1 Variables

2 root

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

3 physical

	var	symbol	documentation	type	units	eqs
98	I_S	I_S	vector of ones of length sepecies	projection		
12	r_{xN}	r_x	x-direction	frame	m	8
14	r_{zN}	r_z	z-direction	frame	m	10
11	ℓ_N	l	length	frame	m	
13	r_{yN}	r_y	y-direction	frame	m	9
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
15	V_N	V	fundamental state - volume	state	m^3	11
18	$n_{N,S}$	n	fundamental state - molar mass	state	mol	129
22	H_N	H	Enthalpy	state	$kg\,m^2\,s^{-2}$	15 128
16	U_N	U	fundamental state - internal energy	state	$kg\,m^2\,s^{-2}$	
17	S_N	S	fundamental state - entropy	state	$kg\,m^2\,K^{-1}\,s^{-2}$	
25	C_N	C	fundamental state - charge	state	$A\,s$	
32	A^v	Av	Avogadro number	constant	mol^{-1}	
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
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
29	v_{zN}	v_z	velocity in z-direction	secondaryState	ms^{-1}	21
28	v_{yN}	v_y	velocity in y-direction	secondaryState	ms^{-1}	20

Continued on next page

	var	symbol	documentation	type	units	eqs
27	v_{xN}	v_x	velocity in x-direction	secondaryState	ms^{-1}	19

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
134	$K^o{}_K$	Ko	Arrhenius frequency factor – a strange construction	properties	$m^{-3}\,mol\,s^{-1}$	118
131	$\phi_{N,K}$	interactionProbability	probability for the species to meet to undergo reaction	properties		115
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
115	$E_{a\,N,K}$	Ea	Arrhenius activation energy	properties	$kg\,m^2\,mol^{-1}\,s^{-2}$	100
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
107	$h_{AA,S}$	h_A	partial molar enthalpies of transport system	property	$kg\,m^2\,mol^{-1}\,s^{-2}$	93
50	k^c_{yA}	kc_y_A	convective mass conductivity in y-direction in arc	property	$m^{-1}\,s$	40
42	$k^d_{yN,S}$	kd_y	diffusional mass conductivity in z-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	33
51	k^c_{zA}	kc_z_A	convective mass conductivity in z-direction in arc	property	$m^{-1}\,s$	41
26	λ_S	Mm	species' molecular mass	property	$kg\,mol^{-1}$	
63	$k^{d,Fick}_{z\ A,S}$	kd_z_Fick	Fick's diffusivity in arc and z-direction	property	ms^{-1}	53
54	$k^d_{zA,S}$	kd_z_A	diffusional mass conductivity in z-direction in arc	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	44
47	$h_{N,S}$	h	partial molar enthalpies	property	$kg\,m^2\,mol^{-1}\,s^{-2}$	38
44	k^c_{xN}	kc_x	convective mass conductivity in x-direction	property	$m^{-1}\,s$	35
37	C_{vN}	Cv	total heat capacity at constant volume	property	$kg\,m^2\,K^{-1}\,s^{-2}$	28
56	k^q_{yA}	kq_y_A	thermal conductivity in y-direction in arc	property	$kg\,K^{-1}\,s^{-3}$	46
58	m_N	m	mass	property	kg	48
38	k^q_{xN}	kq_x	thermal conductivity in x-direction	property	$kg\,K^{-1}\,s^{-3}$	29
57	k^q_{zA}	kq_z_A	thermal conductivity in z-direction in arc	property	$kg\,K^{-1}\,s^{-3}$	47
40	k^q_{zN}	kq_z	thermal conductivity in z-direction	property	$kg\,K^{-1}\,s^{-3}$	31
59	ρ_N	density	density	property	$kg\,m^{-3}$	49
43	$k^d_{zN,S}$	kd_z	diffusional mass conductivity in z-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	34
46	k^c_{zN}	kc_z	convective mass conductivity in z-direction	property	$m^{-1}\,s$	37
49	k^c_{xA}	kc_x_A	convective mass conductivity in x-direction in arc	property	$m^{-1}\,s$	39
45	k^c_{yN}	kc_y	convective mass conductivity in y-direction	property	$m^{-1}\,s$	36
61	$k^{d,Fick}_{x\ A,S}$	kd_x_Fick	Fick's diffusivity in arc and x-direction	property	ms^{-1}	51
36	C_{pN}	Cp	total heat capacity at constant pressure	property	$kg\,m^2\,K^{-1}\,s^{-2}$	27
41	$k^d_{xN,S}$	kd_x	diffusional mass conductivity in x-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	32

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	var	symbol	documentation	type	units	eqs
52	$k^d_{xA,S}$	kd_x_A	diffusional mass conductivity in x-direction in arc	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	42
89	ρ_A	density_A	density of arc material	property	$kg\,m^{-3}$	78
60	v_S	v	molar volume of species	property	$m^3\,mol^{-1}$	50
39	k^q_{yN}	kq_y	thermal conductivity in y-direction	property	$kg\,K^{-1}\,s^{-3}$	30
62	$k^{d,Fick}_{y\ A,S}$	kd_y_Fick	Fick's diffusivity in arc and y-direction	property	$m\,s^{-1}$	52
53	$k^d_{yA,S}$	kd_y_A	diffusional mass conductivity in y-direction in arc	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	43
55	k^q_{xA}	kq_x_A	thermal conductivity in x-direction in arc	property	$kg\,K^{-1}\,s^{-3}$	45
102	$\mu^o_{N,S}$	chemPot_o	standard chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	86

6 macroscopic

	var	symbol	documentation	type	units	eqs
141	$\hat{w}_A$	fw	just an numerical work flow term – as a starter	transport	$kg\,m^2\,s^{-3}$	125
84	$\dot{q}_N$	aq	accumulation due to conductive heat flow	transport	$kg\,m^2\,s^{-3}$	73
83	$\hat{q}_{xA}$	fq_x	heat flow in arc and x-direction	transport	$kg\,m^2\,s^{-3}$	72
111	$\dot{H}^c{}_N$	aHc	enthalpy accumulation due to convective mass flow	transport	$kg\,m^2\,s^{-3}$	97
110	$\hat{H}^d{}_A$	fHd	enthalpy flow due to diffusive mass flow	transport	$kg\,m^2\,s^{-3}$	96
86	d_A	d	fow direction of convective flow	transport		75
109	$\hat{H}^c{}_A$	fHc	enthalpy flow due to convective mass flow	transport	$kg\,m^2\,s^{-3}$	95
92	$\hat{n}^c{}_{A,S}$	fnc	convective mass flow in an arc	transport	$mol\,s^{-1}$	81
93	$\dot{n}^c{}_{N,S}$	anc	accumulation due to convective mass flow	transport	$mol\,s^{-1}$	82
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
101	$\hat{n}^d{}_{A,S}$	fnd	diffusional mass flow in arc	transport	$mol\,s^{-1}$	85 89
87	$c_{A,S}$	c_A	concentration in convective mass flow	transport	$m^{-3}\,mol$	76
91	$\dot{V}_A$	fV	volumetric flow	transport	$m^3\,s^{-1}$	80
104	$\dot{n}^d{}_{N,S}$	and	accumulation due to diffusional mass transfer	transport	$mol\,s^{-1}$	90
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
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
67	A_{yzN}	A_yz	cross sectional area yz	geometry	m^2	56
64	$D_{N,A}$	D	difference operator	differenceOperator		
144	Ho_N	Ho	initial enthalpy	state	$kg\,m^2\,s^{-2}$	130

	var	symbol	documentation	type	units	eqs
145	$no_{N,S}$	no	initial species masses	state	mol	131
85	$c_{N,S}$	c	molar concentration	secondaryState	$m^{-3}\,mol$	74
100	$x_{N,S}$	x	concentration mole fraction	secondaryState		84
99	$n^t{}_N$	nt	total amount	secondaryState	mol	83
138	$\dot{n}_{N,S}$	anProduction	production term	conversion	$mol\,s^{-1}$	122
139	$\dot{n}_{N,S}$	an	differential species balance	diffState	$mol\,s^{-1}$	123
143	$\dot{H}_N$	aH	differential enthalpy balance	diffState	$kg\,m^2\,s^{-3}$	127

7   macroscopic–material

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

8   reactions–macroscopic

	var	symbol	documentation	type	units	eqs
137	$\_\tilde{n}_{N,S}$	`_nProd`	link variable nProd to interface reactions »> macroscopic	get	$mol\,s^{-1}$	121
119	$\_E^a{}_{N,K}$	`_Ea`	link variable Ea to interface reactions »> macroscopic	get	$kg\,m^2\,mol^{-1}\,s^{-2}$	103
123	$\_T_{N,K}$	`_T_K`	link variable T K to interface reactions »> macroscopic	get	K	107
122	$_{NS,K}$	`_N`	link variable N to interface reactions »> macroscopic	get		106

9   material–macroscopic

	var	symbol	documentation	type	units	eqs
108	$\_h_{A,S}$	`_h_A`	link variable h A to interface material »> macroscopic	get	$kg\,m^2\,mol^{-1}\,s^{-2}$	94
79	$\_k_z^{d,Fick}{}_{A,S}$	`_kd_z_Fick`	link variable kd z Fick to interface material »> macroscopic	get	ms^{-1}	68
72	$\_k_{yA}^c$	`_kc_y_A`	link variable kc y A to interface material »> macroscopic	get	$m^{-1}\,s$	61
75	$\_k_x^{d,Fick}{}_{A,S}$	`_kd_x_Fick`	link variable kd x Fick to interface material »> macroscopic	get	ms^{-1}	64
90	$\_\rho_A$	`_density_A`	link variable density A to interface material »> macroscopic	get	$kg\,m^{-3}$	79
73	$\_k_{zA}^c$	`_kc_z_A`	link variable kc z A to interface material »> macroscopic	get	$m^{-1}\,s$	62
80	$\_k_{xA}^q$	`_kq_x_A`	link variable kq x A to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	69
77	$\_k_{yA,S}^d$	`_kd_y_A`	link variable kd y A to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	66
81	$\_k_{yA}^q$	`_kq_y_A`	link variable kq y A to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	70
71	$\_k_{xA}^c$	`_kc_x_A`	link variable kc x A to interface material »> macroscopic	get	$m^{-1}\,s$	60
106	$\_h_{N,S}$	`_h`	link variable h to interface material »> macroscopic	get	$kg\,m^2\,mol^{-1}\,s^{-2}$	92
30	$\_\lambda_S$	`_Mm`	link variable Mm to interface material »> macroscopic	get	$kg\,mol^{-1}$	22
74	$\_k_{xA,S}^d$	`_kd_x_A`	link variable kd x A to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	63
78	$\_k_{zA,S}^d$	`_kd_z_A`	link variable kd z A to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	67

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	var	symbol	documentation	type	units	eqs
88	$\_\rho_N$	`_density`	link variable density to interface material »> macroscopic	get	$kg\,m^{-3}$	77
82	$\_k^q_{z\,A}$	`_kq_z_A`	link variable kq z A to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	71
76	$\_k^{d,Fick}_{y\ A,S}$	`_kd_y_Fick`	link variable kd y Fick to interface material »> macroscopic	get	ms^{-1}	65

10   macroscopic–reactions

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

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

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	$U^e{}_N := (C_N)^{-1} \cdot U_N$	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	$k^q_{xN} := (V_N)^{-1} \cdot C_{pN} \cdot v_{xN}$	thermal conductivity in x-direction	material
30	$k^q_{yN} := (V_N)^{-1} \cdot C_{pN} \cdot v_{yN}$	thermal conductivity in y-direction	material
31	$k^q_{zN} := (V_N)^{-1} \cdot C_{pN} \cdot v_{zN}$	thermal conductivity in z-direction	material
32	$k^d_{xN,S} := (\mu_{N,S})^{-1} \cdot \left(v_{xN} \cdot \left((V_N)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \right) \right)$	diffusional mass conductivity in x-direction	material
33	$k^d_{yN,S} := (\mu_{N,S})^{-1} \cdot \left(v_{yN} \cdot \left((V_N)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \right) \right)$	diffusional mass conductivity in y-direction	material
34	$k^d_{zN,S} := (\mu_{N,S})^{-1} \cdot \left(v_{zN} \cdot \left((V_N)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \right) \right)$	diffusional mass conductivity in z-direction	material
35	$k^c_{xN} := \left(\lambda_S \star (\mu_{N,S})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass conductivity in x-direction	material

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

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	$k_x^{d,Fick}{}_{A,S} := I_{N,A} \star \left(v_{xN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$	Fick's diffusivity in arc and x-direction	material
52	$k_y^{d,Fick}{}_{A,S} := I_{N,A} \star \left(v_{yN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$	Fick's diffusivity in arc and y-direction	material
53	$k_z^{d,Fick}{}_{A,S} := I_{N,A} \star \left(v_{zN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$	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	$d_A := \mathrm{sign}\,(D_{N,A} \star p_N)$	fow 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

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

no	equation	documentation	layer
100	$E_{aN,K} := \text{Instantiate}(R_N \,.\, T_{N,K}, \#)$	Arrhenius activation energy	reactions
110	$c^n{}_{N,S} := \text{Instantiate}(\_c_{N,S}, \#)$	norming concentration used in the definition of the species interaction probability	reactions
112	$\bar{n}_{N,S} := (c^n{}_{N,S})^{-1} \,.\, \_c_{N,S}$	normed concentration	reactions
113	$\bar{n}_{N,S,K} := P_{N,K} \,.\, \bar{n}_{N,S}$	normed concentration – context node and conversion	reactions
115	$\phi_{N,K} := \prod_S cn_N K_{N,S,K}$	probability for the species to meet to undergo reaction	reactions
118	$K^o{}_K := \text{Instantiate}\left(I_S \star \left(P_{N,K} \star \left((t)^{-1} \,.\, (V_N)^{-1} \,.\, n_{N,S}\right)\right), \#\right)$	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	$\dot{n}_{N,S} := \_\tilde{n}_{N,S}$	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	$H_N := \int_{t^o}^{t^e} \dot{H}_N \; dt + Ho_N$	Enthalpy	macroscopic

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

13   Interface Link Equation

no	equation	documentation	layer
22	$\_\lambda_S := \lambda_S$	interface equation	material –> macroscopic
60	$\_k^c_{xA} := k^c_{xA}$	interface equation	material –> macroscopic
61	$\_k^c_{yA} := k^c_{yA}$	interface equation	material –> macroscopic
62	$\_k^c_{zA} := k^c_{zA}$	interface equation	material –> macroscopic
63	$\_k^d_{xA,S} := k^d_{xA,S}$	interface equation	material –> macroscopic
64	$\_k^{d,Fick}_{x\ A,S} := k^{d,Fick}_{x\ A,S}$	interface equation	material –> macroscopic
65	$\_k^{d,Fick}_{y\ A,S} := k^{d,Fick}_{y\ A,S}$	interface equation	material –> macroscopic
66	$\_k^d_{yA,S} := k^d_{yA,S}$	interface equation	material –> macroscopic
67	$\_k^d_{zA,S} := k^d_{zA,S}$	interface equation	material –> macroscopic
68	$\_k^{d,Fick}_{z\ A,S} := k^{d,Fick}_{z\ A,S}$	interface equation	material –> macroscopic
69	$\_k^q_{xA} := k^q_{xA}$	interface equation	material –> macroscopic

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