

# 1 Variables

## 2 root

	var	symbol	documentation	type	units	eqs
10	$F_{N,A}$	<b>F</b>	basic directed graph incidence matrix	network		
96	$I_{NN}$	<b>I_N</b>	vector of ones of length nodes	projection		
48	$I_{NAN,A}$	<b>I_N_A</b>	project node on arc	projection		
97	$I_{AA}$	<b>I_A</b>	vector of ones of length arcs	projection		
9	$\Delta$	<b>pulse</b>	pulse of length time interval	frame		7
4	$t$	<b>t</b>	time	frame	s	
6	$t^e$	<b>te</b>	time end	frame	s	4
7	$\Delta t$	<b>t_interval</b>	time interval	frame	s	5
5	$t^o$	<b>to</b>	time zero	frame	s	3
8	0.5	<b>onehalf</b>	numerical one half	constant		6
2	1	<b>one</b>	numerical one	constant		1
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
98	$I_{SS}$	I_S	vector of ones of length sepecies	projection		
14	$r_{zN}$	r_z	z-direction	frame	$m$	10
13	$r_{yN}$	r_y	y-direction	frame	$m$	9
11	$\ell_N$	l	length	frame	$m$	
12	$r_{xN}$	r_x	x-direction	frame	$m$	8
23	$A_N$	A	Helmholts energy	state	$kg\ m^2\ s^{-2}$	17
18	$n_{N,S}$	n	fundamental state - molar mass	state	$mol$	
22	$H_N$	H	Enthalpy	state	$kg\ m^2\ s^{-2}$	15
16	$U_N$	U	fundamental state - internal energy	state	$kg\ m^2\ s^{-2}$	
24	$G_N$	G	Gibbs free energy	state	$kg\ m^2\ s^{-2}$	18
25	$C_N$	C	fundamental state - charge	state	$A\ s$	
15	$V_N$	V	fundamental state - volume	state	$m^3$	11
17	$S_N$	S	fundamental state - entropy	state	$kg\ m^2\ K^{-1}\ s^{-2}$	
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	$mol^{-1}$	
20	$p_N$	p	pressure	effort	$kg\ m^{-1}\ s^{-2}$	13
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
29	$v_{zN}$	v_z	velocity in z-direction	secondaryState	$ms^{-1}$	21
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

## 4 material

	var	symbol	documentation	type	units	eqs
47	$h_{N,S}$	h	partial molar enthalpies	property	$kg\ m^2\ mol^{-1}\ s^{-2}$	38
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
44	$k_{xN}^c$	kc_x	convective mass conductivity in x-direction	property	$m^{-1}\ s$	35
50	$k_{yA}^c$	kc_y_A	convective mass conductivity in y-direction in arc	property	$m^{-1}\ s$	40
45	$k_{yN}^c$	kc_y	convective mass conductivity in y-direction	property	$m^{-1}\ s$	36
39	$k_{yN}^q$	kq_y	thermal conductivity in y-direction	property	$kg\ K^{-1}\ s^{-3}$	30
59	$\rho_N$	density	density	property	$kg\ m^{-3}$	49
56	$k_{yA}^q$	kq_y_A	thermal conductivity in y-direction in arc	property	$kg\ K^{-1}\ s^{-3}$	46
26	$\lambda_S$	Mm	species' molecular mass	property	$kg\ mol^{-1}$	
40	$k_{zN}^q$	kq_z	thermal conductivity in z-direction	property	$kg\ K^{-1}\ s^{-3}$	31
41	$k_{xN,S}^d$	kd_x	diffusional mass conductivity in x-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	32
38	$k_{xN}^q$	kq_x	thermal conductivity in x-direction	property	$kg\ K^{-1}\ s^{-3}$	29
62	$k_{yA,S}^{d,Fick}$	kd_y_Fick	Fick's diffusivity in arc and y-direction	property	$ms^{-1}$	52
60	$v_S$	v	molar volume of species	property	$m^3\ mol^{-1}$	50
49	$k_{xA}^c$	kc_x_A	convective mass conductivity in x-direction in arc	property	$m^{-1}\ s$	39
46	$k_{zN}^c$	kc_z	convective mass conductivity in z-direction	property	$m^{-1}\ s$	37
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
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
51	$k_{zA}^c$	kc_z_A	convective mass conductivity in z-direction in arc	property	$m^{-1}\ s$	41
36	$C_{pN}$	Cp	total heat capacity at constant pressure	property	$kg\ m^2\ K^{-1}\ s^{-2}$	27
58	$m_N$	m	mass	property	$kg$	48
61	$k_{xA,S}^{d,Fick}$	kd_x_Fick	Fick's diffusivity in arc and x-direction	property	$ms^{-1}$	51

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	var	symbol	documentation	type	units	eqs
42	$k_{yN,S}^d$	kd_y	diffusional mass conductivity in z-direction	property	$kg^{-1} m^{-4} mol^2 s$	33
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
63	$k_z^{d,Fick}{}_{A,S}$	kd_z_Fick	Fick's diffusivity in arc and z-direction	property	$ms^{-1}$	53
89	$\rho_A$	density_A	density of arc material	property	$kg m^{-3}$	78
43	$k_{zN,S}^d$	kd_z	diffusional mass conductivity in z-direction	property	$kg^{-1} m^{-4} mol^2 s$	34
57	$k_{zA}^q$	kq_z_A	thermal conductivity in z-direction in arc	property	$kg K^{-1} s^{-3}$	47
102	$\mu_{N,S}^o$	chemPot_o	standard chemical potential	effort	$kg m^2 mol^{-1} s^{-2}$	86

## 5 macroscopic

	var	symbol	documentation	type	units	eqs
92	$\hat{n}_{A,S}^c$	fnc_A	convective mass flow in an arc	transport	$mol\ s^{-1}$	81
83	$\hat{q}_{xA}$	fq_x_A	heat flow in arc and x-direction	transport	$kg\ m^2\ s^{-3}$	72
86	$d_A$	d	flow direction of convective flow	transport		75
101	$\hat{n}_{A,S}^d$	fnd_A	diffusional mass flow in arc	transport	$mol\ s^{-1}$	85 89
93	$\hat{n}_{N,S}^c$	anc	accumulation due to convective mass flow	transport	$mol\ s^{-1}$	82
91	$\dot{V}_A$	fV	volumetric flow	transport	$m^3\ s^{-1}$	80
87	$c_{A,S}$	c_A	concentration in convective mass flow	transport	$m^{-3}\ mol$	76
84	$\dot{q}_N$	aq	accumulation due to conductive heat flow	transport	$kg\ m^2\ s^{-3}$	73
68	$A_{xyA}$	A_xy_A	cross sectional area yz of arc	geometry	$m^2$	57
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
67	$A_{yzN}$	A_yz	cross sectional area yz	geometry	$m^2$	56
66	$A_{xzN}$	A_xz	cross sectional area xz	geometry	$m^2$	55
65	$A_{xyN}$	A_xy	cross sectional area xy	geometry	$m^2$	54
64	$D_{N,A}$	D	difference operator	differenceOperator		
85	$c_{N,S}$	c	molar concentration	secondaryState	$m^{-3}\ mol$	74
100	$x_{N,S}$	x	concentration mole fraction	secondaryState		84
99	$nt_N$	nt	total amount	secondaryState	$mol$	83

## 6 material–macroscopic

	var	symbol	documentation	type	units	eqs
90	$_{\rho A}$	$_{\text{density\_A}}$	link variable density A to interface material »> macroscopic	get	$kg\,m^{-3}$	79
88	$_{\rho N}$	$_{\text{density}}$	link variable density to interface material »> macroscopic	get	$kg\,m^{-3}$	77
72	$_{k_y^c A}$	$_{\text{kc\_y\_A}}$	link variable kc y A to interface material »> macroscopic	get	$m^{-1}\,s$	61
30	$_{\lambda S}$	$_{\text{Mm}}$	link variable Mm to interface material »> macroscopic	get	$kg\,mol^{-1}$	22
77	$_{k_y^d A,S}$	$_{\text{kd\_y\_A}}$	link variable kd y A to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	66
81	$_{k_y^q A}$	$_{\text{kq\_y\_A}}$	link variable kq y A to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	70
76	$_{k_y^{d,Fick} A,S}$	$_{\text{kd\_y\_Fick}}$	link variable kd y Fick to interface material »> macroscopic	get	$ms^{-1}$	65
74	$_{k_x^d A,S}$	$_{\text{kd\_x\_A}}$	link variable kd x A to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	63
78	$_{k_z^d A,S}$	$_{\text{kd\_z\_A}}$	link variable kd z A to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	67
82	$_{k_z^q A}$	$_{\text{kq\_z\_A}}$	link variable kq z A to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	71
71	$_{k_x^c A}$	$_{\text{kc\_x\_A}}$	link variable kc x A to interface material »> macroscopic	get	$m^{-1}\,s$	60
73	$_{k_z^c A}$	$_{\text{kc\_z\_A}}$	link variable kc z A to interface material »> macroscopic	get	$m^{-1}\,s$	62
80	$_{k_x^q A}$	$_{\text{kq\_x\_A}}$	link variable kq x A to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	69
75	$_{k_x^{d,Fick} A,S}$	$_{\text{kd\_x\_Fick}}$	link variable kd x Fick to interface material »> macroscopic	get	$ms^{-1}$	64

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	var	symbol	documentation	type	units	eqs
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

## 7 macroscopic-material

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



## 8 Equations

## 9 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	$k_{xA}^c := I_{NAN,A} \star k_{xN}^c$	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	material
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

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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	$k_{x,A,S}^{d,Fick} := I_{NAN,A} \star \left( v_{xN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$	Fick's diffusivity in arc and x-direction	material
52	$k_{y,A,S}^{d,Fick} := I_{NAN,A} \star \left( v_{yN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$	Fick's diffusivity in arc and y-direction	material
53	$k_{z,A,S}^{d,Fick} := I_{NAN,A} \star \left( v_{zN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$	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	$c_{N,S} := (V_N)^{-1} \cdot n_{N,S}$	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	$\rho_A := I_{NAN,A} \star \rho_N$	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	$nt_N := I_{SS} \star n_{N,S}$	total amount	macroscopic
84	$x_{N,S} := (nt_N)^{-1} \cdot n_{N,S}$	concentration mole fraction	macroscopic
85	$\dot{n}_{A,S}^d := A_{yzA} \cdot (-_x k_{A,S}^{d,Fick}) \cdot (D_{N,A} \star c_{N,S})$	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	$\dot{n}_{A,S}^d := A_{yzA} \cdot (-_x k_{A,S}^d) \cdot (D_{N,A} \star \mu_{N,S})$	diffusional mass flow in arc	macroscopic

## 10 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 material $\rightarrow$