

## 1 Variables

### 2 root

	var	symbol	documentation	type	units	eqs
8	$F_{N,A}$	F_N_A	fundamental 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
162	$P_{N,NS}$	P_N_NS	projection of nodes onto the node species	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
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	$A\,s$	
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	$mol^{-1}$	

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	var	symbol	documentation	type	units	eqs
17	$p_N$	<b>p</b>	thermodynamic pressure	effort	$kg\,m^{-1}\,s^{-2}$	<b>6</b>
18	$T_N$	<b>T</b>	temperature	effort	$K$	<b>7</b>
19	$\mu_{NS}$	<b>chemPot</b>	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	<b>8 136</b>
27	$Ue_N$	<b>Ue</b>	electrical potential – voltage	effort	$kg\,m^2\,A^{-1}\,s^{-3}$	<b>14 95</b>
28	$v_{xN}$	<b>v_x</b>	velocity in x-direction	secondaryState	$ms^{-1}$	<b>15</b>
29	$v_{yN}$	<b>v_y</b>	velocity in y-direction	secondaryState	$ms^{-1}$	<b>16</b>
30	$v_{zN}$	<b>v_z</b>	velocity in z-direction	secondaryState	$ms^{-1}$	<b>17</b>

## 4 control

	var	symbol	documentation	type	units	eqs
136	$x_N$	<b>x</b>	state	state		<a href="#">111</a>
137	$x_{oN}$	<b>xo</b>	initial state	state		<a href="#">109</a>
129	$A_{N,D}$	<b>A</b>	dynamic matrix	constant	$s^{-1}$	
130	$B_{A,D}$	<b>B</b>	input matrix	constant	$s^{-1}$	
131	$C_{N,A}$	<b>C</b>	measurement matrix	constant		
132	$D_A$	<b>D</b>	diagonal event matrix (no dimensional problems)	constant		
133	$y^o_A$	<b>setPoint</b>	set point	constant		<a href="#">119</a>
134	$m_A$	<b>meas</b>	measurements	constant		
135	$e_A$	<b>e</b>	control error	constant		<a href="#">108</a>
139	$1_{N,D}$	<b>I_N_D</b>	space transformation D to N	constant		
138	$\dot{x}_D$	<b>dxdt</b>	differential state (ABCD) model	diffState	$s^{-1}$	<a href="#">110</a>
141	$\tilde{I}_N$	<b>Imeasured</b>	measured current	algebraic	$A$	<a href="#">113</a>
143	$\tilde{U}^e_N$	<b>UeMeasured</b>	measured electrical potential	algebraic	$kg\,m^2\,A^{-1}s^{-3}$	<a href="#">115</a>
144	$\tilde{\xi}$	<b>addMeasured</b>	measured additive fraction	algebraic		<a href="#">116</a>
145	$R_N$	<b>RComputed</b>	measured resistance	algebraic	$kg\,m^2\,A^{-2}s^{-3}$	<a href="#">117</a>
146	$S$	<b>store</b>	quantities to be stored	algebraic		<a href="#">118</a>
154	$y_A$	<b>y</b>	output equation	algebraic		<a href="#">126</a>
171	$s$	<b>switch</b>	switches at to	algebraic		<a href="#">138</a>

## 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	$\phi_{NK}$	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
185	$I_{N,A}$	I_N_A	mapping from between node and arc – used for properties being used in arcs	projection		
186	$I_{NS,AS}$	I_NS_AS	mapping from between node and arc – used for properties being used in arcs	projection		
112	$\xi$	additive	fraction of additives	constant		88
40	$\lambda_S$	Mm	species molecular mass	constant	$kg\ mol^{-1}$	
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	$k_{dFick_{NS}}$	k_d_Fick	Fick's diffusivity	property	$ms^{-1}$	
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

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	var	symbol	documentation	type	units	eqs
56	$h_{NS}$	<b>h</b>	partial molar enthalpies	property	$kg\,m^2\,mol^{-1}\,s^{-2}$	35
59	$\rho_N$	<b>density</b>	density	property	$kg\,m^{-3}$	38

## 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
173	$\hat{n}_{AS}^{c,controlled}$	fnc_AS_controlled	switched flow	transport	$mol\ s^{-1}$	141
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
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		
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

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	var	symbol	documentation	type	units	eqs
110	$n_{NS}^o$	<b>no</b>	initial species	state	<i>mol</i>	<b>85</b>
127	$1_S$	<b>one_S</b>	a vector of ones with the length of the ordinal number of S	constant		
126	$\phi$	<b>intensities</b>	collected intensities	secondaryState		<b>106</b>
128	$n_N^t$	<b>nTotal</b>	total number of moles	secondaryState	<i>mol</i>	<b>107</b>
168	$n_{tN}$	<b>nt</b>	total number of species in a node	secondaryState	<i>mol</i>	<b>134</b>
169	$\xi_{NS}$	<b>xi</b>	mole fraction	secondaryState		<b>135</b>
176	$g_{NS}$	<b>g</b>		secondaryState	<i>mol</i>	<b>145</b>
57	$m_N$	<b>m</b>	total mass	secondaryState	<i>kg</i>	<b>36</b>
66	$c_{NS}$	<b>c</b>	molar composition	secondaryState	$m^{-3} mol$	<b>44</b>
98	$c_{AS}$	<b>c_AS</b>	concentration in convectional flow	secondaryState	$m^{-3} mol$	<b>73</b>
170	$\tilde{n}_{NS}$	<b>nProd</b>	production term	conversion	$mol s^{-1}$	<b>137</b>
101	$\dot{n}_{NS}$	<b>dndt</b>	differential species balance	diffState	$mol s^{-1}$	<b>76</b> <b>142</b>
108	$\dot{H}_N$	<b>dHdt</b>	differential enthalpy balance	diffState	$kg m^2 s^{-3}$	<b>83</b>
118	$\dot{U}_N^e$	<b>dUedt</b>	Kirkhoffs first law	diffState	$kg m^2 A^{-1} s^{-3}$	<b>96</b> <b>97</b> <b>98</b>
113	$I_N$	<b>i</b>	electrical current definition	internalTransport	<i>A</i>	<b>89</b>

## 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 liquid

	var	symbol	documentation	type	units	eqs
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## 11 gas

	var	symbol	documentation	type	units	eqs
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## 12 control-control

	var	symbol	documentation	type	units	eqs
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## 13 gas–liquid

	var	symbol	documentation	type	units	eqs
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## 14 gas–gas

	var	symbol	documentation	type	units	eqs
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## 15 liquid–liquid

	var	symbol	documentation	type	units	eqs
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## 16 gas–solid

	var	symbol	documentation	type	units	eqs
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## 17 solid-solid

	var	symbol	documentation	type	units	eqs
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## 18 liquid–solid

	var	symbol	documentation	type	units	eqs
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## 19 material–material

	var	symbol	documentation	type	units	eqs
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## 20 reactions-reactions

	var	symbol	documentation	type	units	eqs
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## 21 control-reactions

	var	symbol	documentation	type	units	eqs
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## 22 reactions-control

	var	symbol	documentation	type	units	eqs
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## 23 control-material

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

## 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
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## 28 material-reactions

	var	symbol	documentation	type	units	eqs
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## 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
117	$_{R^e_N}$	<code>_elConductC</code>	link variable elConductC to interface material »> macroscopic	get	$kg^{-1} m^{-2} A^2 s^3$	<a href="#">94</a>
140	$_{\xi}$	<code>_additive</code>	link variable additive to interface material »> macroscopic	get		<a href="#">112</a>
184	$_{k^{d,Fick}_{NS}}$	<code>_k_d_Fick</code>	link variable k d Fick to interface material »> macroscopic	get	$ms^{-1}$	<a href="#">151</a>
41	$_{\lambda_S}$	<code>_Mm</code>	link variable Mm to interface material »> macroscopic	get	$kg mol^{-1}$	<a href="#">20</a>
74	$_{\rho_N}$	<code>_density</code>	link variable density to interface material »> macroscopic	get	$kg m^{-3}$	<a href="#">51</a>
75	$_{h_{NS}}$	<code>_h</code>	link variable h to interface material »> macroscopic	get	$kg m^2 mol^{-1} s^{-2}$	<a href="#">52</a>
76	$_{k^q_{xN}}$	<code>_kq_x</code>	link variable kq x to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	<a href="#">53</a>
77	$_{Cv_N}$	<code>_Cv</code>	link variable Cv to interface material »> macroscopic	get	$kg m^2 K^{-1} s^{-2}$	<a href="#">54</a>
78	$_{k^q_{yN}}$	<code>_kq_y</code>	link variable kq y to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	<a href="#">55</a>
79	$_{k^q_{zN}}$	<code>_kq_z</code>	link variable kq z to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	<a href="#">56</a>
80	$_{k^q_N}$	<code>_kq</code>	link variable kq to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	<a href="#">57</a>
81	$_{k^c_{xN}}$	<code>_kc_x</code>	link variable kc x to interface material »> macroscopic	get	$m^{-1} s$	<a href="#">58</a>
82	$_{Cp_N}$	<code>_Cp</code>	link variable Cp to interface material »> macroscopic	get	$kg m^2 K^{-1} s^{-2}$	<a href="#">59</a>
83	$_{k^c_{yN}}$	<code>_kc_y</code>	link variable kc y to interface material »> macroscopic	get	$m^{-1} s$	<a href="#">60</a>
84	$_{k^c_{zN}}$	<code>_kc_z</code>	link variable kc z to interface material »> macroscopic	get	$m^{-1} s$	<a href="#">61</a>
85	$_{k^c_N}$	<code>_kc</code>	link variable kc to interface material »> macroscopic	get	$m^{-1} s$	<a href="#">62</a>

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	var	symbol	documentation	type	units	eqs
86	$_{k_x^d NS}$	<code>_kd_x</code>	link variable kd x to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	<b>63</b>
87	$_{k_y^d NS}$	<code>_kd_y</code>	link variable kd y to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	<b>64</b>
88	$_{k_z^d NS}$	<code>_kd_z</code>	link variable kd z to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	<b>65</b>
89	$_{k^d NS}$	<code>_kd</code>	link variable kd to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	<b>66</b>

## 32 macroscopic-material

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

### 33 Equations

### 34 Generic

no	equation	documentation	layer
10	$A_N := U_N - T_N \cdot S_N$	Helmholtz energy	physical
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
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	$\check{U}^e_N := Ue_N$	measured electrical potential	control
116	$\check{\xi} := \mapsto \xi$	measured additive fraction	control
117	$R_N := (\check{I}_N)^{-1} \cdot \check{U}^e_N$	measured resistance	control
118	$S := \text{MixedStack}(\check{I}_N, \check{U}^e_N, R_N, \check{\xi})$	quantities to be stored	control
123	$c_{NK,KS} := P_{NK} \cdot (P_{NS,KS} \overset{NS}{\star} c_{NS})$	var doc :	reactions
125	$x_{NK,KS} := (c^o_{NK,KS})^{-1} \cdot c_{NK,KS}$	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

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no	equation	documentation	layer
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
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 $\rightarrow$ macroscopic
14	$Ue_N := (C_N)^{-1} . U_N$	electrical potential – voltage	physical
141	$\hat{n}^{c,controlled}_{AS} := s . \hat{n}^c_{AS}$	switched flow	macroscopic
142	$\dot{n}_{NS} := F_{NS,AS} \overset{AS}{\star} \text{Stack}(\hat{n}^c_{AS}, \hat{n}^{c,controlled}_{AS})$	differential species balance switched	macroscopic
145	$g_{NS} := n_{NS} + n_{NS}$		macroscopic
15	$v_{xN} := \frac{\partial r_{xN}}{\partial t}$	velocity in x-direction	physical
152	$\hat{n}^d_{AS} := A_{yzN} \odot (-_k^{d,Fick}_{NS}) . D_{NS,AS} \overset{NS}{\star} c_{NS}$	diffusional mass flow in a given stream	macroscopic

Continued on next page

no	equation	documentation	layer
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	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
26	$k_N^q := \text{Stack}(k_{xN}^q, k_{yN}^q, k_{zN}^q)$	thermal conductivity	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
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

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no	equation	documentation	layer
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	$m_N := \_ \lambda_S \overset{S \in NS}{\star} n_{NS}$	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
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
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	$\hat{n}_{AS}^d := A_{yzN} \odot (\_ k_{xNS}^d) \cdot D_{NS,AS} \overset{NS}{\star} \mu_{NS}$	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
71	$\hat{H}_N^d := F_{N,A} \overset{A}{\star} \hat{H}_A^d$	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

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no	equation	documentation	layer
73	$c_{AS} := (0.5 \cdot (F_{NS,AS} - d_A \odot  F_{NS,AS} )) \overset{NS}{\star} c_{NS}$	concentration in convectonal 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 convectonal 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 convectonal 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
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

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no	equation	documentation	layer
96	$\dot{U}^e_N := 1 . U e_N$	Kirkhoff first law	macroscopic
97	$\dot{U}^e_N := Root (U e_N)$	Kirkhoff first law	macroscopic

## 35 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	$R^e_N := (I_N)^{-1} . Ue_N$	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

## 36 Instantiation Equation

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

## 37 Interface Link Equation

no	equation	documentation	layer
104	$\mapsto \xi := \xi$	interface equation	material $\rightarrow$ control
105	$T_N := T_N$	interface equation	macroscopic $\rightarrow$ control
112	$\_ \xi := \xi$	interface equation	material $\rightarrow$ macroscopic
114	$Ue_N := Ue_N$	interface equation	macroscopic $\rightarrow$ control
131	$\tilde{n}_{NS} := \tilde{n}_{NS}$	interface equation	reactions $\rightarrow$ macroscopic
151	$\_k^{d,Fick}_{NS} := k_{dFick_{NS}}$	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
52	$\_ h_{NS} := h_{NS}$	interface equation	material $\rightarrow$ macroscopic

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no	equation	documentation	layer
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
57	$\_k_N^q := k_N^q$	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
62	$\_k_N^c := k_N^c$	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

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no	equation	documentation	layer
65	$\_k_z^d_{NS} := k_z^d_{NS}$	interface equation	material $\rightarrow$ macroscopic
66	$\_k^d_{NS} := k^d_{NS}$	interface equation	material $\rightarrow$ macroscopic
90	$I_N := I_N$	interface equation	macroscopic $\rightarrow$ material
94	$\_R^e_N := k^{e,\xi}_N$	interface equation	material $\rightarrow$ macroscopic
99	$I_N := I_N$	interface equation	macroscopic $\rightarrow$ control