf{Instantiate}(\dot{V}_A, \#)$	valve constant – pressure difference must be dimensionless	macroscopic
172	$\dot{V}_A := _ u_A^v \cdot k^{valve}_A \cdot \mathbf{sqrt}\left(\left(D_{N,A} \star \left(p_N \cdot (p_N^o)^{-1}\right)\right)\right)$	volumetric flow	macroscopic

Continued on next page

no	equation	documentation	layer
174	$\hat{m}_A := _ \rho_A \cdot \dot{V}_A$	mass flow rate	macroscopic
175	$\dot{V}_A := (I_{N,A} \star v_{xN}) \cdot A_{yzA}$	volumetric flow	macroscopic
176	$h_N := \mathbf{Instantiate}(\ell_N, \#)$	height	physical
177	$v_{xA} := I_{N,A} \star v_{xN}$	velocity in arc	macroscopic
179	$height_{AA} := I_{N,A} \star h_N$	height in arc node	macroscopic
180	$fE_{potential}_A := \hat{m}_A \cdot g \cdot height_{AA}$	flow of potential energy	macroscopic
181	$length_{pipe}_A := I_{N,A} \star \ell_N$	length of pipe	macroscopic
182	$friction_{coeflinear}_A := \mathbf{Instantiate}(fE_{potential}_A \cdot (length_{pipe}_A)^{-1}, \#)$	friction factor for linear friction model	macroscopic
183	$fw_{friction} := (-friction_{coeflinear}_A) \star length_{pipe}_A$	flow of energy loss due to friction – linear model	macroscopic
184	$\hat{E}_A^k := \hat{m}_A \cdot v_{xA} \cdot v_{xA}$	flow of kinetic energy	macroscopic

16 Interface Link Equation

no	equation	documentation	layer
22	$_{-}\lambda_S := \lambda_S$	interface equation	material -> macroscopic
60	$_{-}k_{xA}^c := k_{xA}^c$	interface equation	material -> macroscopic
61	$_{-}k_{yA}^c := k_{yA}^c$	interface equation	material -> macroscopic
62	$_{-}k_{zA}^c := k_{zA}^c$	interface equation	material -> macroscopic
63	$_{-}k_{xA,S}^d := k_{xA,S}^d$	interface equation	material -> macroscopic
64	$_{-}k_{x,A,S}^{d,Fick} := k_{x,A,S}^{d,Fick}$	interface equation	material -> macroscopic
65	$_{-}k_{y,A,S}^{d,Fick} := k_{y,A,S}^{d,Fick}$	interface equation	material -> macroscopic
66	$_{-}k_{yA,S}^d := k_{yA,S}^d$	interface equation	material -> macroscopic
67	$_{-}k_{zA,S}^d := k_{zA,S}^d$	interface equation	material -> macroscopic
68	$_{-}k_{z,A,S}^{d,Fick} := k_{z,A,S}^{d,Fick}$	interface equation	material -> macroscopic
69	$_{-}k_{xA}^q := k_{xA}^q$	interface equation	material -> macroscopic

Continued on next page

no	equation	documentation	layer
70	$_k_{yA}^q := k_{yA}^q$	interface equation	material \rightarrow macroscopic
71	$_k_{zA}^q := k_{zA}^q$	interface equation	material \rightarrow macroscopic
77	$_\rho_N := \rho_N$	interface equation	material \rightarrow macroscopic
79	$_\rho_A := \rho_A$	interface equation	material \rightarrow macroscopic
87	$_x_{N,S} := x_{N,S}$	interface equation	macroscopic \rightarrow material
92	$_h_{N,S} := h_{N,S}$	interface equation	material \rightarrow macroscopic
94	$_h_{A,S} := h_{A,S}$	interface equation	material \rightarrow macroscopic
103	$_E^a_{N,K} := E_{aN,K}$	interface equation	reactions \rightarrow macroscopic
106	$_N_{S,K} := N_{S,K}$	interface equation	reactions \rightarrow macroscopic
107	$_T_{N,K} := T_{N,K}$	interface equation	reactions \rightarrow macroscopic
109	$_c_{N,S} := c_{N,S}$	interface equation	macroscopic \rightarrow reactions
121	$_\tilde{n}_{N,S} := \tilde{n}_{N,S}$	interface equation	reactions \rightarrow 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	$_{I_N} := I_N$	interface equation	macroscopic material →
157	$_{c_{pN}} := c_{pN}$	interface equation	material → macroscopic
173	$_{u^v_A} := u^v_A$	interface equation	control → macroscopic