

# 1 Variables

## 2 root

	var	symbol	documentation	type	units	eqs
10	$F_{N,A}$	<b>F</b>	basic directed graph incidence matrix	network		
97	$I_A$	<b>I_A</b>	vector of ones of length arcs	projection		
96	$I_N$	<b>I_N</b>	vector of ones of length nodes	projection		
48	$I_{N,A}$	<b>I_N_A</b>	project node on arc	projection		
4	$t$	<b>t</b>	time	frame	<i>s</i>	
7	$\Delta t$	<b>t_interval</b>	time interval	frame	<i>s</i>	5
5	$t^o$	<b>to</b>	time zero	frame	<i>s</i>	3
6	$t^e$	<b>te</b>	time end	frame	<i>s</i>	4
9	$\Delta$	<b>pulse</b>	pulse of length time interval	frame		7
2	1	<b>one</b>	numerical one	constant		1
8	0.5	<b>onehalf</b>	numerical one half	constant		6
3	0	<b>zero</b>	numerical value zero	constant		2
1	#	<b>value</b>	numerical value	constant		

### 3 physical

	var	symbol	documentation	type	units	eqs
170	$S_S$	S_S	species selection	projection		
98	$I_S$	I_S	vector of ones of length sepecies	projection		
11	$\ell_N$	l	length	frame	$m$	
13	$r_{yN}$	r_y	y-direction	frame	$m$	9
14	$r_{zN}$	r_z	z-direction	frame	$m$	10
12	$r_{xN}$	r_x	x-direction	frame	$m$	8
25	$C_N$	C	fundamental state - charge	state	$A s$	
16	$U_N$	U	fundamental state - internal energy	state	$kg m^2 s^{-2}$	
18	$n_{N,S}$	n	fundamental state - molar mass	state	$mol$	129
15	$V_N$	V	fundamental state - volume	state	$m^3$	11
22	$H_N$	H	Enthalpy	state	$kg m^2 s^{-2}$	15 128
17	$S_N$	S	fundamental state - entropy	state	$kg m^2 K^{-1} s^{-2}$	
23	$A_N$	A	Helmholts energy	state	$kg m^2 s^{-2}$	17
24	$G_N$	G	Gibbs free energy	state	$kg m^2 s^{-2}$	18
34	$R_N$	R	Gas constant	constant	$kg m^2 mol^{-1} K^{-1} s^{-2}$	25
33	$B_N$	Boltz	Boltzmann constant	constant	$kg m^2 K^{-1} s^{-2}$	24
32	$A^v$	Av	Avogadro number	constant	$mol^{-1}$	
21	$\mu_{N,S}$	chemPot	chemical potential	effort	$kg m^2 mol^{-1} s^{-2}$	14 88
19	$T_N$	T	temperature	effort	$K$	16
35	$U^e_N$	Ue	electrical potential – voltage	effort	$kg m^2 A^{-1} s^{-3}$	26
20	$p_N$	p	pressure	effort	$kg m^{-1} s^{-2}$	13
28	$v_{yN}$	v_y	velocity in y-direction	secondaryState	$ms^{-1}$	20

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	var	symbol	documentation	type	units	eqs
27	$v_{xN}$	<b>v_x</b>	velocity in x-direction	secondaryState	$ms^{-1}$	19
29	$v_{zN}$	<b>v_z</b>	velocity in z-direction	secondaryState	$ms^{-1}$	21

## 4 reactions

	var	symbol	documentation	type	units	eqs
113	$P_{N,K}$	P_N_K	what node has what reaction	projection		
114	$T_{N,K}$	T_K	temparature of the nodes with reactions	effort	$K$	99
128	$\bar{n}_{N,S}$	cn	normed concentration	secondaryState		112
129	$\bar{n}_{N,S,K}$	cn_NK	normed concentration – context node and conversion	secondaryState		113
115	$E_{aN,K}$	Ea	Arrhenius activation energy	properties	$kg\,m^2\,mol^{-1}\,s^{-2}$	100
126	$c^n_{N,S}$	c_norming	norming concentration used in the definition of the species interaction probability	properties	$m^{-3}\,mol$	110
131	$\phi_{N,K}$	interactionProbability	probability for the species to meet to undergo reaction	properties		115
134	$K^o_K$	Ko	Arrhenius frequency factor – a strange construction	properties	$m^{-3}\,mol\,s^{-1}$	118
118	$N_{S,K}$	N	stoichiometric matrix	properties		
135	$K_{N,K}$	K	reaction"constant	properties	$m^{-3}\,mol\,s^{-1}$	119
136	$\tilde{n}_{N,S}$	nProd	production term for differential component mass balance	conversion	$mol\,s^{-1}$	120

## 5 material

	var	symbol	documentation	type	units	eqs
52	$k_{xA,S}^d$	kd_x_A	diffusional mass conductivity in x-direction in arc	property	$kg^{-1} m^{-4} mol^2 s$	42
26	$\lambda_S$	Mm	species' molecular mass	property	$kg mol^{-1}$	
50	$k_{yA}^c$	kc_y_A	convective mass conductivity in y-direction in arc	property	$m^{-1} s$	40
54	$k_{zA,S}^d$	kd_z_A	diffusional mass conductivity in z-direction in arc	property	$kg^{-1} m^{-4} mol^2 s$	44
62	$k_{yA,S}^{d,Fick}$	kd_y_Fick	Fick's diffusivity in arc and y-direction	property	$ms^{-1}$	52
56	$k_{yA}^q$	kq_y_A	thermal conductivity in y-direction in arc	property	$kg K^{-1} s^{-3}$	46
49	$k_{xA}^c$	kc_x_A	convective mass conductivity in x-direction in arc	property	$m^{-1} s$	39
57	$k_{zA}^q$	kq_z_A	thermal conductivity in z-direction in arc	property	$kg K^{-1} s^{-3}$	47
59	$\rho_N$	density	density	property	$kg m^{-3}$	49
168	$R_N^e$	Re	electrical resistance	property	$kg m^2 A^{-2} s^{-3}$	154
47	$h_{N,S}$	h	partial molar enthalpies	property	$kg m^2 mol^{-1} s^{-2}$	38
61	$k_{xA,S}^{d,Fick}$	kd_x_Fick	Fick's diffusivity in arc and x-direction	property	$ms^{-1}$	51
53	$k_{yA,S}^d$	kd_y_A	diffusional mass conductivity in y-direction in arc	property	$kg^{-1} m^{-4} mol^2 s$	43
60	$v_S$	v	molar volume of species	property	$m^3 mol^{-1}$	50
172	$cp_N$	cp	specific heat capacity at constant pressure	property	$m^2 K^{-1} s^{-2}$	156
89	$\rho_A$	density_A	density of arc material	property	$kg m^{-3}$	78
45	$k_{yN}^c$	kc_y	convective mass conductivity in y-direction	property	$m^{-1} s$	36
171	$k^{e,x}_N$	kex	electrical conductivity – a simple model being a function of a selected set of species	property	$kg^{-1} m^{-2} A^2 s^3$	155
40	$k_{zN}^q$	kq_z	thermal conductivity in z-direction	property	$kg K^{-1} s^{-3}$	31
51	$k_{zA}^c$	kc_z_A	convective mass conductivity in z-direction in arc	property	$m^{-1} s$	41
43	$k_{zN,S}^d$	kd_z	diffusional mass conductivity in z-direction	property	$kg^{-1} m^{-4} mol^2 s$	34
39	$k_{yN}^q$	kq_y	thermal conductivity in y-direction	property	$kg K^{-1} s^{-3}$	30
63	$k_{zA,S}^{d,Fick}$	kd_z_Fick	Fick's diffusivity in arc and z-direction	property	$ms^{-1}$	53

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	var	symbol	documentation	type	units	eqs
38	$k_{xN}^q$	kq_x	thermal conductivity in x-direction	property	$kg\ K^{-1}\ s^{-3}$	29
42	$k_{yN,S}^d$	kd_y	diffusional mass conductivity in z-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	33
44	$k_{xN}^c$	kc_x	convective mass conductivity in x-direction	property	$m^{-1}\ s$	35
36	$C_{pN}$	Cp	total heat capacity at constant pressure	property	$kg\ m^2\ K^{-1}\ s^{-2}$	27
37	$C_{vN}$	Cv	total heat capacity at constant volume	property	$kg\ m^2\ K^{-1}\ s^{-2}$	28
55	$k_{xA}^q$	kq_x_A	thermal conductivity in x-direction in arc	property	$kg\ K^{-1}\ s^{-3}$	45
107	$h_{AA,S}$	h_A	partial molar enthalpies of transport system	property	$kg\ m^2\ mol^{-1}\ s^{-2}$	93
58	$m_N$	m	mass	property	$kg$	48
46	$k_{zN}^c$	kc_z	convective mass conductivity in z-direction	property	$m^{-1}\ s$	37
41	$k_{xN,S}^d$	kd_x	diffusional mass conductivity in x-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	32
102	$\mu_{N,S}^o$	chemPot_o	standard chemical potential	effort	$kg\ m^2\ mol^{-1}\ s^{-2}$	86

## 6 macroscopic

	var	symbol	documentation	type	units	eqs
111	$\dot{H}^c_N$	aHc	enthalpy accumulation due to convective mass flow	transport	$kg\,m^2\,s^{-3}$	97
83	$\hat{q}_{xA}$	fq_x	heat flow in arc and x-direction	transport	$kg\,m^2\,s^{-3}$	72
109	$\hat{H}^c_A$	fHc	enthalpy flow due to convective mass flow	transport	$kg\,m^2\,s^{-3}$	95
166	$I_N$	I	electric current definition	transport	A	152
84	$\dot{q}_N$	aq	accumulation due to conductive heat flow	transport	$kg\,m^2\,s^{-3}$	73
87	$c_{A,S}$	c_A	concentration in convective mass flow	transport	$m^{-3}\,mol$	76
110	$\hat{H}^d_A$	fHd	enthalpy flow due to diffusive mass flow	transport	$kg\,m^2\,s^{-3}$	96
91	$\dot{V}_A$	fV	volumetric flow	transport	$m^3\,s^{-1}$	80
92	$\hat{n}^c_{A,S}$	fnc	convective mass flow in an arc	transport	$mol\,s^{-1}$	81
101	$\hat{n}^d_{A,S}$	fnd	diffusional mass flow in arc	transport	$mol\,s^{-1}$	85 89
141	$\hat{w}_A$	fw	just an numerical work flow term – as a starter	transport	$kg\,m^2\,s^{-3}$	125
86	$d_A$	d	flow direction of convective flow	transport		75
142	$\dot{w}_N$	aw	enthalpy accumulation due to work flows	transport	$kg\,m^2\,s^{-3}$	126
112	$\dot{H}^d_N$	aHd	enthalpy accumulation due to diffusive mass flow	transport	$kg\,m^2\,s^{-3}$	98
104	$\dot{n}^d_{N,S}$	and	accumulation due to diffusional mass transfer	transport	$mol\,s^{-1}$	90
93	$\dot{n}^c_{N,S}$	anc	accumulation due to convective mass flow	transport	$mol\,s^{-1}$	82
65	$A_{xyN}$	A_xy	cross sectional area xy	geometry	$m^2$	54
69	$A_{xzA}$	A_xz_A	cross sectional area xz of arc	geometry	$m^2$	58
70	$A_{yzA}$	A_yz_A	cross sectional area yz of arc	geometry	$m^2$	59
66	$A_{xzN}$	A_xz	cross sectional area xz	geometry	$m^2$	55
67	$A_{yzN}$	A_yz	cross sectional area yz	geometry	$m^2$	56
68	$A_{xyA}$	A_xy_A	cross sectional area yz of arc	geometry	$m^2$	57
64	$D_{N,A}$	D	difference operator	differenceOperator		

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	var	symbol	documentation	type	units	eqs
144	$H^o_N$	Ho	initial enthalpy	state	$kg\,m^2\,s^{-2}$	<a href="#">130</a>
145	$n^o_{N,S}$	no	initial species masses	state	$mol$	<a href="#">131</a>
146	$T^o_N$	T_norming	norming temperature	secondaryState	$K$	<a href="#">132</a>
147	$p^o_N$	p_norming	normed pressure	secondaryState	$kg\,m^{-1}\,s^{-2}$	<a href="#">133</a>
150	$\bar{p}^o_N$	p_normed	normed pressure	secondaryState		<a href="#">136</a>
149	$\bar{T}^o_N$	T_normed	normed temperature	secondaryState		<a href="#">135</a>
85	$c_{N,S}$	c	molar concentration	secondaryState	$m^{-3}\,mol$	<a href="#">74</a>
100	$x_{N,S}$	x	concentration mole fraction	secondaryState		<a href="#">84</a>
99	$n^t_N$	nt	total amount	secondaryState	$mol$	<a href="#">83</a>
148	$c^o_{N,S}$	c_norming	norming concentration	secondaryState	$m^{-3}\,mol$	<a href="#">134</a>
174	$m_N$	m	mass	secondaryState	$kg$	<a href="#">158</a>
151	$\bar{c}^o_{N,S}$	c_normed	normed concentration	secondaryState		<a href="#">137</a>
138	$\dot{n}^p_{N,S}$	anProduction	production term	conversion	$mol\,s^{-1}$	<a href="#">122</a>
143	$\dot{H}_N$	aH	differential enthalpy balance	diffState	$kg\,m^2\,s^{-3}$	<a href="#">127</a>
139	$\dot{n}_{N,S}$	an	differential species balance	diffState	$mol\,s^{-1}$	<a href="#">123</a>



## 7 control

	var	symbol	documentation	type	units	eqs
159	$P$	P	gain	constant		
158	$m^{m*}_{A,S}$	setpoint_matrix	setpoiint for measurment matrix	constant		145
157	$m^{v*}_A$	setpoint_vector	setpoint for measurement vector	constant		144
162	$u^v_A$	u_vector	control ouput vector	algebraic		148
155	$m_A$	measurement_vector	normed measurements of temparatures	algebraic		141 142
163	$u^m_{A,S}$	u_matrix	control output matrix	algebraic		149
156	$m_{A,S}$	measurement_matrix	normed measurment of concentration	algebraic		143
160	$e^v_A$	error_vector	output error vector	algebraic		146
161	$e^m_{A,S}$	error_matrix	output error matrix	algebraic		147

## 8 reactions–macroscopic

	var	symbol	documentation	type	units	eqs
119	$_{E^a_{N,K}}$	<code>_Ea</code>	link variable Ea to interface reactions »> macroscopic	get	$kg\,m^2\,mol^{-1}\,s^{-2}$	<a href="#">103</a>
123	$_{T_{N,K}}$	<code>_T_K</code>	link variable T K to interface reactions »> macroscopic	get	$K$	<a href="#">107</a>
122	$_{NS,K}$	<code>_N</code>	link variable N to interface reactions »> macroscopic	get		<a href="#">106</a>
137	$_{\tilde{n}_{N,S}}$	<code>_nProd</code>	link variable nProd to interface reactions »> macroscopic	get	$mol\,s^{-1}$	<a href="#">121</a>

## 9 control-macroscopic

	var	symbol	documentation	type	units	eqs
164	$_m^{m_{A,S}}$	<code>_setpoint_matrix</code>	link variable setpoint matrix to interface control »> macroscopic	get		150
165	$_m^v_A$	<code>_setpoint_vector</code>	link variable setpoint vector to interface control »> macroscopic	get		151

## 10 macroscopic-control

	var	symbol	documentation	type	units	eqs
152	$_{\bar{p}N}$	<code>_p_normed</code>	link variable p normed to interface macroscopic »> control	get		<a href="#">138</a>
153	$_{\bar{T}N}$	<code>_T_normed</code>	link variable T normed to interface macroscopic »> control	get		<a href="#">139</a>
154	$_{\bar{c}N,S}$	<code>_c_normed</code>	link variable c normed to interface macroscopic »> control	get		<a href="#">140</a>

## 11 macroscopic-material

	var	symbol	documentation	type	units	eqs
103	$_{x_{N,S}}$	$_{\mathbf{x}}$	link variable x to interface macroscopic »> material	get		87
167	$_{I N}$	$_{\mathbf{I}}$	link variable I to interface macroscopic »> material	get	$A$	153

## 12 material–macroscopic

	var	symbol	documentation	type	units	eqs
81	$_{k_y^q A}$	<code>_kq_y_A</code>	link variable kq y A to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	70
79	$_{k_z^{d,Fick} A,S}$	<code>_kd_z_Fick</code>	link variable kd z Fick to interface material »> macroscopic	get	$ms^{-1}$	68
90	$_{\rho A}$	<code>_density_A</code>	link variable density A to interface material »> macroscopic	get	$kg m^{-3}$	79
77	$_{k_y^d A,S}$	<code>_kd_y_A</code>	link variable kd y A to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	66
106	$_{h_{N,S}}$	<code>_h</code>	link variable h to interface material »> macroscopic	get	$kg m^2 mol^{-1} s^{-2}$	92
75	$_{k_x^{d,Fick} A,S}$	<code>_kd_x_Fick</code>	link variable kd x Fick to interface material »> macroscopic	get	$ms^{-1}$	64
173	$_{c_{pN}}$	<code>_cp</code>	link variable cp to interface material »> macroscopic	get	$m^2 K^{-1} s^{-2}$	157
80	$_{k_x^q A}$	<code>_kq_x_A</code>	link variable kq x A to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	69
72	$_{k_y^c A}$	<code>_kc_y_A</code>	link variable kc y A to interface material »> macroscopic	get	$m^{-1} s$	61
30	$_{\lambda_S}$	<code>_Mm</code>	link variable Mm to interface material »> macroscopic	get	$kg mol^{-1}$	22
78	$_{k_z^d A,S}$	<code>_kd_z_A</code>	link variable kd z A to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	67
73	$_{k_z^c A}$	<code>_kc_z_A</code>	link variable kc z A to interface material »> macroscopic	get	$m^{-1} s$	62
88	$_{\rho_N}$	<code>_density</code>	link variable density to interface material »> macroscopic	get	$kg m^{-3}$	77
74	$_{k_x^d A,S}$	<code>_kd_x_A</code>	link variable kd x A to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	63

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	var	symbol	documentation	type	units	eqs
71	$_{k^c_{xA}}$	<code>_kc_x_A</code>	link variable kc x A to interface material »> macroscopic	get	$m^{-1} s$	60
108	$_{h_{A,S}}$	<code>_h_A</code>	link variable h A to interface material »> macroscopic	get	$kg\,m^2\,mol^{-1}\,s^{-2}$	94
82	$_{k^q_{zA}}$	<code>_kq_z_A</code>	link variable kq z A to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	71
76	$_{k^{d,Fick}_{y_{A,S}}}$	<code>_kd_y_Fick</code>	link variable kd y Fick to interface material »> macroscopic	get	$ms^{-1}$	65

## 13 macroscopic-reactions

	var	symbol	documentation	type	units	eqs
125	<code>_c<sub>N,S</sub></code>	<code>_c</code>	link variable c to interface macroscopic »> reactions	get	$m^{-3} mol$	109



## 14 Equations

## 15 Generic

no	equation	documentation	layer
1	$1 := \text{Instantiate}(\#, \#)$	numerical one	root
2	$0 := \text{Instantiate}(\#, \#)$	numerical value zero	root
3	$t^o := \text{Instantiate}(t, 0)$	time zero	root
4	$t^e := \text{Instantiate}(t, \#)$	time end	root
5	$\Delta t := \text{Instantiate}(t, \#)$	time interval	root
6	$0.5 := \text{Instantiate}(\#, \#)$	numerical one half	root
7	$\Delta := \text{sign}(t - t^o) - \text{sign}(t - (t^o - \Delta t))$	pulse of length time interval	root
8	$r_{xN} := \text{Instantiate}(\ell_N, \#)$	x-direction	physical
9	$r_{yN} := \text{Instantiate}(\ell_N, \#)$	y-direction	physical
10	$r_{zN} := \text{Instantiate}(\ell_N, \#)$	z-direction	physical
11	$V_N := r_{xN} \cdot r_{yN} \cdot r_{zN}$	volume	physical
13	$p_N := \frac{\partial U_N}{\partial V_N}$	pressure	physical
14	$\mu_{N,S} := \frac{\partial U_N}{\partial n_{N,S}}$	chemical potential	physical
15	$H_N := U_N - p_N \cdot V_N$	Enthalpy	physical
16	$T_N := \frac{\partial U_N}{\partial S_N}$	temperature	physical
17	$A_N := U_N - T_N \cdot S_N$	Helmholts energy	physical

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no	equation	documentation	layer
18	$G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$	Gibbs free energy	physical
19	$v_{xN} := (t)^{-1} \cdot r_{xN}$	velocity in x-direction	physical
20	$v_{yN} := (t)^{-1} \cdot r_{yN}$	velocity in y-direction	physical
21	$v_{zN} := (t)^{-1} \cdot r_{zN}$	velocity in z-direction	physical
24	$B_N := \text{Instantiate}(S_N, \#)$	Boltzmann constant	physical
25	$R_N := A^v \cdot B_N$	Gas constant	physical
26	$U_N^e := (C_N)^{-1} \cdot U_N$	electrical potential – voltage	physical
27	$C_{pN} := \frac{\partial H_N}{\partial T_N}$	total heat capacity at constant pressure	material
28	$C_{vN} := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	material
29	$k_{xN}^q := (V_N)^{-1} \cdot C_{pN} \cdot v_{xN}$	thermal conductivity in x-direction	material
30	$k_{yN}^q := (V_N)^{-1} \cdot C_{pN} \cdot v_{yN}$	thermal conductivity in y-direction	material
31	$k_{zN}^q := (V_N)^{-1} \cdot C_{pN} \cdot v_{zN}$	thermal conductivity in z-direction	material
32	$k_{xN,S}^d := (\mu_{N,S})^{-1} \cdot \left( v_{xN} \cdot \left( (V_N)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \right) \right)$	diffusional mass conductivity in x-direction	material
33	$k_{yN,S}^d := (\mu_{N,S})^{-1} \cdot \left( v_{yN} \cdot \left( (V_N)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \right) \right)$	diffusional mass conductivity in y-direction	material
34	$k_{zN,S}^d := (\mu_{N,S})^{-1} \cdot \left( v_{zN} \cdot \left( (V_N)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \right) \right)$	diffusional mass conductivity in z-direction	material
35	$k_{xN}^c := \left( \lambda_S \star (\mu_{N,S})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass conductivity in x-direction	material

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no	equation	documentation	layer
36	$k_{yN}^c := \left( \lambda_S \star (\mu_{N,S})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$	convective mass conductivity in y-direction	material
37	$k_{zN}^c := \left( \lambda_S \star (\mu_{N,S})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convective mass conductivity in z-direction	material
38	$h_{N,S} := H_N \cdot (n_{N,S})^{-1}$	partial molar enthalpies	material
39	$k_{xA}^c := I_{N,A} \star k_{xN}^c$	convective mass conductivity in x-direction in arc	material
40	$k_{yA}^c := I_{N,A} \star k_{yN}^c$	convective mass conductivity in y-direction in arc	material
41	$k_{zA}^c := I_{N,A} \star k_{zN}^c$	convective mass conductivity in z-direction in arc	material
42	$k_{xA,S}^d := I_{N,A} \star k_{xN,S}^d$	diffusional mass conductivity in x-direction in arc	material
43	$k_{yA,S}^d := I_{N,A} \star k_{yN,S}^d$	diffusional mass conductivity in z-direction in arc	material
44	$k_{zA,S}^d := I_{N,A} \star k_{zN,S}^d$	diffusional mass conductivity in z-direction in arc	material
45	$k_{xA}^q := I_{N,A} \star k_{xN}^q$	thermal conductivity in x-direction in arc	material
46	$k_{yA}^q := I_{N,A} \star k_{yN}^q$	thermal conductivity in y-direction in arc	material
47	$k_{zA}^q := I_{N,A} \star k_{zN}^q$	thermal conductivity in z-direction in arc	material
48	$m_N := \lambda_S \star n_{N,S}$	mass	material

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no	equation	documentation	layer
49	$\rho_N := (V_N)^{-1} \cdot m_N$	density	material
50	$v_S := V_N \star (n_{N,S})^{-1}$	molar volume of species	material
51	$k_{x,A,S}^{d,Fick} := I_{N,A} \star \left( v_{xN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$	Fick's diffusivity in arc and x-direction	material
52	$k_{y,A,S}^{d,Fick} := I_{N,A} \star \left( v_{yN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$	Fick's diffusivity in arc and y-direction	material
53	$k_{z,A,S}^{d,Fick} := I_{N,A} \star \left( v_{zN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$	Fick's diffusivity in arc and z-direction	material
54	$A_{xyN} := r_{xN} \cdot r_{yN}$	cross sectional area xy	macroscopic
55	$A_{xzN} := r_{xN} \cdot r_{zN}$	cross sectional area xz	macroscopic
56	$A_{yzN} := r_{yN} \cdot r_{zN}$	cross sectional area yz	macroscopic
57	$A_{xyA} := I_{N,A} \star A_{xyN}$	cross sectional area yz of arc	macroscopic
58	$A_{xzA} := I_{N,A} \star A_{xzN}$	cross sectional area xz of arc	macroscopic
59	$A_{yzA} := I_{N,A} \star A_{yzN}$	cross sectional area yz of arc	macroscopic
72	$\hat{q}_{xA} := A_{yzA} \cdot \_k_{xA}^q \cdot (D_{N,A} \star T_N)$	heat flow in arc and x-direction	macroscopic
73	$\dot{q}_N := F_{N,A} \star \hat{q}_{xA}$	accumulation due to conductive heat flow	macroscopic
74	$c_{N,S} := (V_N)^{-1} \cdot n_{N,S}$	molar concentration	macroscopic
75	$d_A := \text{sign}(D_{N,A} \star p_N)$	flow direction of convective flow	macroscopic
76	$c_{A,S} := (0.5 \cdot (D_{N,A} - d_A \cdot  D_{N,A} )) \star c_{N,S}$	concentration in convective mass flow	macroscopic
78	$\rho_A := I_{N,A} \star \rho_N$	density of arc material	material
80	$\dot{V}_A := (\_ \rho_A)^{-1} \cdot \_k_{xA}^c \cdot A_{yzA} \cdot (D_{N,A} \star p_N)$	volumetric flow	macroscopic

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no	equation	documentation	layer
81	$\hat{n}_{A,S}^c := \dot{V}_A \cdot c_{A,S}$	convective mass flow in an arc	macroscopic
82	$\dot{n}_{N,S}^c := F_{N,A} \star \hat{n}_{A,S}^c$	accumulation due to convective mass flow	macroscopic
83	$n_N^t := I_S \star n_{N,S}$	total amount	macroscopic
84	$x_{N,S} := (n_N^t)^{-1} \cdot n_{N,S}$	concentration mole fraction	macroscopic
85	$\hat{n}_{A,S}^d := A_{yzA} \cdot (-_x k_{A,S}^{d,Fick}) \cdot (D_{N,A} \star c_{N,S})$	diffusional mass flow in arc	macroscopic
86	$\mu_{N,S}^o := \text{Instantiate}(\mu_{N,S}, \#)$	standard chemical potential	material
88	$\mu_{N,S} := \mu_{N,S}^o + R_N \cdot T_N \cdot \ln(_x x_{N,S})$	chemical potential standard model with mole fraction	material
89	$\hat{n}_{A,S}^d := A_{yzA} \cdot (-_x k_{A,S}^d) \cdot (D_{N,A} \star \mu_{N,S})$	diffusional mass flow in arc	macroscopic
90	$\dot{n}_{N,S}^d := F_{N,A} \star \hat{n}_{A,S}^d$	accumulation due to diffusional mass transfer	macroscopic
93	$h_{AA,S} := I_{N,A} \star h_{N,S}$	partial molar enthalpies of transport system	material
95	$\hat{H}_A^c := I_S \star (_h h_{A,S} \cdot \hat{n}_{A,S}^c)$	enthalpy flow due to convective mass flow	macroscopic
96	$\hat{H}_A^d := I_S \star (_h h_{A,S} \cdot \hat{n}_{A,S}^d)$	enthalpy flow due to diffusive mass flow	macroscopic
97	$\dot{H}_N^c := F_{N,A} \star \hat{H}_A^c$	enthalpy accumulation due to convective mass flow	macroscopic
98	$\dot{H}_N^d := F_{N,A} \star \hat{H}_A^d$	enthalpy accumulation due to diffusive mass flow	macroscopic
99	$T_{N,K} := T_N \cdot P_{N,K}$	temparature of the nodes with reactions	reactions

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no	equation	documentation	layer
100	$E_{aN,K} := \text{Instantiate}(R_N . T_{N,K}, \#)$	Arrhenius activation energy	reactions
110	$c^n_{N,S} := \text{Instantiate}(_c c_{N,S}, \#)$	norming concentration used in the definition of the species interaction probability	reactions
112	$\bar{n}_{N,S} := (c^n_{N,S})^{-1} . _c c_{N,S}$	normed concentration	reactions
113	$\bar{n}_{N,S,K} := P_{N,K} . \bar{n}_{N,S}$	normed concentration – context node and conversion	reactions
115	$\phi_{N,K} := \prod_S \bar{n}_{N,S,K}^{(N_{S,K})}$	probability for the species to meet to undergo reaction	reactions
118	$K^o_K := \text{Instantiate}(I_S \star (P_{N,K} \star ((t)^{-1} . (V_N)^{-1} . n_{N,S}))), \#)$	Arrhenius frequency factor – a strange construction	reactions
119	$K_{N,K} := K^o_K . \exp((-E_{aN,K}) . (R_N . T_{N,K})^{-1})$	reaction"constant	reactions
120	$\tilde{n}_{N,S} := V_N . (N_{S,K} \star (K_{N,K} . \phi_{N,K}))$	production term for differential component mass balance	reactions
122	$\dot{n}^p_{N,S} := _n \tilde{n}_{N,S}$	production term	macroscopic
123	$\dot{n}_{N,S} := \dot{n}^c_{N,S} + \dot{n}^d_{N,S} + \dot{n}^p_{N,S}$	differential species balance	macroscopic
125	$\hat{w}_A := \text{Instantiate}(\hat{H}^c_A, \#)$	just an numerical work flow term – as a starter	macroscopic
126	$\dot{w}_N := F_{N,A} \star \hat{w}_A$	enthalpy accumulation due to work flows	macroscopic
127	$\dot{H}_N := \dot{H}^c_N + \dot{H}^d_N + \dot{q}_N + \dot{w}_N$	differential enthalpy balance	macroscopic
128	$H_N := \int_{t^o}^{t^e} \dot{H}_N dt + H^o_N$	Enthalpy	macroscopic

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no	equation	documentation	layer
129	$n_{N,S} := \int_{t^o}^{t^e} \dot{n}_{N,S} dt + n_{N,S}^o$	fundamental state - molar mass	macroscopic
130	$H_N^o := \text{Instantiate}(H_N, \#)$	initial enthalpy	macroscopic
131	$n_{N,S}^o := \text{Instantiate}(n_{N,S}, \#)$	initial species masses	macroscopic
132	$T_N^o := \text{Instantiate}(T_N, \#)$	norming temperature	macroscopic
133	$p_N^o := \text{Instantiate}(p_N, \#)$	normed pressure	macroscopic
134	$c_{N,S}^o := \text{Instantiate}(c_{N,S}, \#)$	norming concentration	macroscopic
135	$\bar{T}_N^o := T_N \cdot (T_N^o)^{-1}$	normed temperature	macroscopic
136	$\bar{p}_N^o := (p_N)^{-1} \cdot p_N$	normed pressure	macroscopic
137	$\bar{c}_{N,S}^o := (c_{N,S}^o)^{-1} \cdot c_{N,S}$	normed concentration	macroscopic
141	$m_A := F_{N,A} \star \bar{T}_N$	normed measurements of temperatures	control
142	$m_A := F_{N,A} \star \bar{p}_N$	normed measurements of pressures	control
143	$m_{A,S} := F_{N,A} \star \bar{c}_{N,S}$	normed measurement of concentration	control
144	$m^{v\star}_A := \text{Instantiate}(m_A, \#)$	setpoint for measurement vector	control
145	$m^{m\star}_{A,S} := \text{Instantiate}(m_{A,S}, \#)$	setpoint for measurement matrix	control
146	$e^v_A := m^{v\star}_A - m_A$	output error vector	control
147	$e^m_{A,S} := m^{m\star}_{A,S} - m_{A,S}$	output error matrix	control
148	$u^v_A := P \cdot e^v_A$	control output vector	control
149	$u^m_{A,S} := P \cdot e^m_{A,S}$	control output matrix	control

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no	equation	documentation	layer
152	$I_N := \frac{dC_N}{dt}$	electric current definition	macroscopic
154	$R_N^e := (I_N)^{-1} \cdot U_N^e$	electrical resistance	material
155	$k_N^{e,x} := (R_N^e)^{-1} \cdot (S_S \star \_x n_{N,S})$	electrical conductivity – a simple model being a function of a selected set of species	material
156	$cp_N := C_{pN} \cdot (m_N)^{-1}$	specific heat capacity at constant pressure	material
158	$m_N := \_ \lambda_S \star n_{N,S}$	mass	macroscopic



## 16 Interface Link Equation

no	equation	documentation	layer
22	$_{-}\lambda_S := \lambda_S$	interface equation	material -> macroscopic
60	$_{-}k_{xA}^c := k_{xA}^c$	interface equation	material -> macroscopic
61	$_{-}k_{yA}^c := k_{yA}^c$	interface equation	material -> macroscopic
62	$_{-}k_{zA}^c := k_{zA}^c$	interface equation	material -> macroscopic
63	$_{-}k_{xA,S}^d := k_{xA,S}^d$	interface equation	material -> macroscopic
64	$_{-}k_{x,A,S}^{d,Fick} := k_{x,A,S}^{d,Fick}$	interface equation	material -> macroscopic
65	$_{-}k_{y,A,S}^{d,Fick} := k_{y,A,S}^{d,Fick}$	interface equation	material -> macroscopic
66	$_{-}k_{yA,S}^d := k_{yA,S}^d$	interface equation	material -> macroscopic
67	$_{-}k_{zA,S}^d := k_{zA,S}^d$	interface equation	material -> macroscopic
68	$_{-}k_{z,A,S}^{d,Fick} := k_{z,A,S}^{d,Fick}$	interface equation	material -> macroscopic
69	$_{-}k_{xA}^q := k_{xA}^q$	interface equation	material -> macroscopic

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no	equation	documentation	layer
70	$\_k_{yA}^q := k_{yA}^q$	interface equation	material $\rightarrow$ macroscopic
71	$\_k_{zA}^q := k_{zA}^q$	interface equation	material $\rightarrow$ macroscopic
77	$\_\rho_N := \rho_N$	interface equation	material $\rightarrow$ macroscopic
79	$\_\rho_A := \rho_A$	interface equation	material $\rightarrow$ macroscopic
87	$\_x_{N,S} := x_{N,S}$	interface equation	macroscopic $\rightarrow$ material
92	$\_h_{N,S} := h_{N,S}$	interface equation	material $\rightarrow$ macroscopic
94	$\_h_{A,S} := h_{AA,S}$	interface equation	material $\rightarrow$ macroscopic
103	$\_E^a_{N,K} := E_{aN,K}$	interface equation	reactions $\rightarrow$ macroscopic
106	$\_N_{S,K} := N_{S,K}$	interface equation	reactions $\rightarrow$ macroscopic
107	$\_T_{N,K} := T_{N,K}$	interface equation	reactions $\rightarrow$ macroscopic
109	$\_c_{N,S} := c_{N,S}$	interface equation	macroscopic $\rightarrow$ reactions
121	$\_\tilde{n}_{N,S} := \tilde{n}_{N,S}$	interface equation	reactions $\rightarrow$ macroscopic

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no	equation	documentation	layer
138	$_{\bar{p}N} := \bar{p}^o_N$	interface equation	macroscopic control →
139	$_{\bar{T}N} := \bar{T}^o_N$	interface equation	macroscopic control →
140	$_{\bar{c}_{N,S}} := \bar{c}^o_{N,S}$	interface equation	macroscopic control →
150	$_{m^m_{A,S}} := m^{m^*}_{A,S}$	interface equation	control → macroscopic
151	$_{m^v_A} := m^{v^*}_A$	interface equation	control → macroscopic
153	$_{I_N} := I_N$	interface equation	macroscopic material →
157	$_{c_{pN}} := c_{pN}$	interface equation	material → macroscopic