

## 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		
5	$t^o$	<b>to</b>	time zero	frame	<i>s</i>	<b>3</b>
6	$t^e$	<b>te</b>	time end	frame	<i>s</i>	<b>4</b>
4	$t$	<b>t</b>	time	frame	<i>s</i>	
7	$\Delta t$	<b>t_interval</b>	time interval	frame	<i>s</i>	<b>5</b>
9	$\Delta$	<b>pulse</b>	pulse of length time interval	frame		<b>7</b>
1	$\#$	<b>value</b>	numerical value	constant		
8	0.5	<b>onehalf</b>	numerical one half	constant		<b>6</b>
3	0	<b>zero</b>	numerical value zero	constant		<b>2</b>
2	1	<b>one</b>	numerical one	constant		<b>1</b>

### 3 physical

	var	symbol	documentation	type	units	eqs
98	$I_S$	I_S	vector of ones of length sepecies	projection		
14	$r_{zN}$	r_z	z-direction	frame	$m$	10
12	$r_{xN}$	r_x	x-direction	frame	$m$	8
11	$\ell_N$	l	length	frame	$m$	
13	$r_{yN}$	r_y	y-direction	frame	$m$	9
25	$C_N$	C	fundamental state - charge	state	$A s$	
16	$U_N$	U	fundamental state - internal energy	state	$kg m^2 s^{-2}$	
17	$S_N$	S	fundamental state - entropy	state	$kg m^2 K^{-1} s^{-2}$	
15	$V_N$	V	fundamental state - volume	state	$m^3$	11
22	$H_N$	H	Enthalpy	state	$kg m^2 s^{-2}$	15 128
18	$n_{N,S}$	n	fundamental state - molar mass	state	$mol$	129
24	$G_N$	G	Gibbs free energy	state	$kg m^2 s^{-2}$	18
23	$A_N$	A	Helmholts energy	state	$kg m^2 s^{-2}$	17
32	$A^v$	Av	Avogadro number	constant	$mol^{-1}$	
33	$B_N$	Boltz	Boltzmann constant	constant	$kg m^2 K^{-1} s^{-2}$	24
34	$R_N$	R	Gas constant	constant	$kg m^2 mol^{-1} K^{-1} s^{-2}$	25
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
21	$\mu_{N,S}$	chemPot	chemical potential	effort	$kg m^2 mol^{-1} s^{-2}$	14 88
20	$p_N$	p	pressure	effort	$kg m^{-1} s^{-2}$	13
27	$v_{xN}$	v_x	velocity in x-direction	secondaryState	$ms^{-1}$	19
29	$v_{zN}$	v_z	velocity in z-direction	secondaryState	$ms^{-1}$	21

Continued on next page

	var	symbol	documentation	type	units	eqs
28	$v_{yN}$	<b>v_y</b>	velocity in y-direction	secondaryState	$ms^{-1}$	20

## 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
135	$K_{N,K}$	K	reaction"constant	properties	$m^{-3} mol s^{-1}$	119
134	$K^o_K$	Ko	Arrhenius frequency factor – a strange construction	properties	$m^{-3} mol s^{-1}$	118
115	$E_{a,N,K}$	Ea	Arrhenius activation energy	properties	$kg m^2 mol^{-1} s^{-2}$	100
118	$N_{S,K}$	N	stoichiometric matrix	properties		
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
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
60	$v_S$	<b>v</b>	molar volume of species	property	$m^3 mol^{-1}$	<a href="#">50</a>
40	$k_{zN}^q$	<b>kq_z</b>	thermal conductivity in z-direction	property	$kg K^{-1} s^{-3}$	<a href="#">31</a>
62	$k_y^{d,Fick}{}_{A,S}$	<b>kd_y_Fick</b>	Fick's diffusivity in arc and y-direction	property	$ms^{-1}$	<a href="#">52</a>
52	$k_{xA,S}^d$	<b>kd_x_A</b>	diffusional mass conductivity in x-direction in arc	property	$kg^{-1} m^{-4} mol^2 s$	<a href="#">42</a>
63	$k_z^{d,Fick}{}_{A,S}$	<b>kd_z_Fick</b>	Fick's diffusivity in arc and z-direction	property	$ms^{-1}$	<a href="#">53</a>
61	$k_x^{d,Fick}{}_{A,S}$	<b>kd_x_Fick</b>	Fick's diffusivity in arc and x-direction	property	$ms^{-1}$	<a href="#">51</a>
51	$k_{zA}^c$	<b>kc_z_A</b>	convective mass conductivity in z-direction in arc	property	$m^{-1} s$	<a href="#">41</a>
107	$h_{AA,S}$	<b>h_A</b>	partial molar enthalpies of transport system	property	$kg m^2 mol^{-1} s^{-2}$	<a href="#">93</a>
42	$k_{yN,S}^d$	<b>kd_y</b>	diffusional mass conductivity in z-direction	property	$kg^{-1} m^{-4} mol^2 s$	<a href="#">33</a>
44	$k_{xN}^c$	<b>kc_x</b>	convective mass conductivity in x-direction	property	$m^{-1} s$	<a href="#">35</a>
47	$h_{N,S}$	<b>h</b>	partial molar enthalpies	property	$kg m^2 mol^{-1} s^{-2}$	<a href="#">38</a>
49	$k_{xA}^c$	<b>kc_x_A</b>	convective mass conductivity in x-direction in arc	property	$m^{-1} s$	<a href="#">39</a>
58	$m_N$	<b>m</b>	mass	property	$kg$	<a href="#">48</a>
26	$\lambda_S$	<b>Mm</b>	species' molecular mass	property	$kg mol^{-1}$	
89	$\rho_A$	<b>density_A</b>	density of arc material	property	$kg m^{-3}$	<a href="#">78</a>
59	$\rho_N$	<b>density</b>	density	property	$kg m^{-3}$	<a href="#">49</a>
50	$k_{yA}^c$	<b>kc_y_A</b>	convective mass conductivity in y-direction in arc	property	$m^{-1} s$	<a href="#">40</a>
45	$k_{yN}^c$	<b>kc_y</b>	convective mass conductivity in y-direction	property	$m^{-1} s$	<a href="#">36</a>
54	$k_{zA,S}^d$	<b>kd_z_A</b>	diffusional mass conductivity in z-direction in arc	property	$kg^{-1} m^{-4} mol^2 s$	<a href="#">44</a>
55	$k_{xA}^q$	<b>kq_x_A</b>	thermal conductivity in x-direction in arc	property	$kg K^{-1} s^{-3}$	<a href="#">45</a>
43	$k_{zN,S}^d$	<b>kd_z</b>	diffusional mass conductivity in z-direction	property	$kg^{-1} m^{-4} mol^2 s$	<a href="#">34</a>
36	$C_{pN}$	<b>Cp</b>	total heat capacity at constant pressure	property	$kg m^2 K^{-1} s^{-2}$	<a href="#">27</a>
37	$C_{vN}$	<b>Cv</b>	total heat capacity at constant volume	property	$kg m^2 K^{-1} s^{-2}$	<a href="#">28</a>

*Continued on next page*

	var	symbol	documentation	type	units	eqs
56	$k_{yA}^q$	kq_y_A	thermal conductivity in y-direction in arc	property	$kg\ K^{-1}\ s^{-3}$	46
39	$k_{yN}^q$	kq_y	thermal conductivity in y-direction	property	$kg\ K^{-1}\ s^{-3}$	30
46	$k_{zN}^c$	kc_z	convective mass conductivity in z-direction	property	$m^{-1}\ s$	37
38	$k_{xN}^q$	kq_x	thermal conductivity in x-direction	property	$kg\ K^{-1}\ s^{-3}$	29
57	$k_{zA}^q$	kq_z_A	thermal conductivity in z-direction in arc	property	$kg\ K^{-1}\ s^{-3}$	47
41	$k_{xN,S}^d$	kd_x	diffusional mass conductivity in x-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	32
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
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
93	$\dot{n}_{N,S}^c$	anc	accumulation due to convective mass flow	transport	$mol\ s^{-1}$	82
104	$\dot{n}_{N,S}^d$	and	accumulation due to diffusional mass transfer	transport	$mol\ s^{-1}$	90
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
141	$\hat{w}_A$	fw	just an numerical work flow term – as a starter	transport	$kg\ m^2\ s^{-3}$	125
101	$\hat{n}_{A,S}^d$	fnd	diffusional mass flow in arc	transport	$mol\ s^{-1}$	85 89
142	$\dot{w}_N$	aw	enthalpy accumulation due to work flows	transport	$kg\ m^2\ s^{-3}$	126
83	$\hat{q}_{xA}$	fq_x	heat flow in arc and x-direction	transport	$kg\ m^2\ s^{-3}$	72
92	$\hat{n}_{A,S}^c$	fnc	convective mass flow in an arc	transport	$mol\ s^{-1}$	81
110	$\hat{H}_A^d$	fHd	enthalpy flow due to diffusive mass flow	transport	$kg\ m^2\ s^{-3}$	96
112	$\dot{H}_N^d$	aHd	enthalpy accumulation due to diffusive mass flow	transport	$kg\ m^2\ s^{-3}$	98
111	$\dot{H}_N^c$	aHc	enthalpy accumulation due to convective mass flow	transport	$kg\ m^2\ s^{-3}$	97
86	$d_A$	d	fow direction of convective flow	transport		75
91	$\dot{V}_A$	fV	volumetric flow	transport	$m^3\ s^{-1}$	80
109	$\hat{H}_A^c$	fHc	enthalpy flow due to convective mass flow	transport	$kg\ m^2\ s^{-3}$	95
67	$A_{yzN}$	A_yz	cross sectional area yz	geometry	$m^2$	56
69	$A_{xzA}$	A_xz_A	cross sectional area xz of arc	geometry	$m^2$	58
66	$A_{xzN}$	A_xz	cross sectional area xz	geometry	$m^2$	55
68	$A_{xyA}$	A_xy_A	cross sectional area yz of arc	geometry	$m^2$	57
65	$A_{xyN}$	A_xy	cross sectional area xy	geometry	$m^2$	54
70	$A_{yzA}$	A_yz_A	cross sectional area yz of arc	geometry	$m^2$	59
64	$D_{N,A}$	D	difference operator	differenceOperator		
145	$n_{N,S}^o$	no	initial species masses	state	$mol$	131

Continued on next page

	var	symbol	documentation	type	units	eqs
144	$H^o_N$	<b>Ho</b>	initial enthalpy	state	$kg\,m^2\,s^{-2}$	<b>130</b>
85	$c_{N,S}$	<b>c</b>	molar concentration	secondaryState	$m^{-3}\,mol$	<b>74</b>
100	$x_{N,S}$	<b>x</b>	concentration mole fraction	secondaryState		<b>84</b>
99	$n^t_N$	<b>nt</b>	total amount	secondaryState	$mol$	<b>83</b>
138	$\dot{n}_{N,S}$	<b>anProduction</b>	production term	conversion	$mol\,s^{-1}$	<b>122</b>
139	$\dot{n}_{N,S}$	<b>an</b>	differential species balance	diffState	$mol\,s^{-1}$	<b>123</b>
143	$\dot{H}_N$	<b>aH</b>	differential enthalpy balance	diffState	$kg\,m^2\,s^{-3}$	<b>127</b>



## 7 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

## 8 macroscopic-material

	var	symbol	documentation	type	units	eqs
103	$_x_{N,S}$	$_x$	link variable x to interface macroscopic »> material	get		87

## 9 reactions–macroscopic

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

## 10 material–macroscopic

	var	symbol	documentation	type	units	eqs
71	$_{kc_x A}$	<code>_kc_x_A</code>	link variable kc x A to interface material »> macroscopic	get	$m^{-1} s$	60
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
82	$_{k_z^q A}$	<code>_kq_z_A</code>	link variable kq z A to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	71
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
90	$_{\rho A}$	<code>_density_A</code>	link variable density A to interface material »> macroscopic	get	$kg m^{-3}$	79
88	$_{\rho N}$	<code>_density</code>	link variable density to interface material »> macroscopic	get	$kg m^{-3}$	77
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
72	$_{kc_y A}$	<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
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
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
106	$_{h_{N,S}}$	<code>_h</code>	link variable h to interface material »> macroscopic	get	$kg m^2 mol^{-1} s^{-2}$	92
73	$_{kc_z A}$	<code>_kc_z_A</code>	link variable kc z A to interface material »> macroscopic	get	$m^{-1} s$	62
76	$_{k_y^{d,Fick} A,S}$	<code>_kd_y_Fick</code>	link variable kd y Fick to interface material »> macroscopic	get	$ms^{-1}$	65

*Continued on next page*

	var	symbol	documentation	type	units	eqs
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
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
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

## 11 Equations

## 12 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

*Continued on next page*

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

*Continued on next page*

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

*Continued on next page*



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

*Continued on next page*

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

*Continued on next page*

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	$\dot{n}_{N,S} := _\dot{n}_{N,S}$	production term	macroscopic
123	$\dot{n}_{N,S} := \dot{n}^c_{N,S} + \dot{n}^d_{N,S} + \dot{n}_{N,S}$	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

*Continued on next page*

no	equation	documentation	layer
129	$n_{N,S} := \int_{t^o}^{t^e} \dot{n}_{N,S} dt + n^o_{N,S}$	fundamental state - molar mass	macroscopic
130	$H^o_N := \text{Instantiate}(H_N, \#)$	initial enthalpy	macroscopic
131	$n^o_{N,S} := \text{Instantiate}(n_{N,S}, \#)$	initial species masses	macroscopic

## 13 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

*Continued on next page*

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