

## 1 Variables

## 2 root

	var	symbol	documentation	type	units	tokens	eqs
5	$F_{N,A}$	<b>F</b>	incidence matrix of a directed graph	network		[]	
170	$1_N$	<b>ones_N</b>	ones with length number of nodes	network		[]	
171	$1_A$	<b>ones_A</b>	ones with length of number of arcs	network		[]	
6	$t$	<b>t</b>	time	frame	<i>s</i>	[]	
7	$t_o$	<b>to</b>	starting time	frame	<i>s</i>	[]	4
8	$t_e$	<b>te</b>	end time	frame	<i>s</i>	[]	5
1	#	<b>value</b>	numerical value	constant		[]	
2	0	<b>zero</b>	numerical value zero	constant		[]	1
3	1	<b>one</b>	numerical value one	constant		[]	2
4	0.5	<b>onehalf</b>	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
159	$C_N$	C	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	$\mu_{NS}$	chem_pot	chemical potential	effort	$kg\ m^2\ mol^{-1}\ s^{-2}$	[]	32 114
160	$U^e_N$	Ue	voltage	effort	$kg\ m^2\ A^{-1}\ s^{-3}$	[]	156 177 182
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	$v_{yN}$	<b>v_y</b>	velocity in y direction	secondaryState	$ms^{-1}$	[]	13
24	$v_{zN}$	<b>v_z</b>	velocity in z-direction	secondaryState	$ms^{-1}$	[]	14
25	$v_N$	<b>v</b>	velocity vector	secondaryState	$ms^{-1}$	[]	15

## 4 control

	var	symbol	documentation	type	units	tokens	eqs
139	$m_A$	<b>mc</b>	measurements	input		[]	
158	$u_A$	<b>u</b>	data link	input		[]	155
129	$I_{N,D}$	<b>I_N_D</b>	identity to shift from differential space integral space	network		[]	
130	$I_{A,D}$	<b>I_A_D</b>	identity to shift from differential space to arc	network		[]	
137	$x_N$	<b>x</b>	controller state	state		[]	112
138	$x_N^o$	<b>xo</b>	controller initial condition	state		[]	103
133	$C_{N,A}$	<b>Cx</b>	measurement matrix	constant		[]	144
134	$D_{N,D}$	<b>Dx</b>	event matrix (dimension issue)	constant		[]	145
135	$y_A^o$	<b>setpoint</b>	set point	constant		[]	146
136	$D_A$	<b>D_A</b>	event diagonal matrix (no dimension problem)	constant		[]	147
142	$A_{N,D}$	<b>Ax</b>	dynamic control matrix	constant	$s^{-1}$	[]	148
143	$B_{A,D}$	<b>Bx</b>	input matrix	constant	$s^{-1}$	[]	149
144	$\dot{x}_D$	<b>dxdt</b>	differential controller state	diffState	$s^{-1}$	[]	106
140	$e_A$	<b>e</b>	control error	algebraic		[]	104
155	$y_A$	<b>y</b>	controller output	algebraic		[]	150 153

## 5 reactions

	var	symbol	documentation	type	units	tokens	eqs
86	$N_{S,K}$	N	stoichiometric matrix	constant		[]	
87	$E_{a,NK}$	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	$\phi_{KS}$	phi_KS	probability of species to meet	constant		[]	92

## 6 material

	var	symbol	documentation	type	units	tokens	eqs
29	$\lambda_S$	Mm	species molecular masses	constant	$kg\ mol^{-1}$	[]	142
30	$C_{pN}$	Cp	total heat capacity at constant pressure	property	$kg\ m^2\ K^{-1}\ s^{-2}$	[]	18
31	$C_{vN}$	Cv	total heat capacity at constant volume	property	$kg\ m^2\ K^{-1}\ s^{-2}$	[]	19
34	$k_{xN}^q$	kq_x	thermal conductivity in x-direction	property	$kg\ K^{-1}\ s^{-3}$	[]	22 131
35	$k_{yN}^q$	kq_y	thermal conductivity in y-direction	property	$kg\ K^{-1}\ s^{-3}$	[]	23 132
36	$k_{zN}^q$	kq_z	thermal conductivity in z-direction	property	$kg\ K^{-1}\ s^{-3}$	[]	24 133
37	$k_N^q$	kq	Cartesian thermal conductivity vector	property	$kg\ K^{-1}\ s^{-3}$	[]	25
50	$k_{xN}^c$	kc_x	convective mass conductivity in x-direction	property	$m^{-1}\ s$	[]	37 134
51	$k_{yN}^c$	kc_y	convective mass conductivity in y-direction	property	$m^{-1}\ s$	[]	38 135
52	$k_{zN}^c$	kc_z	convective mass conductivity in z-direction	property	$m^{-1}\ s$	[]	39 136
53	$k_N^c$	kc	Cartesian convective mass conductivity vector	property	$m^{-1}\ s$	[]	40
54	$k_{xNS}^d$	kd_x	diffusional mass conductivity in x-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	[]	41 137
55	$k_{yNS}^d$	kd_y	diffusional mass conductivity in y-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	[]	42 138
56	$k_{zNS}^d$	kd_z	diffusional mass conductivity in z-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	[]	43
57	$k_{NS}^d$	kd	Cartesian diffusional 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
71	$\rho_N$	density	mass density	property	$kg\ m^{-3}$	[]	49 154

Continued on next page

	var	symbol	documentation	type	units	tokens	eqs
148	$c_{pN}$	<b>cp</b>	specific heat capacity at constant pressure	property	$m^2 K^{-1} s^{-2}$	[]	<a href="#">120</a> <a href="#">140</a>
149	$c_{vN}$	<b>cv</b>	specific heat capacity at constant volume	property	$m^2 K^{-1} s^{-2}$	[]	<a href="#">121</a> <a href="#">141</a>
154	$\theta$	<b>data</b>	available data set	property		[]	<a href="#">143</a>
182	$kC_N$	<b>kC</b>	electrical conductiviy	property	$kg^{-1} m^{-2} A^2 s^3$	[]	<a href="#">178</a> <a href="#">195</a>
185	$k^{e,\xi}_N$	<b>k_e_xi</b>	very simple model for electrical conductivity due to species transort	property	$kg^{-1} m^{-2} A^2 s^3$	[]	<a href="#">181</a>
191	$k^{e,\xi}_N$	<b>k_e_o_xi</b>	base electrical conductivity per species	property	$kg^{-1} m^{-2} A^2 s^3$	[]	<a href="#">194</a>

## 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	$\hat{n}_{AS}^d$	fnd_AS	diffusional mass transfer per arc	transport	$mol s^{-1}$	[]	80
105	$\hat{n}_{NS}^d$	fnd	net diffusional mass transfer	transport	$mol s^{-1}$	[]	81
106	$\hat{H}_A^d$	fHd_A	enthalpy flow due to mass diffusion per arc	transport	$kg m^2 s^{-3}$	[]	82
107	$\hat{H}_N^d$	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	$\hat{n}_{AS}^c$	fnc_AS	convective molar mass flow per arc	transport	$mol s^{-1}$	[]	86
111	$\hat{n}_{NS}^c$	fnc	net convective molar mass flow	transport	$mol s^{-1}$	[]	87
120	$\hat{H}_A^c$	fHc_A	enthalpy flow due to convective mass flow	transport	$kg m^2 s^{-3}$	[]	96
121	$\hat{H}_N^c$	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
188	$i_A$	current_A	current in arc of circuit	transport	A	[]	191
95	$A_{yzN}$	Ayz	cross sectional area in x-direction	geometry	$m^2$	[]	71
96	$A_{xzN}$	Axz	cross sectional area in y direction	geometry	$m^2$	[]	72
97	$A_{xyN}$	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		[]	
177	$P_{N,NS}$	P_N_NS	projection of node to node x species	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
187	$i$	current	generic current	state	$A$	[]	
145	$T_{refN}$	T_ref	reference 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		[]	
181	$U^{e,circuit}_N$	Ue_circuit	closed circuit potential (will be set to zero)	effort	$kg\ m^2\ A^{-1}\ s^{-3}$	[]	175 176
69	$m_N$	m	mass	secondaryState	$kg$	[]	47
108	$c_{NS}$	c	molar concentration	secondaryState	$m^{-3}\ mol$	[]	84 127
152	$\psi$	intensities	collected intensities	secondaryState		[]	126
165	$n^t_N$	cnorm	moles per node	secondaryState	$m^{-3}\ mol$	[]	161
166	$\xi_{NS}$	x_frac	mole fractions	secondaryState		[]	162
77	$T_{NK}$	T_NK	temperature in reactive systems	conversion	$K$	[]	55

Continued on next page

	var	symbol	documentation	type	units	tokens	eqs
93	$N_{NS,NK}$	<b>N_NS_NK</b>	extended stoichiometric matrix	conversion		[]	<a href="#">69</a>
117	$\xi_{NK}$	<b>xi</b>	extend of reaction per volume	conversion	$m^{-3} mol s^{-1}$	[]	<a href="#">93</a>
118	$\tilde{n}_{NS}$	<b>pn</b>	production term	conversion	$mol s^{-1}$	[]	<a href="#">94</a>
119	$\dot{n}_{NS}$	<b>dndt</b>	differential molar mass balance	diffState	$mol s^{-1}$	[]	<a href="#">95</a> <a href="#">129</a>
126	$\dot{H}_N$	<b>dHdt</b>	differential enthalpy balance	diffState	$kg m^2 s^{-3}$	[]	<a href="#">102</a> <a href="#">128</a>
173	$current_{interenal_N}$	<b>current_interenal</b>	internal current	internalTransport	$A$	[]	<a href="#">168</a> <a href="#">196</a>
183	$i_{NS}$	<b>i_NS</b>	current due to species transport	internalTransport	$A$	[]	<a href="#">179</a>

## 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	$H_N := U_N - p_N \cdot V_N$	enthalpy	physical
10	$A_N := U_N - T_N \cdot S_N$	Helmholtz energy	physical
11	$G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$	Gibbs energy	physical
12	$v_{xN} := \frac{\partial r_{xN}}{\partial t}$	velocity in x-direction	physical
13	$v_{yN} := \frac{\partial r_{yN}}{\partial t}$	velocity in y direction	physical
14	$v_{zN} := \frac{\partial r_{zN}}{\partial t}$	velocity in z-direction	physical
15	$v_N := \text{Stack}(v_{xN}, v_{yN}, v_{zN})$	velocity vector	physical
16	$Bo_N := \text{Instantiate}(S_N, \#)$	Boltzmann constant	physical
17	$R_N := A^v \cdot Bo_N$	Gas constant	physical

*Continued on next page*



no	equation	documentation	layer
18	$C_{pN} := \frac{\partial H_N}{\partial T_N}$	total heat capacity	material
19	$C_{vN} := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	material
22	$k_{xN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}$	thermal conductivity in x-direction	material
23	$k_{yN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{yN}$	thermal conductivity in y-direction	material
24	$k_{zN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{zN}$	thermal conductivity in z-direction	material
25	$k_N^q := \text{Stack}(k_{xN}^q, k_{yN}^q, k_{zN}^q)$	Cartesian thermal conductivity vector	material
32	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	chemical potential	physical
37	$k_{xN}^c := \left( \lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass conductivity in x-direction	material
38	$k_{yN}^c := \left( \lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$	convective mass conductivity in y-direction	material
39	$k_{zN}^c := \left( \lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convective mass conductivity in z-direction	material
40	$k_N^c := \text{Stack}(k_{xN}^c, k_{yN}^c, k_{zN}^c)$	Cartesian convective mass conductivity vector	material
41	$k_{xNS}^d := (\mu_{NS})^{-1} \cdot \left( v_{xN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in x-direction	material
42	$k_{yNS}^d := (\mu_{NS})^{-1} \cdot \left( v_{yN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in y-direction	material
43	$k_{zNS}^d := (\mu_{NS})^{-1} \cdot \left( v_{zN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in z-direction	material

Continued on next page

no	equation	documentation	layer
44	$k_{NS}^d := \text{Stack}(k_{xNS}^d, k_{yNS}^d, k_{zNS}^d)$	Cartesian diffusional mass conductivity vector	material
45	$h_{NS} := H_N \odot (n_{NS})^{-1}$	partial molar enthalpies	material
46	$d_A := \text{sign}\left(F_{N,A} \stackrel{N}{\star} p_N\right)$	direction of convective ow	macroscopic
47	$m_N := \lambda_S \stackrel{S \in NS}{\star} n_{NS}$	mass	macroscopic
49	$\rho_N := m_N \cdot (V_N)^{-1}$	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	$T_{NK} := P_{N,NK} \stackrel{N}{\star} T_N$	temperature in reactive systems	macroscopic
64	$E_{aNK} := \text{Instantiate}(P_{N,NK} \stackrel{N}{\star} R_N \cdot T_{NK}, \#)$	Arrhenius's activation energy	reactions
65	$K_{NK} := K^o_K \odot \exp((-E_{aNK}) \cdot (R_N \stackrel{N}{\star} P_{N,NK} \cdot T_{NK})^{-1})$	Arrhenius reaction constant	reactions
69	$N_{NS,NK} := P_{S,NS} \stackrel{S}{\star} \left( (P_{K,NK} \cdot T_{NK} \cdot (T_{NK})^{-1}) \stackrel{K}{\star} N_{S,K} \right)$	extended stoichiometric matrix	macroscopic
71	$A_{yzN} := r_{yN} \cdot r_{zN}$	cross sectional area in x-direction	macroscopic
72	$A_{xzN} := r_{xN} \cdot r_{zN}$	cross sectional area in y direction	macroscopic
73	$A_{xyN} := r_{xN} \cdot r_{yN}$	cross sectional area in z-direction	macroscopic
74	$\hat{V}_A := (\rho_N)^{-1} \cdot k_{xN}^c \cdot A_{yzN} \cdot D_{N,A} \stackrel{N}{\star} p_N$	volumetric flow in x-direction	macroscopic
80	$\hat{n}_{AS}^d := A_{yzN} \odot (-k_{xNS}^d) \cdot D_{NS,AS} \stackrel{NS}{\star} \mu_{NS}$	diffusional mass transfer per arc	macroscopic
81	$\hat{n}_{NS}^d := F_{NS,AS} \stackrel{AS}{\star} \hat{n}_{AS}^d$	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	$c_{AS} := (0.5 \cdot (F_{NS,AS} - d_A \odot  F_{NS,AS} )) \overset{NS}{\star} c_{NS}$	molar 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	$\phi_{KS} := \prod \left( c_{KS} \cdot (c^o_{KS})^{-1} \right)$	probability of species to meet	reactions
93	$\xi_{NK} := K_{NK} \cdot P_{NK,KS} \overset{KS}{\star} \phi_{KS}$	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	$\hat{q}_A := A_{yzN} \cdot k_{xN}^q \cdot D_{N,A} \overset{N}{\star} T_N$	heat flow in x-direction	macroscopic
101	$\hat{q}_N := F_{N,A} \overset{A}{\star} \hat{q}_A$	net heat flow	macroscopic
102	$\dot{H}_N := \hat{H}_N^c + \hat{H}_N^d + \hat{q}_N + \hat{w}_N$	differential enthalpy balance	macroscopic
103	$x_N^o := \text{Instantiate}(x_N, \#)$	controller initial condition	control
104	$e_A := m_A - y_A^o$	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	$n_{NS} := \int_{t_o}^{t_e} \dot{n}_{NS} \, dt + n_{NS}^o$	species molar mass	macroscopic
117	$T_{refN} := \text{Instantiate}(T_N, \#)$	reference temperature	macroscopic

*Continued on next page*

no	equation	documentation	layer
120	$c_{pN} := C_{pN} \cdot (m_N)^{-1}$	specific heat capacity at constant pressure	material
121	$c_{vN} := C_{vN} \cdot (m_N)^{-1}$	specific heat capacity at constant volume	material
122	$H_N := m_N \cdot \int_{T_{refN}}^{T_N} c_{pN} dT_N$	enthalpy	macroscopic
123	$H_N := \int_{t_o}^{t_e} \dot{H}_N dt + H_N^o$	enthalpy	macroscopic
124	$n_{NS}^o := \text{Instantiate}(n_{NS}, \#)$	initial condition for species mass in nodes	macroscopic
125	$H_N^o := \text{Instantiate}(H_N, \#)$	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	$k_{xN}^q := \text{Instantiate}(k_{xN}^q, \#)$	thermal conductivity in x-direction	material

*Continued on next page*

no	equation	documentation	layer
132	$k_{yN}^q := \text{Instantiate}(k_{yN}^q, \#)$	thermal conductivity in y-direction	material
133	$k_{zN}^q := \text{Instantiate}(k_{zN}^q, \#)$	thermal conductivity in z-direction	material
134	$k_{xN}^c := \text{Instantiate}(k_{xN}^c, \#)$	convective mass convectivity in x-direction	material
135	$k_{yN}^c := \text{Instantiate}(k_{yN}^c, \#)$	convective mass convectivity in y-direction	material
136	$k_{zN}^c := \text{Instantiate}(k_{zN}^c, \#, -)$	convective mass convectivity in z-direction	material
137	$k_{xNS}^d := \text{Instantiate}(k_{xNS}^d, \#)$	diffusional mass conductivity in x-direction	material
138	$k_{yNS}^d := \text{Instantiate}(k_{yNS}^d, \#)$	diffusional mass conductivity in y-direction	material
139	$h_{NS} := \text{Instantiate}(h_{NS}, \#)$	partial molar enthalpies	material
140	$c_{pN} := \text{Instantiate}(c_{pN}, \#)$	specific heat capacity at constant pressure	material
141	$c_{vN} := \text{Instantiate}(c_{vN}, \#)$	specific heat capacity at constant volume	material
142	$\lambda_S := \text{Instantiate}(\lambda_S, \#)$	species molecular masses	material
143	$\theta := \text{MixedStack}(k_{yN}^q, k_{zN}^q, k_{xNS}^d, h_{NS}, c_{pN}, c_{vN}, \lambda_S, \rho_N)$	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	$y_A := C_{N,A} \overset{N}{\star} x_N + D_A \cdot e_A$	controller output	control
153	$y_A := D_A \cdot e_A$	controller output	control
154	$\rho_N := \text{Instantiate}(\rho_N, \#)$	mass density	material
155	$u_A := 1 \cdot y_A$	data link	control
156	$U^e_N := (C_N)^{-1} \cdot U_N$	voltage	physical
161	$n^t_N := 1_{NS} \overset{S \in NS}{\star} c_{NS}$	moles per node	macroscopic

*Continued on next page*

no	equation	documentation	layer
162	$\xi_{NS} := (n_N^t)^{-1} \odot c_{NS}$	mole fractions	macroscopic
168	$current_{interenal}_N := \frac{dC_N}{dt}$	internal current	macroscopic
175	$U^{e,circuit}_N := 1_N \cdot U^e_N$	closed circuit potential (will be set to zero)	macroscopic
176	$U^{e,circuit}_N := \text{Instantiate}(U^{e,circuit}_N, 0)$	closed circuit potential (will be set to zero)	macroscopic
177	$U^e_N := \text{Instantiate}(U^e_N, \#)$	voltage	macroscopic
178	$kC_N := current_{interenal}_N \cdot (U^e_N)^{-1}$	electrical conductivity	material
179	$i_{NS} := P_{N,NS} \overset{N}{\star} current_{interenal}_N$	current due to species transport	macroscopic
181	$k^{e,\xi}_N := (U^e_N)^{-1} \cdot \left( i_{NS} \overset{S \in NS}{\star} \ln(\xi_{NS}) \right)$	very simple model for electrical conductivity due to species transport	material
182	$U^e_N := (k^{e,\xi}_N)^{-1} \cdot current_{interenal}_N$	voltage	macroscopic
191	$i_A := 1_A \cdot i$	current in arc of circuit	macroscopic
194	$k^{e,\xi}_N := \text{Instantiate}(k^{e,\xi}_N, \#)$	base electrical conductivity per species	material
195	$kC_N := k^{e,\xi}_N \overset{S \in NS}{\star} \xi_{NS}$	electrical conductivity in node	material

Continued on next page



no	equation	documentation	layer
196	$current_{internal_N} := kC_N . U^e_N$	internal current	macroscopic