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	$r_{x\,N}$	r_x	x-coordinate	frame	m	
11	$r_{y\,N}$	r_y	y-coordinate	frame	m	
12	$r_{z\,N}$	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
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	$v_{x\,N}$	`v_x`	velocity in x-direction	secondaryState	ms^{-1}	15
29	$v_{y\,N}$	`v_y`	velocity in y-direction	secondaryState	ms^{-1}	16
30	$v_{z\,N}$	`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	$\check{I}_N$	`Imeasured`	measured current	algebraic	A	113
143	${\check{U}^e}_N$	`UeMeasured`	measured electrical potential	algebraic	$kg\,m^2\,A^{-1}s^{-3}$	115
144	$\check{\xi}$	`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

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	${R^e}_N$	`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	$kg^{-1}\,m^{-2}\,A^2s^3$	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	$kg^{-1}\,m^{-2}\,A^2s^3$	156
191	${k^c_x}_A$	`kc_x_A`	convective mass conductivity in x-direction (arc)	property	$m^{-1}\,s$	157
192	${k^c_y}_A$	`kc_y_A`	convective mass conductivity in y-direction (arc)	property	$m^{-1}\,s$	158
193	${k^c_z}_A$	`kc_z_A`	convective mass conductivity in z-direction	property	$m^{-1}\,s$	159
194	${k^d_x}_{AS}$	`kd_x_A`	diffusional mass conductivity in x-direction (arc)	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	160
195	${k^d_y}_{AS}$	`kd_y_A`	diffusional mass conductivity in y-direction (arc)	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	161
196	${k^d_z}_{AS}$	`kd_z_A`	diffusional mass conductivity in z-direction (arc)	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	162
197	${k^q_x}_A$	`kq_x_A`	thermal conductivity in x-direction (arc)	property	$kg\,K^{-1}\,s^{-3}$	163
198	${k^q_y}_A$	`kq_y_A`	thermal conductivity in y-direction (arc)	property	$kg\,K^{-1}\,s^{-3}$	164
199	${k^q_z}_A$	`kq_z_A`	thermal conductivity in z-direction (arc)	property	$kg\,K^{-1}\,s^{-3}$	165
42	${C_p}_N$	`Cp`	total heat capacity at constant pressure	property	$kg\,m^2\,K^{-1}\,s^{-2}$	21
43	${C_V}_N$	`Cv`	total heat capacity at constant volume	property	$kg\,m^2\,K^{-1}\,s^{-2}$	22
44	${k^q_x}_N$	`kq_x`	thermal conductivity in x-direction	property	$kg\,K^{-1}\,s^{-3}$	23
45	${k^q_y}_N$	`kq_y`	thermal conductivity in y-direction	property	$kg\,K^{-1}\,s^{-3}$	24
46	${k^q_z}_N$	`kq_z`	thermal conductivity in z-direction	property	$kg\,K^{-1}\,s^{-3}$	25
48	${k^c_x}_N$	`kc_x`	convective mass conductivity in x-direction	property	$m^{-1}\,s$	27

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	var	symbol	documentation	type	units	eqs
49	${k^c_y}_N$	kc_y	convective mass conductivity in y-direction	property	$m^{-1}\,s$	28
50	${k^c_z}_N$	kc_z	convective mass conductivity in z-direction	property	$m^{-1}\,s$	29
52	${k^d_x}_{NS}$	kd_x	diffusional mass conductivity in x-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	31
53	${k^d_y}_{NS}$	kd_y	diffusional mass conductivity in y-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	32
54	${k^d_z}_{NS}$	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	${R^e}_N$	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	$kg^{-1}\,m^{-2}\,A^2s^3$	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	$kg^{-1}\,m^{-2}\,A^2s^3$	156
191	${k^c_x}_A$	kc_x_A	convective mass conductivity in x-direction (arc)	property	$m^{-1}\,s$	157
192	${k^c_y}_A$	kc_y_A	convective mass conductivity in y-direction (arc)	property	$m^{-1}\,s$	158
193	${k^c_z}_A$	kc_z_A	convective mass conductivity in z-direction	property	$m^{-1}\,s$	159
194	${k^d_x}_{AS}$	kd_x_A	diffusional mass conductivity in x-direction (arc)	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	160
195	${k^d_y}_{AS}$	kd_y_A	diffusional mass conductivity in y-direction (arc)	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	161
196	${k^d_z}_{AS}$	kd_z_A	diffusional mass conductivity in z-direction (arc)	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	162
197	${k^q_x}_A$	kq_x_A	thermal conductivity in x-direction (arc)	property	$kg\,K^{-1}\,s^{-3}$	163
198	${k^q_y}_A$	kq_y_A	thermal conductivity in y-direction (arc)	property	$kg\,K^{-1}\,s^{-3}$	164
199	${k^q_z}_A$	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	$k^q_{x\,N}$	`kq_x`	thermal conductivity in x-direction	property	$kg\,K^{-1}\,s^{-3}$	23
45	$k^q_{y\,N}$	`kq_y`	thermal conductivity in y-direction	property	$kg\,K^{-1}\,s^{-3}$	24
46	$k^q_{z\,N}$	`kq_z`	thermal conductivity in z-direction	property	$kg\,K^{-1}\,s^{-3}$	25
48	$k^c_{x\,N}$	`kc_x`	convective mass conductivity in x-direction	property	$m^{-1}\,s$	27
49	$k^c_{y\,N}$	`kc_y`	convective mass conductivity in y-direction	property	$m^{-1}\,s$	28
50	$k^c_{z\,N}$	`kc_z`	convective mass conductivity in z-direction	property	$m^{-1}\,s$	29
52	$k^d_{x\,NS}$	`kd_x`	diffusional mass conductivity in x-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	31
53	$k^d_{y\,NS}$	`kd_y`	diffusional mass conductivity in y-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	32
54	$k^d_{z\,NS}$	`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	$\hat{n}^{c}{}_{NS}$	`fnc`	net molar convectional mass flow	transport	$mol\, s^{-1}$	75
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	$\hat{q}_{x\,A}$	`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
173	$\hat{n}^{c,controlled}{}_{AS}$	`fnc_AS_controlled`	switched flow	transport	$mol\, s^{-1}$	141 181
92	$\hat{V}_{A}$	`fV`	volumetric flow	transport	$m^3\, s^{-1}$	67 140
93	$\hat{n}^{d}{}_{AS}$	`fnd_AS`	diffusional mass flow in a given stream	transport	$mol\, s^{-1}$	68 152
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
99	$\hat{n}^{c}{}_{AS}$	`fnc_AS`	molar convectional mass flow in the given stream	transport	$mol\, s^{-1}$	74
215	$Ayz_{A\,A}$	`Ayz_A`	cross sectional area yz (arc)	geometry	m^2	179
71	$A_{yz\,N}$	`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	$H^{o}{}_{N}$	`Ho`	initial enthalpy	state	$kg\, m^2\, s^{-2}$	84

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	var	symbol	documentation	type	units	eqs
110	${n^o}_{NS}$	no	initial species	state	mol	85
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	$mol\,s^{-1}$	76 182
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
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 energy

	var	symbol	documentation	type	units	eqs

11 liquid

	var	symbol	documentation	type	units	eqs

12 gas

	var	symbol	documentation	type	units	eqs

13 control–control

	var	symbol	documentation	type	units	eqs

14 energy–gas

	var	symbol	documentation	type	units	eqs

15 energy–energy

	var	symbol	documentation	type	units	eqs

16 gas–gas

	var	symbol	documentation	type	units	eqs

17 energy–liquid

	var	symbol	documentation	type	units	eqs

18 liquid–liquid

	var	symbol	documentation	type	units	eqs

19 energy–solid

	var	symbol	documentation	type	units	eqs

20 solid–solid

	var	symbol	documentation	type	units	eqs

21 gas–liquid

	var	symbol	documentation	type	units	eqs

22 gas–solid

	var	symbol	documentation	type	units	eqs

23 liquid–solid

	var	symbol	documentation	type	units	eqs

24 material–material

	var	symbol	documentation	type	units	eqs

25 reactions–reactions

	var	symbol	documentation	type	units	eqs

26 control–reactions

	var	symbol	documentation	type	units	eqs

27 reactions–control

	var	symbol	documentation	type	units	eqs

28 control–material

	var	symbol	documentation	type	units	eqs

29 material–control

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

30 control–macroscopic

	var	symbol	documentation	type	units	eqs
172	s	`_switch`	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	Ue_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

33 material–reactions

	var	symbol	documentation	type	units	eqs

34 reactions–macroscopic

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

35 macroscopic–reactions

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

36 material–macroscopic

	var	symbol	documentation	type	units	eqs
117	$\_{R^e}_N$	`_elConductC`	link variable elConductC to interface material »> macroscopic	get	$kg^{-1}\,m^{-2}\,A^2 s^3$	94
140	$\_\xi$	`_additive`	link variable additive to interface material »> macroscopic	get		112
184	$\_{k^{d,Fick}}_{NS}$	`_k_d_Fick`	link variable k d Fick to interface material »> macroscopic	get	ms^{-1}	151
202	$\_\rho_A$	`_density_A`	link variable density A to interface material »> macroscopic	get	$kg\,m^{-3}$	166
203	$\_{R^e}_A$	`_elConductC_A`	link variable elConductC A to interface material »> macroscopic	get	$kg^{-1}\,m^{-2}\,A^2 s^3$	167
204	$\_h_{AS}$	`_h_A`	link variable h A to interface material »> macroscopic	get	$kg\,m^2\,mol^{-1}\,s^{-2}$	168
205	$\_{k^{d,Fick,A}}_{AS}$	`_k_d_Fick_A`	link variable k d Fick A to interface material »> macroscopic	get	ms^{-1}	169
206	$\_{k^c_x}_A$	`_kc_x_A`	link variable kc x A to interface material »> macroscopic	get	$m^{-1}\,s$	170
207	$\_{k^c_y}_A$	`_kc_y_A`	link variable kc y A to interface material »> macroscopic	get	$m^{-1}\,s$	171
208	$\_{k^c_z}_A$	`_kc_z_A`	link variable kc z A to interface material »> macroscopic	get	$m^{-1}\,s$	172
209	$\_{k^d_x}_{AS}$	`_kd_x_A`	link variable kd x A to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	173
210	$\_{k^d_y}_{AS}$	`_kd_y_A`	link variable kd y A to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	174
211	$\_{k^d_z}_{AS}$	`_kd_z_A`	link variable kd z A to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	175
212	$\_{k^c_x}_A$	`_kq_x_A`	link variable kq x A to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	176

Continued on next page

	var	symbol	documentation	type	units	eqs
213	$\_k^c_{yA}$	`_kq_y_A`	link variable kq y A to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	177
214	$\_k^c_{zA}$	`_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	$\_k^q_{xN}$	`_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	$\_k^q_{yN}$	`_kq_y`	link variable kq y to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	55
79	$\_k^q_{zN}$	`_kq_z`	link variable kq z to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	56
81	$\_k^c_{xN}$	`_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	$\_k^c_{yN}$	`_kc_y`	link variable kc y to interface material »> macroscopic	get	$m^{-1}\,s$	60
84	$\_k^c_{zN}$	`_kc_z`	link variable kc z to interface material »> macroscopic	get	$m^{-1}\,s$	61
86	$\_k^d_{xNS}$	`_kd_x`	link variable kd x to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	63
87	$\_k^d_{yNS}$	`_kd_y`	link variable kd y to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	64
88	$\_k^d_{zNS}$	`_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	$A_N := U_N - T_N \, . \, S_N$	Helmholtz energy	physical
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
11	$G_N := U_N + p_N \, . \, V_N - T_N \, . \, S_N$	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	$\check{U}^e{}_N := Ue_N$	measured electrical potential	control
116	$\check{\xi} := \mapsto \xi$	measured additive fraction	control
117	$R_N := \left(\check{I}_N\right)^{-1} . \, \check{U}^e{}_N$	measured resistance	control
123	$c_{NK,KS} := P_{NK} \, . \, \left(P_{NS,KS} \overset{NS}{\star} c_{NS}\right)$	var doc :	reactions
125	$x_{NK,KS} := \left(c^o{}_{NK,KS}\right)^{-1} . \, c_{NK,KS}$	matrix of normed, dimensionless mole fractions	reactions
126	$y_A := C_{N,A} \overset{N}{\star} x_N + D_A \, . \, e_A$	output equation	control
127	$R := A^v \, . \, B$	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	$\tilde{n}_{NS} := V_N \overset{N}{\star} \left(P_{N,NK} \overset{NK}{\star} \left((K_{NK} \,.\, \phi_{NK}) \,.\, \left(P_{NS,KS} \overset{KS}{\star} N_{NK,KS}\right)\right)\right)$	the species production term	reactions
132	$B_N := \text{Instantiate}(S_N, \#)$	Boltzmann constant	physical
133	$R_N := A^v \,.\, B_N$	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	$\mu_{NS} := (R_N \,.\, T_N) \odot ln(\xi_{NS})$	chemical potential	macroscopic
137	$\tilde{n}_{NS} := \tilde{n}_{NS}$	production term	macroscopic
138	$s := 0.5 \,.\, (1 + \text{sign}\,(t^o))$	switches at to	control
139	$s := s$	switches at to	control –> macro-scopic
14	$U^e{}_N := (C_N)^{-1} \,.\, U_N$	electrical potential – voltage	physical
141	$\hat{n}^{c,controlled}{}_{AS} := s \,.\, \hat{n}^c{}_{AS}$	switched flow	macroscopic
145	$g_{NS} := n_{NS} + n_{NS}$		macroscopic
15	$v_{xN} := \frac{\partial r_{xN}}{\partial t}$	velocitiy in x-direction	physical
152	$\hat{n}^d{}_{AS} := Ayz_{AA} \odot \left(-\_k^{d,Fick,A}{}_{AS}\right) \,.\, D_{NS,AS} \overset{NS}{\star} c_{NS}$	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	$k^{e,\xi}{}_{A} := I_{N,A} \overset{N}{\star} k^{e,\xi}{}_{N}$	simple model for the electrical conductivity as a function of the additive (arc)	material
157	$k^{c}_{x\,A} := I_{N,A} \overset{N}{\star} k^{c}_{x\,N}$	convective mass conductivity in x-direction (arc)	material
158	$k^{c}_{y\,A} := I_{N,A} \overset{N}{\star} k^{c}_{y\,N}$	convective mass conductivity in y-direction (arc)	material
159	$k^{c}_{z\,A} := I_{N,A} \overset{N}{\star} k^{c}_{z\,N}$	convective mass conductivity in z-direction	material
16	$v_{y\,N} := \frac{\partial\, r_{y\,N}}{\partial\, t}$	velocity in y direction	physical
160	$k^{d}_{x\,AS} := I_{NS,AS} \overset{NS}{\star} k^{d}_{x\,NS}$	diffusional mass conductivity in x-direction (arc)	material
161	$k^{d}_{y\,AS} := I_{NS,AS} \overset{NS}{\star} k^{d}_{y\,NS}$	diffusional mass conductivity in y-direction (arc)	material
162	$k^{d}_{z\,AS} := I_{NS,AS} \overset{NS}{\star} k^{d}_{z\,NS}$	diffusional mass conductivity in z-direction (arc)	material
163	$k^{q}_{x\,A} := I_{N,A} \overset{N}{\star} k^{q}_{x\,N}$	thermal conductivity in x-direction	material
164	$k^{q}_{y\,A} := I_{N,A} \overset{N}{\star} k^{q}_{y\,N}$	thermal conductivity in y-direction (arc)	material
165	$k^{q}_{z\,A} := I_{N,A} \overset{N}{\star} k^{q}_{z\,N}$	thermal conductivity in z-direction (arc)	material
17	$v_{z\,N} := \frac{\partial\, r_{z\,N}}{\partial\, t}$	velocity in z-direction	macroscopic
179	$Ayz_{A\,A} := I_{N,A} \overset{N}{\star} A_{yz\,N}$	cross sectional area yz (arc)	macroscopic
180	$pulse := \text{sign}\,(t - t^{o}) - \text{sign}\,(t - (t^{o} + \Delta t))$	pulse function	root

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no	equation	documentation	layer
181	$\hat{n}^{c,controlled}{}_{AS} := pulse \,.\, \hat{n}^{c}{}_{AS}$	manipulate flow	macroscopic
182	$\dot{n}_{NS} := \text{Instantiate}(\dot{n}_{NS}, 0)$	differential species balance – event dynamic	macroscopic
183	$T_ref_N := \text{Instantiate}(T_N, -)$	reference temperature	macroscopic
184	$H_N := \_Cp_N \,.\, (T_N - T_ref_N)$	enthalpy from constant heat capacity	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	$k^q_{xN} := (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial T_N} \,.\, v_{xN}$	thermal conductivity in x-direction	material
24	$k^q_{yN} := (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial T_N} \,.\, v_{yN}$	thermal conductivity in y-direction	material
25	$k^q_{zN} := (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial T_N} \,.\, v_{zN}$	thermal conductivity in z-direction'	material
27	$k^c_{xN} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \,.\, (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial p_N} \,.\, v_{xN}$	convecitve mass conductivity in x-direction	material
28	$k^c_{yN} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \,.\, (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial p_N} \,.\, v_{yN}$	convecitve mass conductivity in y-direction	material
29	$k^c_{zN} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \,.\, (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial p_N} \,.\, v_{zN}$	convecitve mass conductivity in z-direction	material
31	$k^d_{xNS} := (\mu_{NS})^{-1} \,.\, \left(v_{xN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in x-direction	material
32	$k^d_{yNS} := (\mu_{NS})^{-1} \,.\, \left(v_{yN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in y-direction	material
33	$k^d_{zNS} := (\mu_{NS})^{-1} \,.\, \left(v_{zN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in z-direction	material

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no	equation	documentation	layer
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	$\rho_N := m_N \,.\, (V_N)^{-1}$	density	material
39	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature of the reactive system	reactions
42	$K_{NK} := K^o{}_K \odot exp((-E^a{}_{NK}) \,.\, (R \,.\, T_{NK})^{-1})$	Arrhenius reaction 'constant'	reactions
44	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar composition	macroscopic
48	$A_{yzN} := r_{yN} \,.\, r_{zN}$	cross sectional area yz	macroscopic
6	$p_N := \left(-\frac{\partial U_N}{\partial V_N}\right)$	thermodynamic pressure	physical
67	$\hat{V}_A := (\_\rho_N)^{-1} \,.\, \_k^c_{xN} \,.\, A_{yzN} \,.\, D_{N,A} \overset{N}{\star} p_N$	volumetric flow	macroscopic
68	$\hat{n}^d{}_{AS} := Ayz_{AA} \odot \left(-\_k^d_{xAS}\right) \,.\, D_{NS,AS} \overset{NS}{\star} \mu_{NS}$	diffusional mass flow in a given stream	macroscopic
69	$\hat{n}^d{}_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^d{}_{AS}$	net diffusional mass flow	macroscopic
7	$T_N := \frac{\partial U_N}{\partial S_N}$	temperature	physical
70	$\hat{H}^d{}_A := \left(F_{NS,AS} \overset{NS}{\star} \_h_{NS}\right) \overset{S \in AS}{\star} \hat{n}^d{}_{AS}$	enthalpy flow per diffusional mass stream	macroscopic
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	$c_{AS} := (0.5 \,.\, (F_{NS,AS} - d_A \odot \lvert F_{NS,AS} \rvert)) \overset{NS}{\star} c_{NS}$	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

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no	equation	documentation	layer
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	$\hat{q}_{xA} := A_{yzN} \,.\, \_k^q_{xN} \,.\, D_{N,A} \overset{N}{\star} T_N$	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	$H_N := U_N - p_N \,.\, V_N$	enthalpy	physical
93	$k^{e,\xi}{}_N := \left(R^e{}_N\right)^{-1} \,.\, \xi$	simple model for the electrical conductivity as a function of the additive	material
95	$U^e{}_N := \left(\_R^e{}_N\right)^{-1} \,.\, I_N$	electrical potential – voltage	macroscopic
96	$\dot{U}^e{}_N := 1 \,.\, U^e{}_N$	Kirkhoff first law	macroscopic
97	$\dot{U}^e{}_N := Root\left(U^e{}_N\right)$	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	$\mapsto \xi := \xi$	interface equation	material –> control
105	$T_N := T_N$	interface equation	macroscopic –> control
112	$\_\xi := \xi$	interface equation	material –> macroscopic
114	$Ue_N := U^e{}_N$	interface equation	macroscopic –> control
131	$\tilde{n}_{NS} := \tilde{n}_{NS}$	interface equation	reactions –> macroscopic
151	$\_k^{d,Fick}{}_{NS} := k^{d,Fick}{}_{NS}$	interface equation	material –> macroscopic
166	$\_\rho_A := \rho_A$	interface equation	material –> macroscopic
167	$\_R^e{}_A := k^{e,\xi}{}_A$	interface equation	material –> macroscopic
168	$\_h_{AS} := h_{AS}$	interface equation	material –> macroscopic
169	$\_k^{d,Fick,A}{}_{AS} := k^{d,Fick}{}_{AS}$	interface equation	material –> macroscopic
170	$\_k^c_{x A} := k^c_{x A}$	interface equation	material –> macroscopic

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no	equation	documentation	layer
171	$\_k^c_{yA} := k^c_{yA}$	interface equation	material –> macroscopic
172	$\_k^c_{zA} := k^c_{zA}$	interface equation	material –> macroscopic
173	$\_k^d_{xAS} := k^d_{xAS}$	interface equation	material –> macroscopic
174	$\_k^d_{yAS} := k^d_{yAS}$	interface equation	material –> macroscopic
175	$\_k^d_{zAS} := k^d_{zAS}$	interface equation	material –> macroscopic
176	$\_k^c_{xA} := k^q_{xA}$	interface equation	material –> macroscopic
177	$\_k^c_{yA} := k^q_{yA}$	interface equation	material –> macroscopic
178	$\_k^c_{zA} := k^q_{zA}$	interface equation	material –> macroscopic
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

Continued on next page

no	equation	documentation	layer
52	$\_h_{NS} := h_{NS}$	interface equation	material –> macro-scopic
53	$\_k^q_{x}{}_N := k^q_{x}{}_N$	interface equation	material –> macro-scopic
54	$\_Cv_N := C_{VN}$	interface equation	material –> macro-scopic
55	$\_k^q_{y}{}_N := k^q_{y}{}_N$	interface equation	material –> macro-scopic
56	$\_k^q_{z}{}_N := k^q_{z}{}_N$	interface equation	material –> macro-scopic
58	$\_k^c_{x}{}_N := k^c_{x}{}_N$	interface equation	material –> macro-scopic
59	$\_Cp_N := C_{pN}$	interface equation	material –> macro-scopic
60	$\_k^c_{y}{}_N := k^c_{y}{}_N$	interface equation	material –> macro-scopic
61	$\_k^c_{z}{}_N := k^c_{z}{}_N$	interface equation	material –> macro-scopic
63	$\_k^d_{x}{}_{NS} := k^d_{x}{}_{NS}$	interface equation	material –> macro-scopic
64	$\_k^d_{y}{}_{NS} := k^d_{y}{}_{NS}$	interface equation	material –> macro-scopic
65	$\_k^d_{z}{}_{NS} := k^d_{z}{}_{NS}$	interface equation	material –> macro-scopic

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