

1 Variables

2 root

	var	symbol	documentation	type	units	eqs
8	$F_{N,A}$	F_N_A	fundamental incidence matrix	network		
216	Δt	dt_pulse	lenth of pulse	frame	s	
217	$pulse$	pulse	pulse function	frame		180
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
162	$P_{N,NS}$	P_N_NS	projection of nodes onto the node species	projection		
200	$I_{NS,AS}$	I_NS_AS	projection species to node species	projection		
201	$I_{N,A}$	I_N_A	projection of nodes and arcs	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		
9	$P_{N,A}$	P_N_A	projection from node to arc for arc properties	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	
16	n_{NS}	n	fundamental state – molar mass	state	mol	86
20	H_N	H	enthalpy	state	$kg\,m^2\,s^{-2}$	9 87 184
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	$A\,s$	

Continued on next page

	var	symbol	documentation	type	units	eqs
165	B_N	boz	Boltzmann constant	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	132
166	R_N	R	gas constant	constant	$kg\,m^2\,mol^{-1}\,K^{-1}\,s^{-2}$	133
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	7 185 191
19	μ_{NS}	chemPot	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	8 136
27	U^e_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		
219	T^*_N	T_norm	temprature transmitter constant	constant	K	186
138	\dot{x}_D	dxdt	differential state (ABCD) model	diffState	s^{-1}	110
141	\tilde{I}_N	I_measured	measured current	algebraic	A	113
143	\tilde{U}^e_N	U_measured	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
154	y_A	y	output equation	algebraic		126
171	s	switch	switches at to	algebraic		138
220	\ddot{T}_N	T_measured	temperature signal	algebraic		187

5 reactions

	var	symbol	documentation	type	units	eqs
147	P_{NK}	P_NK	reactions per node	projection		
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 stoichiometric matrix	constant		128
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
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
115	R_N^e	elResist	electrical resistant	property	$kg\,m^2\,A^{-2}\,s^{-3}$	91 92
116	$k_N^{e,\xi}$	elConductC	simple model for the electrical conductivity as a function of the additive	property	$kg^{-1}\,m^{-2}\,A^2\,s^3$	93
183	$k_{NS}^{d,Fick}$	k_d_Fick	Fick's diffusivity	property	ms^{-1}	
187	h_{AS}	h_A	partial molar enthalpies (arc)	property	$kg\,m^2\,mol^{-1}\,s^{-2}$	153
188	$k_{AS}^{d,Fick}$	k_d_Fick_A	Fick's diffusivity (arc)	property	ms^{-1}	154
189	ρ_A	density_A	density (arc)	property	$kg\,m^{-3}$	155
190	$k_A^{e,\xi}$	elConductC_A	simple model for the electrical conductivity as a function of the additive (arc)	property	$kg^{-1}\,m^{-2}\,A^2\,s^3$	156
191	k_{xA}^c	kc_x_A	convective mass conductivity in x-direction (arc)	property	$m^{-1}\,s$	157
192	k_{yA}^c	kc_y_A	convective mass conductivity in y-direction (arc)	property	$m^{-1}\,s$	158
193	k_{zA}^c	kc_z_A	convective mass conductivity in z-direction	property	$m^{-1}\,s$	159
194	k_{xAS}^d	kd_x_A	diffusional mass conductivity in x-direction (arc)	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	160
195	k_{yAS}^d	kd_y_A	diffusional mass conductivity in y-direction (arc)	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	161
196	k_{zAS}^d	kd_z_A	diffusional mass conductivity in z-direction (arc)	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	162
197	k_{xA}^q	kq_x_A	thermal conductivity in x-direction (arc)	property	$kg\,K^{-1}\,s^{-3}$	163
198	k_{yA}^q	kq_y_A	thermal conductivity in y-direction (arc)	property	$kg\,K^{-1}\,s^{-3}$	164
199	k_{zA}^q	kq_z_A	thermal conductivity in z-direction (arc)	property	$kg\,K^{-1}\,s^{-3}$	165
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
48	k_{xN}^c	kc_x	convective mass conductivity in x-direction	property	$m^{-1}\,s$	27

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	var	symbol	documentation	type	units	eqs
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
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
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
183	$k^{d,Fick}_{NS}$	k_d_Fick	Fick's diffusivity	property	ms^{-1}	
187	h_{AS}	h_A	partial molar enthalpies (arc)	property	$kg m^2 mol^{-1} s^{-2}$	153
188	$k^{d,Fick}_{AS}$	k_d_Fick_A	Fick's diffusivity (arc)	property	ms^{-1}	154
189	ρ_A	density_A	density (arc)	property	$kg m^{-3}$	155
190	$k^{e,\xi}_A$	elConductC_A	simple model for the electrical conductivity as a function of the additive (arc)	property	$kg^{-1} m^{-2} A^2 s^3$	156
191	k_{xA}^c	kc_x_A	convective mass conductivity in x-direction (arc)	property	$m^{-1} s$	157
192	k_{yA}^c	kc_y_A	convective mass conductivity in y-direction (arc)	property	$m^{-1} s$	158
193	k_{zA}^c	kc_z_A	convective mass conductivity in z-direction	property	$m^{-1} s$	159
194	k_{xAS}^d	kd_x_A	diffusional mass conductivity in x-direction (arc)	property	$kg^{-1} m^{-4} mol^2 s$	160
195	k_{yAS}^d	kd_y_A	diffusional mass conductivity in y-direction (arc)	property	$kg^{-1} m^{-4} mol^2 s$	161
196	k_{zAS}^d	kd_z_A	diffusional mass conductivity in z-direction (arc)	property	$kg^{-1} m^{-4} mol^2 s$	162
197	k_{xA}^q	kq_x_A	thermal conductivity in x-direction (arc)	property	$kg K^{-1} s^{-3}$	163
198	k_{yA}^q	kq_y_A	thermal conductivity in y-direction (arc)	property	$kg K^{-1} s^{-3}$	164
199	k_{zA}^q	kq_z_A	thermal conductivity in z-direction (arc)	property	$kg K^{-1} s^{-3}$	165

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	var	symbol	documentation	type	units	eqs
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
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
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
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
112	ξ	additive	fraction of additives	constant		88
40	λ_S	Mm	species molecular mass	constant	$kg\,mol^{-1}$	

7 macroscopic

	var	symbol	documentation	type	units	eqs
100	\hat{n}_{NS}^c	fnc	net molar convectional mass flow	transport	$mol\ s^{-1}$	75
102	\hat{H}_A^c	fHc_A	convective enthalpy flow for given stream	transport	$kg\ m^2\ s^{-3}$	77
103	\hat{H}_N^c	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
92	\hat{V}_A	fV	volumetric flow	transport	$m^3\ s^{-1}$	67 140
93	\hat{n}_{AS}^d	fnd_AS	diffusional mass flow in a given stream	transport	$mol\ s^{-1}$	68 152
94	\hat{n}_{NS}^d	fnd	net diffusional mass flow	transport	$mol\ s^{-1}$	69
95	\hat{H}_A^d	fHd_A	enthalpy flow per diffusional mass stream	transport	$kg\ m^2\ s^{-3}$	70
96	\hat{H}_N^d	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
99	\hat{n}_{AS}^c	fnc_AS	molar convectional mass flow in the given stream	transport	$mol\ s^{-1}$	74
215	A_{yzA}	Ayz_A	cross sectional area yz (arc)	geometry	m^2	179
71	A_{yzN}	Ayz	cross sectional area yz	geometry	m^2	48
70	$F_{NS,AS}$	F_NS_AS	species related incidence matrix	network		
90	$D_{N,A}$	D	difference operator	differenceOperator		
91	$D_{NS,AS}$	D_NS_AS	difference operator for species topology	differenceOperator		
109	H_N^o	Ho	initial enthalpy	state	$kg\ m^2\ s^{-2}$	84
110	n_{NS}^o	no	initial species	state	mol	85

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	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		
218	T^{ref}_N	T_ref	reference temperature	effort	K	183
128	n^t_N	nTotal	total number of moles	secondaryState	mol	107
168	n_{tN}	nt	total number of species in a node	secondaryState	mol	134
169	ξ_{NS}	xi	mole fraction	secondaryState		135
176	g_{NS}	g		secondaryState	mol	145
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
170	\tilde{n}_{NS}	nProd	production term	conversion	$mol s^{-1}$	137
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	Kirkhoffs first law	diffState	$kg m^2 A^{-1} s^{-3}$	96 97 98
221	0_N	dHdt_0	event-discrete differential enthalpy balance	diffState	$kg m^2 s^{-3}$	188
222	0_{NS}	dndt_0	event-dynamic differential species balance	diffState	$mol s^{-1}$	189
113	I_N	i	electrical current definition	internalTransport	A	89

8 solid

	var	symbol	documentation	type	units	eqs
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9 fluid

	var	symbol	documentation	type	units	eqs
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10 energy

	var	symbol	documentation	type	units	eqs
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11 liquid

	var	symbol	documentation	type	units	eqs
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12 gas

	var	symbol	documentation	type	units	eqs
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13 control-control

	var	symbol	documentation	type	units	eqs
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14 energy–gas

	var	symbol	documentation	type	units	eqs
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15 energy–energy

	var	symbol	documentation	type	units	eqs
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16 gas–gas

	var	symbol	documentation	type	units	eqs
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17 energy-liquid

	var	symbol	documentation	type	units	eqs
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18 liquid–liquid

	var	symbol	documentation	type	units	eqs
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19 energy–solid

	var	symbol	documentation	type	units	eqs
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20 solid-solid

	var	symbol	documentation	type	units	eqs
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21 gas–liquid

	var	symbol	documentation	type	units	eqs
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22 gas-solid

	var	symbol	documentation	type	units	eqs
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23 liquid–solid

	var	symbol	documentation	type	units	eqs
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24 material–material

	var	symbol	documentation	type	units	eqs
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25 reactions-reactions

	var	symbol	documentation	type	units	eqs
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26 control-reactions

	var	symbol	documentation	type	units	eqs
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27 reactions-control

	var	symbol	documentation	type	units	eqs
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28 control-material

	var	symbol	documentation	type	units	eqs
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29 material-control

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

30 control-macroscopic

	var	symbol	documentation	type	units	eqs
172	<i>s</i>	<code>_switch</code>	switches at to	get		139

31 macroscopic-control

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

32 reactions-material

	var	symbol	documentation	type	units	eqs
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33 material-reactions

	var	symbol	documentation	type	units	eqs
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34 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

35 macroscopic-reactions

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

36 material–macroscopic

	var	symbol	documentation	type	units	eqs
117	$_{R^e_N}$	<code>_elConductC</code>	link variable elConductC to interface material »> macroscopic	get	$kg^{-1} m^{-2} A^2 s^3$	94
140	$_{\xi}$	<code>_additive</code>	link variable additive to interface material »> macroscopic	get		112
184	$_{k^{d,Fick}_{NS}}$	<code>_k_d_Fick</code>	link variable k d Fick to interface material »> macroscopic	get	ms^{-1}	151
202	$_{\rho_A}$	<code>_density_A</code>	link variable density A to interface material »> macroscopic	get	$kg m^{-3}$	166
203	$_{R^e_A}$	<code>_elConductC_A</code>	link variable elConductC A to interface material »> macroscopic	get	$kg^{-1} m^{-2} A^2 s^3$	167
204	$_{h_{AS}}$	<code>_h_A</code>	link variable h A to interface material »> macroscopic	get	$kg m^2 mol^{-1} s^{-2}$	168
205	$_{k^{d,Fick,A}_{AS}}$	<code>_k_d_Fick_A</code>	link variable k d Fick A to interface material »> macroscopic	get	ms^{-1}	169
206	$_{k^c_{xA}}$	<code>_kc_x_A</code>	link variable kc x A to interface material »> macroscopic	get	$m^{-1} s$	170
207	$_{k^c_{yA}}$	<code>_kc_y_A</code>	link variable kc y A to interface material »> macroscopic	get	$m^{-1} s$	171
208	$_{k^c_{zA}}$	<code>_kc_z_A</code>	link variable kc z A to interface material »> macroscopic	get	$m^{-1} s$	172
209	$_{k^d_{xAS}}$	<code>_kd_x_A</code>	link variable kd x A to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	173
210	$_{k^d_{yAS}}$	<code>_kd_y_A</code>	link variable kd y A to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	174
211	$_{k^d_{zAS}}$	<code>_kd_z_A</code>	link variable kd z A to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	175
212	$_{k^c_{xA}}$	<code>_kq_x_A</code>	link variable kq x A to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	176

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	var	symbol	documentation	type	units	eqs
213	$_{k_y^c A}$	$_{kq_y_A}$	link variable kq y A to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	177
214	$_{k_z^c A}$	$_{kq_z_A}$	link variable kq z A to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	178
41	$_{\lambda_S}$	$_{Mm}$	link variable Mm to interface material »> macroscopic	get	$kg mol^{-1}$	20
74	$_{\rho_N}$	$_{density}$	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	$_{k_x^q N}$	$_{kq_x}$	link variable kq x to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	53
77	$_{Cv_N}$	$_{Cv}$	link variable Cv to interface material »> macroscopic	get	$kg m^2 K^{-1} s^{-2}$	54
78	$_{k_y^q N}$	$_{kq_y}$	link variable kq y to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	55
79	$_{k_z^q N}$	$_{kq_z}$	link variable kq z to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	56
81	$_{k_x^c N}$	$_{kc_x}$	link variable kc x to interface material »> macroscopic	get	$m^{-1} s$	58
82	$_{Cp_N}$	$_{Cp}$	link variable Cp to interface material »> macroscopic	get	$kg m^2 K^{-1} s^{-2}$	59
83	$_{k_y^c N}$	$_{kc_y}$	link variable kc y to interface material »> macroscopic	get	$m^{-1} s$	60
84	$_{k_z^c N}$	$_{kc_z}$	link variable kc z to interface material »> macroscopic	get	$m^{-1} s$	61
86	$_{k_x^d NS}$	$_{kd_x}$	link variable kd x to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	63
87	$_{k_y^d NS}$	$_{kd_y}$	link variable kd y to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	64
88	$_{k_z^d NS}$	$_{kd_z}$	link variable kd z to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	65

37 macroscopic-material

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

38 Equations

39 Generic

no	equation	documentation	layer
10	$A_N := U_N - T_N \cdot S_N$	Helmholtz energy	physical
107	$n_N^t := 1_S \overset{S \in NS}{\star} n_{NS}$	total number of moles	macroscopic
108	$e_A := m_A - y_A^o$	control error	control
11	$G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$	Gibbs free energy	physical
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
115	$\check{U}_N^e := _U_N^e$	measured electrical potential	control
116	$\check{\xi} := _\xi$	measured additive fraction	control
117	$R_N := (\check{I}_N)^{-1} \cdot \check{U}_N^e$	measured resistance	control
123	$c_{NK,KS} := P_{NK} \cdot (P_{NS,KS} \overset{NS}{\star} _c_{NS})$	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

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no	equation	documentation	layer
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	$B_N := \text{Instantiate}(S_N, \#)$	Boltzmann constant	physical
133	$R_N := A^v \cdot B_N$	gas constant	physical
134	$n_{tN} := 1_S \overset{S \in NS}{\star} n_{NS}$	total number of species in a node	macroscopic
135	$\xi_{NS} := (n_{tN})^{-1} \odot n_{NS}$	mole fraction	macroscopic
136	$\mu_{NS} := (R_N \cdot T_N) \odot \ln(\xi_{NS})$	chemical potential	macroscopic
137	$\tilde{n}_{NS} := _ \tilde{n}_{NS}$	production term	macroscopic
138	$s := 0.5 \cdot (1 + \text{sign}(t^o))$	switches at to	control
139	$s := s$	switches at to	control \rightarrow macroscopic
14	$U^e_N := (C_N)^{-1} \cdot U_N$	electrical potential – voltage	physical
145	$g_{NS} := n_{NS} + n_{NS}$		macroscopic
15	$v_{xN} := \frac{\partial r_{xN}}{\partial t}$	velocity in x-direction	physical
152	$\hat{n}^d_{AS} := A_{yZA} \odot \left(_ k^{d,Fick,A}_{AS} \right) \cdot D_{NS,AS} \overset{NS}{\star} c_{NS}$	diffusional mass flow in a given stream	macroscopic
153	$h_{AS} := I_{NS,AS} \overset{NS}{\star} h_{NS}$	partial molar enthalpies (arc)	material
154	$k^{d,Fick}_{AS} := I_{NS,AS} \overset{NS}{\star} k^{d,Fick}_{NS}$	Fick's diffusivity (arc)	material
155	$\rho_A := I_{N,A} \overset{N}{\star} \rho_N$	density (arc)	material

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no	equation	documentation	layer
156	$k^{e,\xi}_A := I_{N,A} \stackrel{N}{\star} k^{e,\xi}_N$	simple model for the electrical conductivity as a function of the additive (arc)	material
157	$k^c_{xA} := I_{N,A} \stackrel{N}{\star} k^c_{xN}$	convective mass conductivity in x-direction (arc)	material
158	$k^c_{yA} := I_{N,A} \stackrel{N}{\star} k^c_{yN}$	convective mass conductivity in y-direction (arc)	material
159	$k^c_{zA} := I_{N,A} \stackrel{N}{\star} k^c_{zN}$	convective mass conductivity in z-direction	material
16	$v_{yN} := \frac{\partial r_{yN}}{\partial t}$	velocity in y direction	physical
160	$k^d_{xAS} := I_{NS,AS} \stackrel{NS}{\star} k^d_{xNS}$	diffusional mass conductivity in x-direction (arc)	material
161	$k^d_{yAS} := I_{NS,AS} \stackrel{NS}{\star} k^d_{yNS}$	diffusional mass conductivity in y-direction (arc)	material
162	$k^d_{zAS} := I_{NS,AS} \stackrel{NS}{\star} k^d_{zNS}$	diffusional mass conductivity in z-direction (arc)	material
163	$k^q_{xA} := I_{N,A} \stackrel{N}{\star} k^q_{xN}$	thermal conductivity in x-direction	material
164	$k^q_{yA} := I_{N,A} \stackrel{N}{\star} k^q_{yN}$	thermal conductivity in y-direction (arc)	material
165	$k^q_{zA} := I_{N,A} \stackrel{N}{\star} k^q_{zN}$	thermal conductivity in z-direction (arc)	material
17	$v_{zN} := \frac{\partial r_{zN}}{\partial t}$	velocity in z-direction	macroscopic
179	$A_{yzA} := I_{N,A} \stackrel{N}{\star} A_{yzN}$	cross sectional area yz (arc)	macroscopic
180	$pulse := \text{sign}(t - t^o) - \text{sign}(t - (t^o + \Delta t))$	pulse function	root

Continued on next page

no	equation	documentation	layer
183	$T_N^{ref} := \text{Instantiate}(T_N, -)$	reference temperature	macroscopic
184	$H_N := _Cp_N \cdot (T_N - T_N^{ref})$	enthalpy from constant heat capacity	macroscopic
185	$T_N := \text{Root}(H_N)$	temperature	macroscopic
186	$T_N^* := \text{Instantiate}(_T_N, \#)$	temprature transmitter constant	control
187	$\check{T}_N := _T_N \cdot (T_N^*)^{-1}$	temperature signal	control
188	$0_N := \hat{H}_N^c + \hat{H}_N^d + \hat{q}_N + \hat{w}_N - \dot{H}_N$	event-discrete differential enthalpy balance	macroscopic
189	$0_{NS} := \hat{n}_{NS}^c + \hat{n}_{NS}^d + _ \tilde{n}_{NS} - \dot{n}_{NS}$	event-dynamic differential species balance	macroscopic
191	$T_N := \text{Root}(0_N)$	temperature	macroscopic
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
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

Continued on next page

no	equation	documentation	layer
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
35	$h_{NS} := H_N \odot (n_{NS})^{-1}$	partial molar enthalpies	material
36	$m_N := _ \lambda_S \overset{S \in NS}{\star} n_{NS}$	total mass	macroscopic
38	$\rho_N := _ m_N \cdot (V_N)^{-1}$	density	material
39	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	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
6	$p_N := \left(-\frac{\partial U_N}{\partial V_N} \right)$	thermodynamic pressure	physical
67	$\hat{V}_A := (_ \rho_N)^{-1} \cdot _ k_{xN}^c \cdot A_{yzN} \cdot D_{N,A} \overset{N}{\star} p_N$	volumetric flow	macroscopic
68	$\hat{n}_{AS}^d := A_{yzA} \odot \left(-_ k_{xAS}^d \right) \cdot D_{NS,AS} \overset{NS}{\star} \mu_{NS}$	diffusional mass flow in a given stream	macroscopic
69	$\hat{n}_{NS}^d := F_{NS,AS} \overset{AS}{\star} \hat{n}_{AS}^d$	net diffusional mass flow	macroscopic
7	$T_N := \frac{\partial U_N}{\partial S_N}$	temperature	physical
70	$\hat{H}_A^d := \left(F_{NS,AS} \overset{NS}{\star} _ h_{NS} \right) \overset{S \in AS}{\star} \hat{n}_{AS}^d$	enthalpy flow per diffusional mass stream	macroscopic

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no	equation	documentation	layer
71	$\hat{H}^d_N := F_{N,A} \overset{A}{\star} \hat{H}^d_A$	net enthaply stream due to diffusion	macroscopic
72	$d_A := \text{sign} \left(F_{N,A} \overset{N}{\star} p_N \right)$	flow direction of convectional flow	macroscopic
73	$c_{AS} := (0.5 \cdot (F_{NS,AS} - d_A \odot F_{NS,AS})) \overset{NS}{\star} c_{NS}$	concentration in convectional flow	macroscopic
74	$\hat{n}^c_{AS} := \hat{V}_A \odot c_{AS}$	molar convetional mass flow in the given stream	macroscopic
75	$\hat{n}^c_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^c_{AS}$	net molar convectional mass flow	macroscopic
76	$\dot{n}_{NS} := \hat{n}^c_{NS} + \hat{n}^d_{NS} + _ \tilde{n}_{NS}$	differential species balance	macroscopic
77	$\hat{H}^c_A := \left(F_{NS,AS} \overset{NS}{\star} _ h_{NS} \right) \overset{S \in AS}{\star} \hat{n}^c_{AS}$	convective enthalpy flow for given stream	macroscopic
78	$\hat{H}^c_N := F_{N,A} \overset{A}{\star} \hat{H}^c_A$	net convectional enthalpy stream	macroscopic
8	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	chemical potential	physical
80	$\hat{w}_N := F_{N,A} \overset{A}{\star} \hat{w}_A$	net work stream	macroscopic
81	$\hat{q}_{xA} := A_{yzN} \cdot _ k^q_{xN} \cdot D_{N,A} \overset{N}{\star} T_N$	heat flow in x-direction for given stream	macroscopic
82	$\hat{q}_N := F_{N,A} \overset{A}{\star} \hat{q}_{xA}$	net heat flow	macroscopic
83	$\dot{H}_N := \hat{H}^c_N + \hat{H}^d_N + \hat{q}_N + \hat{w}_N$	differential enthalpy balance	macroscopic
86	$n_{NS} := \int_{t^o}^{t^e} \dot{n}_{NS} dt + n^o_{NS}$	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
9	$H_N := U_N - p_N \cdot V_N$	enthalpy	physical

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no	equation	documentation	layer
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	$U^e_N := (_R^e_N)^{-1} \cdot I_N$	electrical potential – voltage	macroscopic
96	$\dot{U}^e_N := 1 \cdot U^e_N$	Kirkhoff first law	macroscopic
97	$\dot{U}^e_N := Root(U^e_N)$	Kirkhoff first law	macroscopic

40 Instantiate

no	equation	documentation	layer
1	$1 := \text{Instantiate}(\#, \#)$	numerical value 1	root
109	$x_{oN} := \text{Instantiate}(x_N, \#)$	initial state	control
119	$y^o_A := \text{Instantiate}(y^o_A, \#)$	set point	control
124	$c^o_{NK,KS} := \text{Instantiate}(c_{NK,KS}, \#)$	norming concentration	reactions
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
41	$E^a_{NK} := \text{Instantiate}(R.T_{NK}, \#)$	Arrhenius activation energy	reactions
5	$t^e := \text{Instantiate}(t, \#)$	end time	root
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	$R^e_N := (_I_N)^{-1} . U^e_N$	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

41 Instantiation Equation

no	equation	documentation	layer
140	$\hat{V}_A := \text{Instantiate}(\hat{V}_A, \#)$	instantiation equation	macroscopic

42 Interface Link Equation

no	equation	documentation	layer
104	$_ \xi := \xi$	interface equation	material -> control
105	$_ T_N := T_N$	interface equation	macroscopic -> control
112	$_ \xi := \xi$	interface equation	material -> macroscopic
114	$_ U_N^e := U_N^e$	interface equation	macroscopic -> control
131	$_ \tilde{n}_{NS} := \tilde{n}_{NS}$	interface equation	reactions -> macroscopic
151	$_ k_{NS}^{d,Fick} := k_{NS}^{d,Fick}$	interface equation	material -> macroscopic
166	$_ \rho_A := \rho_A$	interface equation	material -> macroscopic
167	$_ R_A^e := k_{A}^{e,\xi}$	interface equation	material -> macroscopic
168	$_ h_{AS} := h_{AS}$	interface equation	material -> macroscopic
169	$_ k_{AS}^{d,Fick,A} := k_{AS}^{d,Fick}$	interface equation	material -> macroscopic
170	$_ k_{xA}^c := k_{xA}^c$	interface equation	material -> macroscopic

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no	equation	documentation	layer
171	$_k_{yA}^c := k_{yA}^c$	interface equation	material \rightarrow macroscopic
172	$_k_{zA}^c := k_{zA}^c$	interface equation	material \rightarrow macroscopic
173	$_k_{xAS}^d := k_{xAS}^d$	interface equation	material \rightarrow macroscopic
174	$_k_{yAS}^d := k_{yAS}^d$	interface equation	material \rightarrow macroscopic
175	$_k_{zAS}^d := k_{zAS}^d$	interface equation	material \rightarrow macroscopic
176	$_k_{xA}^c := k_{xA}^q$	interface equation	material \rightarrow macroscopic
177	$_k_{yA}^c := k_{yA}^q$	interface equation	material \rightarrow macroscopic
178	$_k_{zA}^c := k_{zA}^q$	interface equation	material \rightarrow macroscopic
20	$_\lambda_S := \lambda_S$	interface equation	material \rightarrow macroscopic
37	$_m_N := m_N$	interface equation	macroscopic \rightarrow material
45	$_c_{NS} := c_{NS}$	interface equation	macroscopic \rightarrow reactions
51	$_\rho_N := \rho_N$	interface equation	material \rightarrow macroscopic

Continued on next page

no	equation	documentation	layer
52	$_h_{NS} := h_{NS}$	interface equation	material \rightarrow macroscopic
53	$_k_{xN}^q := k_{xN}^q$	interface equation	material \rightarrow macroscopic
54	$_Cv_N := C_{VN}$	interface equation	material \rightarrow macroscopic
55	$_k_{yN}^q := k_{yN}^q$	interface equation	material \rightarrow macroscopic
56	$_k_{zN}^q := k_{zN}^q$	interface equation	material \rightarrow macroscopic
58	$_k_{xN}^c := k_{xN}^c$	interface equation	material \rightarrow macroscopic
59	$_Cp_N := C_{pN}$	interface equation	material \rightarrow macroscopic
60	$_k_{yN}^c := k_{yN}^c$	interface equation	material \rightarrow macroscopic
61	$_k_{zN}^c := k_{zN}^c$	interface equation	material \rightarrow macroscopic
63	$_k_{xNS}^d := k_{xNS}^d$	interface equation	material \rightarrow macroscopic
64	$_k_{yNS}^d := k_{yNS}^d$	interface equation	material \rightarrow macroscopic
65	$_k_{zNS}^d := k_{zNS}^d$	interface equation	material \rightarrow macroscopic

Continued on next page

no	equation	documentation	layer
90	$_I_N := I_N$	interface equation	macroscopic material \rightarrow
94	$_R^e_N := k^{e,\xi}_N$	interface equation	material \rightarrow macroscopic
99	$_I_N := I_N$	interface equation	macroscopic control \rightarrow