1 Variables

2 root

	var	symbol	documentation	type	units	eqs
10	$F_{N,A}$	F	basic directed graph incidence matrix	network		
48	$I_{NAN,A}$	I_N_A	project node on arc	projection		
7	Δt	t_interval	time interval	frame	s	5
9	Δ	pulse	pulse of length time interval	frame		7
5	t^o	to	time zero	frame	s	3
6	t^e	te	time end	frame	s	4
4	t	t	time	frame	s	
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
13	r_{yN}	r_y	y-direction	frame	m	9
12	r_{xN}	r_x	x-direction	frame	$\mid m \mid$	8
14	r_{zN}	r_z	z-direction	frame	$\mid m \mid$	10
11	ℓ_N	1	length	frame	$\mid m \mid$	
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
18	$n_{N,S}$	n	fundamental state - molar mass	state	mol	
16	U_N	U	fundamental state - internal energy	state	$kg m^2 s^{-2}$	
15	V_N	V	fundamental state - volume	state	m^3	11
25	C_N	C	fundamental state - charge	state	As	
17	S_N	S	fundamental state - entropy	state	$kg m^2 K^{-1} s^{-2}$	
22	H_N	н	Enthalpy	state	$kg m^2 s^{-2}$	15
34	R_N	R	Gas constant	constant	$kg m^2 mol^{-1} K^{-1} s^{-2}$	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
35	$U^e{}_N$	Ue	electrical potential – voltage	effort	$kg m^2 A^{-1} s^{-3}$	26
19	T_N	Т	temperature	effort	K	16
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
28	v_{yN}	v_y	velocity in y-direction	secondaryState	ms^{-1}	20
29	v_{zN}	v_z	velocity in z-direction	secondaryState	ms^{-1}	21

4 material

	var	symbol	documentation	type	units	eqs
26	λ_S	Mm	species' molecular mass	property	$kg mol^{-1}$	
56	k_{yA}^q	kq_y_A	thermal conductivity in y-direction in arc	property	$kg K^{-1} s^{-3}$	46
42	$k_{yN,S}^d$	kd_y	diffusional mass conductivity in z-direction	property	$kg^{-1} m^{-4} mol^2 s$	33
43	$k_{zN,S}^d$	kd_z	diffusional mass conductivity in z-direction	property	$kg^{-1} m^{-4} mol^2 s$	34
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
61	$k^(d, Fick_{xA,S}$	kd_x_Fick	Fick's diffusivity in arc and x-direction	property	ms^{-1}	51
44	k_{xN}^c	kc_x	convective mass conductivity in x-direction	property	$m^{-1} s$	35
51	k_{zA}^c	kc_z_A	convective mass conductivity in z-direction in arc	property	$m^{-1} s$	41
63	$k^(d, Fick_{zA,S})$	kd_z_Fick	Fick's diffusivity in arc and z-direction	property	ms^{-1}	53
38	k_{xN}^q	kq_x	thermal conductivity in x-direction	property	$kg K^{-1} s^{-3}$	29
45	k_{yN}^c	kc_y	convective mass conductivity in y-direction	property	$m^{-1} s$	36
47	$h_{N,S}$	h	partial molar enthalpies	property	$kg m^2 mol^{-1} s^{-2}$	38
37	C_{vN}	Cv	total heat capacity at constant volume	property	$kg m^2 K^{-1} s^{-2}$	28
40	k_{zN}^q	kq_z	thermal conductivity in z-direction	property	$kg K^{-1} s^{-3}$	31
60	v_S	v	molar volume of species	property	$m^3 mol^{-1}$	50
46	k_{zN}^c	kc_z	convective mass conductivity in z-direction	property	$m^{-1} s$	37
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
36	C_{pN}	Ср	total heat capacity at constant pressure	property	$kg m^2 K^{-1} s^{-2}$	27
41	$k_{xN,S}^d$	kd_x	diffusional mass conductivity in x-direction	property	$kg^{-1} m^{-4} mol^2 s$	32
39	k_{yN}^q	kq_y	thermal conductivity in y-direction	property	$kg K^{-1} s^{-3}$	30
49	k_{xA}^c	kc_x_A	convective mass conductivity in x-direction in arc	property	$m^{-1} s$	39
59	$density_N$	density	density	property	$kg m^{-3}$	49
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

	var	symbol	documentation	type	units	eqs
62	$k^(d, Fick_{yA,S})$	kd_y_Fick	Fick's diffusivity in arc and y-direction	property	ms^{-1}	52
57	k_{zA}^q	kq_z_A	thermal conductivity in z-direction in arc	property	$kg K^{-1} s^{-3}$	47
55	k_{xA}^q	kq_x_A	thermal conductivity in x-direction in arc	property	$kg K^{-1} s^{-3}$	45
58	m_N	m	mass	property	kg	48
50	k_{yA}^c	kc_y_A	convective mass conductivity in y-direction in arc	property	$m^{-1} s$	40
89	$density_{AA}$	density_A	density of arc material	property	$kg m^{-3}$	78

5 macroscopic

	var	symbol	documentation	type	units	eqs
84	\dot{q}_N	aq	accumulation due to conductive heat flow	transport	kgm^2s^{-3}	73
87	$c_{A,S}$	c_A	concentration in convective mass flow	transport	$m^{-3} mol$	76
83	\hat{q}_{xA}	fq_x_A	heat flow in arc and x-direction	transport	$kg m^2 s^{-3}$	72
91	\dot{V}_A	fV	volumetric flow	transport	$m^3 s^{-1}$	80
92	$\hat{n}^c{}_{A,S}$	fnc_A	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
86	d_A	d	fow direction of convective flow	transport		75
70	A_{yzA}	A_yz_A	cross sectional area yz of arc	geometry	m^2	59
68	A_{xyA}	A_xy_A	cross sectional area yz of arc	geometry	m^2	57
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
69	A_{xzA}	A_xz_A	cross sectional area xz of arc	geometry	m^2	58
65	A_{xyN}	A_xy	cross sectional area xy	geometry	m^2	54
64	$D_{N,A}$	D	difference operator	differenceOperator		
85	$c_{N,S}$	С	molar concentration	secondaryState	$m^{-3} mol$	74

${\small 6} \quad \text{material-macroscopic} \\$

	var	symbol	documentation	type	units	eqs
75	$_{k}d_{xF}ick_{A,S}$	_kd_x_Fick	link variable kd x Fick to interface material »> macroscopic	get	ms^{-1}	64
81	$-k_{yA}^q$	_kq_y_A	link variable kq y A to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	70
73	$_k_{zA}^c$	_kc_z_A	link variable kc z A to interface material »> macroscopic	get	$m^{-1} s$	62
76	$_{k}d_{yF}ick_{A,S}$	_kd_y_Fick	link variable kd y Fick to interface material »> macroscopic	get	ms^{-1}	65
88	$_ ho_N$	_density	link variable density to interface material »> macroscopic	get	$kg m^{-3}$	77
80	$-k_{xA}^q$	_kq_x_A	$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	get	$kg K^{-1} s^{-3}$	69
79	$_{k}d_{zF}ick_{A,S}$	_kd_z_Fick	link variable kd z Fick to interface material »> macroscopic	get	ms^{-1}	68
82	$-k_z^q A$	_kq_z_A	link variable kq z A to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	71
78	$-k_z^d{}_{A,S}$	_kd_z_A	link variable kd z A to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	67
72	$-k_{yA}^{c}$	_kc_y_A	link variable kc y A to interface material »> macroscopic	get	$m^{-1} s$	61
90	_\rho_A	_density_A	link variable density A to interface material »> macroscopic	get	$kg m^{-3}$	79
74	$_k^d_{xA,S}$	_kd_x_A	$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	get	$kg^{-1} m^{-4} mol^2 s$	63
71	$-k_{xA}^c$	_kc_x_A	link variable kc x A to interface material »> macroscopic	get	$m^{-1} s$	60
30	$_{-}\lambda_{S}$	_Mm	link variable Mm to interface material »> macroscopic	get	$kg mol^{-1}$	22

	var	symbol	documentation	type	units	eqs
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

7 Equations

8 Generic

no	equation	documentation	layer
1	1 := Instantiate(#, #)	numerical one	root
2	0 := 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	$\Delta t := \operatorname{Instantiate}(t, \#)$	time interval	root
6	0.5 := Instantiate(#, #)	numerical one half	root
7	$\Delta := \operatorname{sign}(t - t^{o}) - \operatorname{sign}(t - (t^{o} - \Delta t))$	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	$v_{xN} := \left(t\right)^{-1} . r_{xN}$	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	$U^e{}_N := \left(C_N\right)^{-1} . U_N$	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	$k_{xN,S}^d := \left(\mu_{N,S}\right)^{-1} \cdot \left(v_{xN} \cdot \left(\left(V_N\right)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}}\right)\right)$	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

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	mat erial
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	$h_{N,S} := H_N \cdot \left(n_{N,S} \right)^{-1}$	partial molar enthalpies	material
39	$k_{xA}^c := I_{NAN,A} \star k_{xN}^c$	convective mass conductivity in x-direction in arc	material
40	$k_{yA}^c := I_{NAN,A} \star k_{yN}^c$	convective mass conductivity in y-direction in arc	material
41	$k_{zA}^c := I_{NAN,A} \star k_{zN}^c$	convective mass conductivity in z-direction in arc	material
42	$k_{xA,S}^d := I_{NAN,A} \star k_{xN,S}^d$	diffusional mass conductivity in x-direction in arc	material
43	$k_{yA,S}^d := I_{NAN,A} \star k_{yN,S}^d$	diffusional mass conductivity in z- direction in arc	material
44	$k_{zA,S}^d := I_{NAN,A} \star k_{zN,S}^d$	diffusional mass conductivity in z- direction in arc	material
45	$k_{xA}^q := I_{NAN,A} \star k_{xN}^q$	thermal conductivity in x-direction in arc	material
46	$k_{yA}^q := I_{NAN,A} \star k_{yN}^q$	thermal conductivity in y-direction in arc	mat erial
47	$k_{zA}^q := I_{NAN,A} \star k_{zN}^q$	thermal conductivity in z-direction in arc	material
48	$m_N := \lambda_S \star n_{N,S}$	mass	material

no	equation	documentation	layer
49	$density_N := (V_N)^{-1} \cdot m_N$	density	material
50	$v_S := V_N \star (n_{N,S})^{-1}$	molar volume of species	material
51	$k^{(d)}, Fick_{xA,S} := I_{NAN,A} \star \left(v_{xN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1}\right)$	Fick's diffusivity in arc and x-direction	material
52	$k^{(d)}, Fick_{yA,S} := I_{NAN,A} \star \left(v_{yN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1}\right)$	Fick's diffusivity in arc and y-direction	material
53	$k^{(d)}, Fick_{zA,S} := I_{NAN,A} \star \left(v_{zN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1}\right)$	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	$A_{xyA} := I_{NAN,A} \star A_{xyN}$	cross sectional area yz of arc	macroscopic
58	$A_{xzA} := I_{NAN,A} \star A_{xzN}$	cross sectional area xz of arc	macroscopic
59	$A_{yzA} := I_{NAN,A} \star A_{yzN}$	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	$c_{N,S} := \left(V_N\right)^{-1} . n_{N,S}$	molar concentration	macroscopic
75	$d_A := \mathrm{sign}\left(D_{N,A} \star p_N\right)$	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	$density_{AA} := I_{NAN,A} \star density_N$	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	$\hat{n}^c{}_{A,S} := \dot{V}_A \cdot c_{A,S}$	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

9 Interface Link Equation

no	equation	documentation	layer
22	$_{-}\lambda_{S}:=\lambda_{S}$	interface equation	material -> macro- scopic
60	$_k_{xA}^c := k_{xA}^c$	interface equation	material -> macro- scopic
61	$_k_{yA}^c := k_{yA}^c$	interface equation	material -> macro- scopic
62	$_k_{zA}^c := k_{zA}^c$	interface equation	material -> macro- scopic
63	$_k_{xA,S}^d := k_{xA,S}^d$	interface equation	material -> macro- scopic
64	$_kd_{xF}ick_{A,S}:=k^(d,Fick_{xA,S})$	interface equation	material -> macro- scopic
65	$_kd_{yF}ick_{A,S}:=k^(d,Fick_{yA,S})$	interface equation	material -> macro- scopic
66	$_{k_{y}A,S}:=k_{y}^{d}{}_{A,S}$	interface equation	material -> macro- scopic
67	$_k_{zA,S}^d := k_{zA,S}^d$	interface equation	material -> macro- scopic
68	$_kd_{zF}ick_{A,S} := k^{(d)}, Fick_{zA,S}$	interface equation	material -> macro- scopic
69	$_k_{xA}^q := k_{xA}^q$	interface equation	material -> macro- scopic

no	equation	documentation	layer
70	$_k_{yA}^q := k_{yA}^q$	interface equation	material -> macro- scopic
71	$igspace_{zA} := k_{zA}^q$	interface equation	material -> macro- scopic
77	$_ ho_N := density_N$	interface equation	material -> macro- scopic
79	$_ ho_A := density_{AA}$	interface equation	material -> macro- scopic