

1 Variables

2 root

	var	symbol	documentation	type	units	eqs
8	$F_{N,A}$	F_N_A	fudamental incidence matrix	network		
5	t	t	time	frame	s	
6	t^o	to	starting time	frame	s	4
7	t^e	te	end time	frame	s	5
1	#	value	numerical value	constant		
2	1	one	numerical value one	constant		1
3	0	zero	numerical value zero	constant		2
4	0.5	onehalf	numerical value one half	constant		3

3 physical

	var	symbol	documentation	type	units	eqs
9	$P_{N,A}$	P_N_A	projection from node to arc for arc properties	projection		
32	$P_{NS,AS}$	P_NS_AS	projection node species to arc species	projection		
33	$P_{K,NK}$	P_K_NK	projection of conversion to node conversion	projection		
34	$P_{S,NS}$	P_S_NS	projection species to node species	projection		
35	$P_{N,NK}$	P_N_NK	projection node to node conversion	projection		
36	$P_{NS,KS}$	P_NS_KS	projection node species to conversion species	projection		
37	$P_{A,NS}$	P_A_NS	projection arc to node species for conductivity	projection		
65	$P_{NK,KS}$	P_NK_KS	projection node conversion to conversion species	projection		
162	$P_{N,NS}$	P_N_NS	projection of nodes onto the node species	projection		
10	r_{xN}	r_x	x-coordinate	frame	m	
11	r_{yN}	r_y	y-coordinate	frame	m	
12	r_{zN}	r_z	z coordinate	frame	m	
13	U_N	U	fundamental state – internal energy	state	$kg\,m^2\,s^{-2}$	
14	S_N	S	fundamental state – entropy	state	$kg\,m^2\,K^{-1}\,s^{-2}$	
15	V_N	V	fundamental state – volume	state	m^3	133
16	n_{NS}	n	fundamental state – molar mass	state	mol	86
20	H_N	H	enthalpy	state	$kg\,m^2\,s^{-2}$	9 87
21	A_N	A	Helmholtz energy	state	$kg\,m^2\,s^{-2}$	10
22	G_N	G	Gibbs free energy	state	$kg\,m^2\,s^{-2}$	11
23	C_N	charge	fundamental state – charge	state	$A\,s$	
24	A^v	Avogadro	Avogadro number	constant	mol^{-1}	
17	p_N	p	thermodynamic pressure	effort	$kg\,m^{-1}\,s^{-2}$	6
18	T_N	T	temperature	effort	K	7

Continued on next page

	var	symbol	documentation	type	units	eqs
19	μ_{NS}	chemPot	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	8
27	Ue_N	Ue	electrical potential – voltage	effort	$kg\,m^2\,A^{-1}\,s^{-3}$	14 95
28	v_{xN}	v_x	velocity in x-direction	secondaryState	ms^{-1}	15
29	v_{yN}	v_y	velocity in y-direction	secondaryState	ms^{-1}	16
30	v_{zN}	v_z	velocity in z-direction	secondaryState	ms^{-1}	17

4 control

	var	symbol	documentation	type	units	eqs
136	x_N	x	state	state		111
137	x_{oN}	xo	initial state	state		109
129	$A_{N,D}$	A	dynamic matrix	constant	s^{-1}	
130	$B_{A,D}$	B	input matrix	constant	s^{-1}	
131	$C_{N,A}$	C	measurement matrix	constant		
132	D_A	D	diagonal event matrix (no dimensional problems)	constant		
133	y^o_A	setPoint	set point	constant		119
134	m_A	meas	measurements	constant		
135	e_A	e	control error	constant		108
139	$1_{N,D}$	I_N_D	space transformation D to N	constant		
138	\dot{x}_D	dxdt	differential state (ABCD) model	diffState	s^{-1}	110
141	\tilde{I}_N	Imeasured	measured current	algebraic	A	113
143	\tilde{U}^e_N	UeMeasured	measured electrical potential	algebraic	$kg\,m^2\,A^{-1}s^{-3}$	115
144	$\tilde{\xi}$	addMeasured	measured additive fraction	algebraic		116
145	R_N	RComputed	measured resistance	algebraic	$kg\,m^2\,A^{-2}s^{-3}$	117
146	S	store	quantities to be stored	algebraic		118
154	y_A	y	output equation	algebraic		126

5 reactions

	var	symbol	documentation	type	units	eqs
147	P_{NK}	P_NK	reactions per node	projection		
38	K^o_K	Ko	Arrhenius frequency factor	constant	$m^{-3} mol s^{-1}$	
62	E^a_{NK}	Ea	Arrhenius activation energy	constant	$kg m^2 mol^{-1} s^{-2}$	41
63	K_{NK}	K_NK	Arrhenius reaction 'constant'	constant	$m^{-3} mol s^{-1}$	42
155	B	Boltzmann	Boltzmann constant	constant	$kg m^2 K^{-1} s^{-2}$	
157	R	GasConstant	gas constant	constant	$kg m^2 mol^{-1} K^{-1} s^{-2}$	127
158	$N_{K,KS}$	N_K_KS	stoichiometry	constant		
159	$N_{NK,KS}$	N_NK_KS	extended stoichiometrix matrix	constant		128
60	T_{NK}	T_NK	temperature of the reactive system	effort	K	39
151	$c_{NK,KS}$	c	concentration matrix reaction per node and species per reaction	secondaryState	$m^{-3} mol$	123
152	$c^o_{NK,KS}$	co	norming concentration	secondaryState	$m^{-3} mol$	124
153	$x_{NK,KS}$	x	matrix of normed, dimensionless mole fractions	secondaryState		125
160	ϕ_{NK}	phi	probability function for reactions	secondaryState		129
163	\tilde{n}_{NS}	nProd	the species production term	secondaryState	$mol s^{-1}$	130

6 material

	var	symbol	documentation	type	units	eqs
40	λ_S	Mm	species molecular mass	constant	$kg\ mol^{-1}$	
112	ξ	additive	fraction of additives	constant		88
166	<i>DiffCoeff</i>	DiffCoeff	diffusion coefficient	constant	$m^3\ s^{-1}$	
42	C_{pN}	Cp	total heat capacity at constant pressure	property	$kg\ m^2\ K^{-1}\ s^{-2}$	21
43	C_{VN}	Cv	total heat capacity at constant volume	property	$kg\ m^2\ K^{-1}\ s^{-2}$	22
44	k_{xN}^q	kq_x	thermal conductivity in x-direction	property	$kg\ K^{-1}\ s^{-3}$	23
45	k_{yN}^q	kq_y	thermal conductivity in y-direction	property	$kg\ K^{-1}\ s^{-3}$	24
46	k_{zN}^q	kq_z	thermal conductivity in z-direction'	property	$kg\ K^{-1}\ s^{-3}$	25
47	k_N^q	kq	thermal conductivity	property	$kg\ K^{-1}\ s^{-3}$	26
48	k_{xN}^c	kc_x	convective mass conductivity in x-direction	property	$m^{-1}\ s$	27
49	k_{yN}^c	kc_y	convective mass conductivity in y-direction	property	$m^{-1}\ s$	28
50	k_{zN}^c	kc_z	convective mass conductivity in z-direction	property	$m^{-1}\ s$	29
51	k_N^c	kc	convective mass conductivity	property	$m^{-1}\ s$	30
52	k_{xNS}^d	kd_x	diffusional mass conductivity in x-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	31
53	k_{yNS}^d	kd_y	diffusional mass conductivity in y-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	32
54	k_{zNS}^d	kd_z	diffusional mass conductivity in z-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	33
55	k_{NS}^d	kd	diffusional mass conductivity	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	34
56	h_{NS}	h	partial molar enthalpies	property	$kg\ m^2\ mol^{-1}\ s^{-2}$	35
59	ρ_N	density	density	property	$kg\ m^{-3}$	38
115	R_N^e	elResist	electrical resistant	property	$kg\ m^2\ A^{-2}\ s^{-3}$	91 92
116	$k^{e,\xi}_N$	elConductC	simple model for the electrical conductivity as a function of the additive	property	$kg^{-1}\ m^{-2}\ A^2\ s^3$	93

7 macroscopic

	var	symbol	documentation	type	units	eqs
92	\hat{V}_A	fV	volumetric flow	transport	$m^3 s^{-1}$	67
93	\hat{n}^d_{AS}	fnd_AS	diffusional mass flow in a given stream	transport	$mol s^{-1}$	68 132
94	\hat{n}^d_{NS}	fnd	net diffusional mass flow	transport	$mol s^{-1}$	69
95	\hat{H}^d_A	fHd_A	enthalpy flow per diffusional mass stream	transport	$kg m^2 s^{-3}$	70
96	\hat{H}^d_N	fHd	net enthalpy stream due to diffusion	transport	$kg m^2 s^{-3}$	71
97	d_A	d	flow direction of convectional flow	transport		72
102	\hat{H}^c_A	fHc_A	convective enthalpy flow for given stream	transport	$kg m^2 s^{-3}$	77
103	\hat{H}^c_N	fHc	net convectional enthalpy stream	transport	$kg m^2 s^{-3}$	78
104	\hat{w}_A	fw_A	sample work stream	transport	$kg m^2 s^{-3}$	79
105	\hat{w}_N	fw	net work stream	transport	$kg m^2 s^{-3}$	80
106	\hat{q}_{xA}	fq_A_x	heat flow in x-direction for given stream	transport	$kg m^2 s^{-3}$	81
107	\hat{q}_N	fq	net heat flow	transport	$kg m^2 s^{-3}$	82
71	A_{yzN}	Ayz	cross sectional area yz	geometry	m^2	48
72	A_{xzN}	Axz	cross sectional area xz	geometry	m^2	49
73	A_{xyN}	Axy	cross sectional area xy	geometry	m^2	50
70	$F_{NS,AS}$	F_NS_AS	species related incidence matrix	network		
165	$Fd_{NS,AS}$	Fd	species related incidence matrix for diffusion	network		
90	$D_{N,A}$	D	difference operator	differenceOperator		
91	$D_{NS,AS}$	D_NS_AS	difference operator for species topology	differenceOperator		
167	$Dd_{NS,AS}$	Dd_NS_AS	difference operator for species topology (diffusion)	differenceOperator		
109	H^o_N	Ho	initial enthalpy	state	$kg m^2 s^{-2}$	84
110	n^o_{NS}	no	initial species	state	mol	85

Continued on next page

	var	symbol	documentation	type	units	eqs
127	1_S	one_S	a vector of ones with the length of the ordinal number of S	constant		
168	$DiffCoeff_{AS}$	DiffCoeff	Diffusion Coefficient	constant	$m^3 s^{-1}$	
57	m_N	m	total mass	secondaryState	kg	36
66	c_{NS}	c	molar composition	secondaryState	$m^{-3} mol$	44
98	c_{AS}	c_AS	concentration in convectional flow	secondaryState	$m^{-3} mol$	73
99	\hat{n}^c_{AS}	fnc_AS	molar convetional mass flow in the given stream	secondaryState	$mol s^{-1}$	74
100	\hat{n}^c_{NS}	fnc	net molar convectional mass flow	secondaryState	$mol s^{-1}$	75
126	ϕ	intensities	collected intensities	secondaryState		106
128	n^t_N	nTotal	total number of moles	secondaryState	mol	107
101	\dot{n}_{NS}	dndt	differential species balance	diffState	$mol s^{-1}$	76
108	\dot{H}_N	dHdt	differential enthalpy balance	diffState	$kg m^2 s^{-3}$	83
118	\dot{U}^e_N	dUedt	Kirkhoff first law	diffState	$kg m^2 A^{-1} s^{-3}$	96 97 98
113	I_N	i	electrical current definition	internalTransport	A	89

8 solid

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

9 fluid

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

10 liquid

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

11 gas

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

12 control-control

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

13 gas–liquid

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

14 gas–gas

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

15 liquid–liquid

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

16 gas–solid

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

17 solid–solid

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

18 liquid–solid

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

19 material–material

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

20 reactions-reactions

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

21 control-reactions

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

22 reactions-control

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

23 control-material

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

24 material-control

	var	symbol	documentation	type	units	eqs
124	$\mapsto \xi$	<code>_additive</code>	link variable additive to interface material » > control	get		104

25 control-macroscopic

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

26 macroscopic-control

	var	symbol	documentation	type	units	eqs
119	I_N	<code>_i</code>	link variable i to interface macroscopic »> control	get	A	99
125	T_N	<code>_T</code>	link variable T to interface macroscopic »> control	get	K	105
142	Ue_N	<code>_Ue</code>	link variable Ue to interface macroscopic »> control	get	$kg\,m^2\,A^{-1}s^{-3}$	114

27 reactions-material

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

28 material-reactions

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

29 reactions-macroscopic

	var	symbol	documentation	type	units	eqs
164	\tilde{n}_{NS}	_nProd	link variable nProd to interface reactions »> macroscopic	get	$mol\ s^{-1}$	131

30 macroscopic-reactions

	var	symbol	documentation	type	units	eqs
67	c_{NS}	<code>_c</code>	link variable c to interface macroscopic »> reactions	get	$m^{-3} mol$	45

31 material–macroscopic

	var	symbol	documentation	type	units	eqs
41	λ_S	_Mm	link variable Mm to interface material »> macroscopic	get	$kg\,mol^{-1}$	20
74	ρ_N	_density	link variable density to interface material »> macroscopic	get	$kg\,m^{-3}$	51
75	h_{NS}	_h	link variable h to interface material »> macroscopic	get	$kg\,m^2\,mol^{-1}\,s^{-2}$	52
76	k_{xN}^q	_kq_x	link variable kq x to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	53
77	C_{vN}^v	_Cv	link variable Cv to interface material »> macroscopic	get	$kg\,m^2\,K^{-1}\,s^{-2}$	54
78	k_{yN}^q	_kq_y	link variable kq y to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	55
79	k_{zN}^q	_kq_z	link variable kq z to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	56
80	k_N^q	_kq	link variable kq to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	57
81	k_{xN}^c	_kc_x	link variable kc x to interface material »> macroscopic	get	$m^{-1}\,s$	58
82	C_{pN}	_Cp	link variable Cp to interface material »> macroscopic	get	$kg\,m^2\,K^{-1}\,s^{-2}$	59
83	k_{yN}^c	_kc_y	link variable kc y to interface material »> macroscopic	get	$m^{-1}\,s$	60
84	k_{zN}^c	_kc_z	link variable kc z to interface material »> macroscopic	get	$m^{-1}\,s$	61
85	k_N^c	_kc	link variable kc to interface material »> macroscopic	get	$m^{-1}\,s$	62
86	k_{xNS}^d	_kd_x	link variable kd x to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	63
87	k_{yNS}^d	_kd_y	link variable kd y to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	64

Continued on next page

	var	symbol	documentation	type	units	eqs
88	k_{zNS}^d	<code>_kd_z</code>	link variable kd z to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	65
89	k_{NS}^d	<code>_kd</code>	link variable kd to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	66
117	R_N^e	<code>_elConductC</code>	link variable elConductC to interface material »> macroscopic	get	$kg^{-1} m^{-2} A^2 s^3$	94
140	ξ	<code>_additive</code>	link variable additive to interface material »> macroscopic	get		112

32 macroscopic-material

	var	symbol	documentation	type	units	eqs
58	m_N	_m	link variable m to interface macroscopic »> material	get	kg	37
114	I_N	_i	link variable i to interface macroscopic »> material	get	A	90

33 Equations

34 Generic

no	equation	documentation	layer
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
8	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	chemical potential	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 free energy	physical
14	$Ue_N := (C_N)^{-1} \cdot U_N$	electrical potential – voltage	physical
15	$v_{xN} := \frac{\partial r_{xN}}{\partial t}$	velocity in x-direction	physical
16	$v_{yN} := \frac{\partial r_{yN}}{\partial t}$	velocity in y direction	physical
17	$v_{zN} := \frac{\partial r_{zN}}{\partial t}$	velocity in z-direction	physical
21	$C_{pN} := \frac{\partial H_N}{\partial T_N}$	total heat capacity at constant pressure	material
22	$C_{VN} := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	material
23	$k_{xN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}$	thermal conductivity in x-direction	material
24	$k_{yN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{yN}$	thermal conductivity in y-direction	material
25	$k_{zN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{zN}$	thermal conductivity in z-direction'	material
26	$k_N^q := \text{Stack}(k_{xN}^q, k_{yN}^q, k_{zN}^q)$	thermal conductivity	material

Continued on next page

no	equation	documentation	layer
27	$k_{xN}^c := \left(\lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass conductivity in x-direction	material
28	$k_{yN}^c := \left(\lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$	convective mass conductivity in y-direction	material
29	$k_{zN}^c := \left(\lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convective mass conductivity in z-direction	material
30	$k_N^c := \text{Stack}(k_{xN}^c, k_{yN}^c, k_{zN}^c)$	convective mass conductivity	material
31	$k_{xNS}^d := (\mu_{NS})^{-1} \cdot \left(v_{xN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in x-direction	material
32	$k_{yNS}^d := (\mu_{NS})^{-1} \cdot \left(v_{yN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in y-direction	material
33	$k_{zNS}^d := (\mu_{NS})^{-1} \cdot \left(v_{zN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in z-direction	material
34	$k_{NS}^d := \text{Stack}(k_{xNS}^d, k_{yNS}^d, k_{zNS}^d)$	diffusional mass conductivity	material
35	$h_{NS} := H_N \odot (n_{NS})^{-1}$	partial molar enthalpies	material
36	$m_N := \lambda_S^{S \in NS} \star n_{NS}$	total mass	macroscopic
38	$\rho_N := m_N \cdot (V_N)^{-1}$	density	material
39	$T_{NK} := P_{N,NK} \star^N T_N$	temperature of the reactive system	reactions
42	$K_{NK} := K^o_K \odot \exp((-E^a_{NK}) \cdot (R \cdot T_{NK})^{-1})$	Arrhenius reaction 'constant'	reactions
44	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar composition	macroscopic
48	$A_{yzN} := r_{yN} \cdot r_{zN}$	cross sectional area yz	macroscopic

Continued on next page

no	equation	documentation	layer
49	$A_{xzN} := r_{xN} \cdot r_{zN}$	cross sectional area xz	macroscopic
50	$A_{xyN} := r_{xN} \cdot r_{yN}$	cross sectional area xy	macroscopic
67	$\hat{V}_A := (\rho_N)^{-1} \cdot k_{xN}^c \cdot A_{yzN} \cdot D_{N,A} \star^N p_N$	volumetric flow	macroscopic
68	$\hat{n}_{AS}^d := A_{yzN} \odot (-k_{xNS}^d) \cdot D_{NS,AS} \star^{NS} \mu_{NS}$	diffusional mass flow in a given stream	macroscopic
69	$\hat{n}_{NS}^d := F d_{NS,AS} \star^{AS} \hat{n}_{AS}^d$	net diffusional mass flow	macroscopic
70	$\hat{H}_A^d := \left(F_{NS,AS} \star^{NS} h_{NS} \right)^{S \in AS} \star \hat{n}_{AS}^d$	enthalpy flow per diffusional mass stream	macroscopic
71	$\hat{H}_N^d := F_{N,A} \star^A \hat{H}_A^d$	net enthaply stream due to diffusion	macroscopic
72	$d_A := \text{sign} \left(F_{N,A} \star^N p_N \right)$	flow direction of convectional flow	macroscopic
73	$c_{AS} := (0.5 \cdot (F_{NS,AS} - d_A \odot F_{NS,AS})) \star^{NS} c_{NS}$	concentration in convectional flow	macroscopic
74	$\hat{n}_{AS}^c := \hat{V}_A \odot c_{AS}$	molar convetional mass flow in the given stream	macroscopic
75	$\hat{n}_{NS}^c := F_{NS,AS} \star^{AS} \hat{n}_{AS}^c$	net molar convectional mass flow	macroscopic
76	$\dot{n}_{NS} := \hat{n}_{NS}^c + \hat{n}_{NS}^d + \tilde{n}_{NS}$	differential species balance	macroscopic
77	$\hat{H}_A^c := \left(F_{NS,AS} \star^{NS} h_{NS} \right)^{S \in AS} \star \hat{n}_{AS}^c$	convective enthalpy flow for given stream	macroscopic
78	$\hat{H}_N^c := F_{N,A} \star^A \hat{H}_A^c$	net convectional enthalpy stream	macroscopic
80	$\hat{w}_N := F_{N,A} \star^A \hat{w}_A$	net work stream	macroscopic
81	$\hat{q}_{xA} := A_{yzN} \cdot k_{xN}^q \cdot D_{N,A} \star^N T_N$	heat flow in x-direction for given stream	macroscopic
82	$\hat{q}_N := F_{N,A} \star^A \hat{q}_{xA}$	net heat flow	macroscopic

Continued on next page

no	equation	documentation	layer
83	$\dot{H}_N := \hat{H}^c_N + \hat{H}^d_N + \hat{q}_N + \hat{w}_N$	differential enthalpy balance	macroscopic
86	$n_{NS} := \int_{t^o}^{t^e} \dot{n}_{NS} \, dt$	fundamental state – molar mass	macroscopic
87	$H_N := \int_{t^o}^{t^e} \dot{H}_N \, dt$	enthalpy	macroscopic
89	$I_N := \frac{dC_N}{dt}$	electrical current definition	macroscopic
93	$k^{e,\xi}_N := (R^e_N)^{-1} \cdot \xi$	simple model for the electrical conductivity as a function of the additive	material
95	$Ue_N := (R^e_N)^{-1} \cdot I_N$	electrical potential – voltage	macroscopic
96	$\dot{U}^e_N := 1 \cdot Ue_N$	Kirkhoff first law	macroscopic
97	$\dot{U}^e_N := \text{Root}(Ue_N)$	Kirkhoff first law	macroscopic
106	$\phi := \text{MixedStack}(p_N, T_N, \mu_{NS}, c_{NS}, Ue_N)$	collected intensities	macroscopic
107	$n^t_N := 1_S \overset{S \in NS}{\star} n_{NS}$	total number of moles	macroscopic
108	$e_A := m_A - y^o_A$	control error	control
110	$\dot{x}_D := A_{N,D} \overset{N}{\star} x_N + B_{A,D} \overset{A}{\star} e_A$	differential state (ABCD) model	control
111	$x_N := \int_{t^o}^{t^e} 1_{N,D} \overset{D}{\star} \dot{x}_D \, dt$	state	control
113	$\check{I}_N := I_N$	measured current	control

Continued on next page

no	equation	documentation	layer
115	$\check{U}_N^e := U e_N$	measured electrical potential	control
116	$\check{\xi} := \mapsto \xi$	measured additive fraction	control
117	$R_N := (\check{I}_N)^{-1} \cdot \check{U}_N^e$	measured resistance	control
118	$S := \text{MixedStack}(\check{I}_N, \check{U}_N^e, R_N, \check{\xi})$	quantities to be stored	control
123	$c_{NK,KS} := P_{NK} \cdot \left(P_{NS,KS} \overset{NS}{\star} c_{NS} \right)$	var doc :	reactions
125	$x_{NK,KS} := (c_{NK,KS}^o)^{-1} \cdot c_{NK,KS}$	matrix of normed, dimensionless mole fractions	reactions
126	$y_A := C_{N,A} \overset{N}{\star} x_N + D_A \cdot e_A$	output equation	control
127	$R := A^v \cdot B$	gas constant	reactions
128	$N_{NK,KS} := P_{K,NK} \overset{K}{\star} N_{K,KS}$	extended stoichiometrix matrix	reactions
129	$\phi_{NK} := \prod_{KS} x_{NK,KS}^{N_{NK,KS}}$	probability function for reactions	reactions
130	$\tilde{n}_{NS} := V_N \overset{N}{\star} \left(P_{N,NK} \overset{NK}{\star} \left((K_{NK} \cdot \phi_{NK}) \cdot \left(P_{NS,KS} \overset{KS}{\star} N_{NK,KS} \right) \right) \right)$	the species production term	reactions
132	$\hat{n}_{AS}^d := \text{DiffCoeff}_{AS} \cdot \left(D_{NS,AS} \overset{NS}{\star} c_{NS} \right)$	diffusional mass flow in a given stream	macroscopic

Continued on next page

no	equation	documentation	layer
133	$V_N := m_N \cdot (\rho_N)^{-1}$	fundamental state – volume	macroscopic

35 Instantiate

no	equation	documentation	layer
1	$1 := \text{Instantiate}(\#, \#)$	numerical value 1	root
2	$0 := \text{Instantiate}(\#, \#)$	numerical value zero	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
41	$E^a_{NK} := \text{Instantiate}(R.T_{NK}, \#)$	Arrhenius activation energy	reactions
79	$\hat{w}_A := \text{Instantiate}(\hat{H}^c_A, \#)$	sample work stream	macroscopic
84	$H^o_N := \text{Instantiate}(H_N, \#)$	initial enthalpy	macroscopic
85	$n^o_{NS} := \text{Instantiate}(n_{NS}, \#)$	initial species	macroscopic
88	$\xi := \text{Instantiate}(\xi, \#)$	fraction of additives	material
91	$R^e_N := (I_N)^{-1} . Ue_N$	electrical resistant	material
92	$R^e_N := \text{Instantiate}(R^e_N, \#)$	electrical resistant	material
98	$\dot{U}^e_N := \text{Instantiate}(\dot{U}^e_N, 0)$	Kirkhoff first law	macroscopic
109	$xo_N := \text{Instantiate}(x_N, \#)$	initial state	control
119	$y^o_A := \text{Instantiate}(y^o_A, \#)$	set point	control

Continued on next page

no	equation	documentation	layer
124	$c^o_{NK,KS} := \text{Instantiate}(c_{NK,KS}, \#)$	norming concentration	reactions

36 Interface Link Equation

no	equation	documentation	layer
20	$\lambda_S := \lambda_S$	interface equation	material → macroscopic
37	$m_N := m_N$	interface equation	macroscopic → material
45	$c_{NS} := c_{NS}$	interface equation	macroscopic → reactions
51	$\rho_N := \rho_N$	interface equation	material → macroscopic
52	$h_{NS} := h_{NS}$	interface equation	material → macroscopic
53	$k_{xN}^q := k_{xN}^q$	interface equation	material → macroscopic
54	$C^{v_N} := C^{v_N}$	interface equation	material → macroscopic
55	$k_{yN}^q := k_{yN}^q$	interface equation	material → macroscopic
56	$k_{zN}^q := k_{zN}^q$	interface equation	material → macroscopic
57	$k_N^q := k_N^q$	interface equation	material → macroscopic
58	$k_{xN}^c := k_{xN}^c$	interface equation	material → macroscopic

Continued on next page

no	equation	documentation	layer
59	$CP_N := C_{pN}$	interface equation	material → macroscopic
60	$k_{yN}^c := k_{yN}^c$	interface equation	material → macroscopic
61	$k_{zN}^c := k_{zN}^c$	interface equation	material → macroscopic
62	$k_N^c := k_N^c$	interface equation	material → macroscopic
63	$k_{xNS}^d := k_{xNS}^d$	interface equation	material → macroscopic
64	$k_{yNS}^d := k_{yNS}^d$	interface equation	material → macroscopic
65	$k_{zNS}^d := k_{zNS}^d$	interface equation	material → macroscopic
66	$k_{NS}^d := k_{NS}^d$	interface equation	material → macroscopic
90	$I_N := I_N$	interface equation	macroscopic → material
94	$R_N^e := k_N^{e,\xi}$	interface equation	material → macroscopic
99	$I_N := I_N$	interface equation	macroscopic → control
104	$\mapsto \xi := \xi$	interface equation	material → control

Continued on next page

no	equation	documentation	layer
105	$T_N := T_N$	interface equation	macroscopic control →
112	$\xi := \xi$	interface equation	material → macroscopic
114	$Ue_N := Ue_N$	interface equation	macroscopic control →
131	$\tilde{n}_{NS} := \tilde{n}_{NS}$	interface equation	reactions → macroscopic