### 1 Variables

#### 2 root

	var	symbol	documentation	type	units	eqs
9	$S_{I,p}$	S_Ip	selection matrix interface to control input	network		
8	$F^{sink}_{N,A}$	F_NA_sink	incidence matrix NA sink	network		
22	$y_{N,t,u}$	y_Ntu	output signal in control domain	network		
20	$A_{N,t,u}$	A_Ntu	mapping from input elements to outputs	network		
12	$S_{A,p}$	S_Ap	selection matrix interface species-related measures	network		
27	$I_{N,A}$	I_NA	$   \    identity \ mapping \ from \ < N > \ to \ < A > $	network		
13	$S_{I,q}$	S_Aq	selection matrix arcs to outputs	network		
3	$F^{source}_{N,I}$	F_NI_source	incidence matrix NI source	network		
14	$S_{N,p,q}$	S_Npu	selection matrix for stacker	network		
11	$I_{t,u}$	I_tu	$   \   identity \ mapping \ from \ < t > \ to \ < u >$	network		
17	$cz_N$	cz_N	output from control	network		
18	$cz_I$	cz_I	interface variable macro -> control	network		
21	$u_{N,t,u}$	u_Ntu	input signal in control domain	network		
5	$F^{source}{}_{A,I}$	F_AI_source	incidence matrix AI source	network		
6	$F^{sink}{}_{A,I}$	F_AI_sink	incidence matrix AI sink	network		
10	$S_{I,q}$	S_Iq	selection matrix interface to control output	network		
4	$F^{sink}{}_{N,I}$	F_NI_sink	incidence matrix NI sink	network		
15	$S_{N,q,t}$	S_Nqt	selection matrix or splitter	network		
19	$A_{N,p,q}$	A_Npq	mapping from inputs to outputs	network		
7	$F^{source}_{N,A}$	F_NA_source	incidence matrix NA source	network		
16	$mv_I$	mv_I	interface variable macro -> control	network		
2	$F_{N,A}$	F	incidence matrix	network		

	var	symbol	documentation	type	units	eqs
105	$t^o$	to	starting time	frame	s	4
107	$\Delta t$	t_interval	time interval	frame	s	6
1	t	t	time	frame	s	
106	$t^e$	te	end time	frame	s	5
104	0.5	oneHalf	numerical value one half	constant		3
103	1	one	numerical value one	constant		2
101	#	value	numerical value	constant		
102	0	zero	numerical value zero	constant		1

# 3 physical

	var	symbol	documentation	type	units	eqs
25	$r_{zN}$	r_z	z-coordinate	frame	m	
24	$r_{yN}$	r_y	y-coordinate	frame	$\mid m \mid$	
23	$r_{xN}$	r_x	x-coordinate	frame	$\mid m \mid$	
110	$V_N$	V	volume	state	$m^3$	7
108	$U_N$	U	fundamental state – internal energy	state	$kg m^2 s^{-2}$	
144	$C_N$	C	fundamental state – charge	state	As	
111	$n_{N,S}$	n	fundamental state – molar mass	state	mol	93
137	$m_N$	m	mass	state	kg	30
109	$S_N$	S	fundamental state – internal entropy	state	$kg  m^2  K^{-1}  s^{-2}$	
122	$k^B$	Boltz	Boltzmann constant	constant	$kg m^2 K^{-1} s^{-2}$	
123	R	R	gas constant	constant	$kg m^2 mol^{-1} K^{-1} s^{-2}$	17
132	$\lambda_S$	Mm	molecular masses	constant	$kg  mol^{-1}$	
121	$N^A$	Avo	Avogadro constant	constant	$mol^{-1}$	
149	$A_{xzN}$	Axz	cross sectional are xz	secondaryState	$m^2$	41
148	$A_{xyN}$	Axy	cross sectional area xy	secondaryState	$m^2$	40
150	$A_{yzN}$	Ayz	cross sectional area yz	secondaryState	$m^2$	42
143	$ ho_N$	rho	density	secondaryState	$kg m^{-3}$	36

#### 4 macroscopic

	var	symbol	documentation	type	units	eqs
151	$\hat{q}_{xA}$	fq_x	heat flow in x-direction	transport	$kgm^2s^{-3}$	43
205	$\dot{H}^d_{xN}$	aHnd_x	accumulation of enthalpy due to diffusional mass flow in x-direction	transport	$kg m^2 s^{-3}$	100
195	$\dot{n}^d_{xN,S}$	and_x	accumulation due to diffusion in x-direction	transport	$mol  s^{-1}$	88
153	$\hat{q}_{zA}$	fq_z	heat flow in z-direction	transport	$kg m^2 s^{-3}$	45
154	$\hat{n}^d_{xA,S}$	fnd_x	diffusion flow in x-direction	transport	$mol  s^{-1}$	46 89
152	$\hat{q}_{yA}$	fq_y	heat flow in y-direction	transport	$kgm^2s^{-3}$	44
207	$\dot{H}^d_{zN}$	aHnd_z	accumulation of enthalpy due to diffusional mass flow in z-direction	transport	$kg m^2 s^{-3}$	102
211	$\hat{w}_A$	fw	a fixed work flow to start with	transport	$kg m^2 s^{-3}$	106
214	$\dot{w}_N$	aw	accumulation of enthalpy due to work flow	transport	$kgm^2s^{-3}$	109
210	$\dot{q}_{zN}$	aq_z	accumulation due to heat flow in z-direction	transport	$kgm^2s^{-3}$	105
194	$anc_{xN,S}$	anc_x	accumulation of molar mass due to convection	transport	$mol  s^{-1}$	87
206	$\dot{H}^d_{yN}$	aHnd_y	accumulation of enthalpy due to diffusional mass flow in y-direction	transport	$kg m^2 s^{-3}$	101
158	$c_{A,S}$	c_AS	concentration in convective event-dynamic flow	transport	$m^{-3}  mol$	50
208	$\dot{q}_{xN}$	aq_x	accumulation due to heat flow in x-direction	transport	$kgm^2s^{-3}$	103
160	$\hat{n}_{xA,S}^c$	fnc_x	molar convective flow in x-direction	transport	$mol  s^{-1}$	52
157	$d_A$	d	flow direction of convective flow	transport		49
212	$\dot{n}^d_{yN,S}$	and_y	accumulation due to diffusion in y-direction	transport	$mol  s^{-1}$	107
156	$\hat{n}^d_{zA,S}$	fnd_z	diffusion flow in z-direction	transport	$mol  s^{-1}$	48 91
209	$\dot{q}_{yN}$	aq_y	accumulation due to heat flow in y-direction	transport	$kg m^2 s^{-3}$	104
155	$\hat{n}^d_{yA,S}$	fnd_y	diffusion flow in y-direction	transport	$mol  s^{-1}$	47 90
159	$\hat{V}_A$	fV	volumetric flow in x-direction	transport	$m^3  s^{-1}$	51

	var	symbol	documentation	type	units	eqs
204	$\dot{H}_{xN}^{c}$	aHnc_x	accumulation of enthalpy due to convective mass flow in x-direction	transport	$kgm^2s^{-3}$	99
213	$\dot{n}^d_{zN,S}$	and_z	accumulation due to diffusion in z-direction	transport	$mol  s^{-1}$	108
183	$k_{xA}^c$	kcA_x	convective mass conductivity in arc and x diretion	properties	$m^{-1} s$	76
189	$ ho_A$	rhoA	density in arc	properties	$kg  m^{-3}$	82
192	$\hat{k}_z^{d,Fick}{}_{A,S}$	kdAFick_z	Fick diffusivity in arc and z-direction	properties	$ms^{-1}$	85
193	$h_{A,S}$	hA	partial molar enthalpiies in arc	properties	$kg  m^2  mol^{-1}  s^{-2}$	86
188	$k_{zA}^{q}$	kqA_z	thermal conductivity in arc and z-direction	properties	$kg K^{-1} s^{-3}$	81
184	$k_{yA}^c$	kcA_y	convective mass conductivity in arc and y-direction	properties	$m^{-1} s$	77
187	$k_{yA}^q$	kqA_y	thermal conductivity in arc and y-direction	properties	$kg K^{-1} s^{-3}$	80
185	$k_{zA}^{c}$	kcA_z	convecive mass conductivity in arc and y-direction	properties	$m^{-1} s$	78
181	$k_{yA,S}^d$	kdA_y	diffusivity in arc and y-direction	properties	$kg^{-1}  m^{-4}  mol^2  s$	74
190	$\hat{k}_x^{d,Fick}{}_{A,S}$	kdAFick_x	Fick's diffusivity in arc and x-direction	properties	$ms^{-1}$	83
219	$R^e{}_N$	elResistant	electrical resistant	properties	$kg m^2 A^{-2} s^{-3}$	115
180	$k_{xA,S}^d$	kdA_x	diffusivity in arc and x-direction	properties	$kg^{-1} m^{-4} mol^2 s$	73
186	$k_{xA}^q$	kqA_x	thermal conductivity in arc and x-direction	properties	$kg K^{-1} s^{-3}$	79
182	$k_{zA,S}^d$	kdA_z	diffusivity in arc and z-direction	properties	$kg^{-1} m^{-4} mol^2 s$	75
191	$\hat{k}_y^{d,Fick}{}_{A,S}$	kdAFick_y	Fick diffusivity in arc and y-direction	properties	$ms^{-1}$	84
117	$G_N$	G	Gibbs free energy	state	$kg m^2 s^{-2}$	13
203	$n^o{}_{N,S}$	no	initial mass	state	mol	98
115	$H_N$	Н	Enthalpy	state	$kgm^2s^{-2}$	11 112
216	$H^o{}_N$	Но	initial enthalpy	state	$kgm^2s^{-2}$	111
116	$A_N$	A	Helmholtz energy	state	$kgm^2s^{-2}$	12
113	$T_N$	Т	temperature	effort	K	9

	var	symbol	documentation	type	units	eqs
217	$U^e{}_N$	Ue	electrical potential – voltage	effort	$kg  m^2  A^{-1} s^{-3}$	113
112	$p_N$	p	thermodynamic pressure	effort	$kg  m^{-1}  s^{-2}$	8
114	$\mu_{N,S}$	chemPot	chemical potential	effort	$kg  m^2  mol^{-1}  s^{-2}$	10 54
161	$\mu^o{}_{N,S}$	chemPotStandard	instantiating standard chemical potential	effort	$kg  m^2  mol^{-1}  s^{-2}$	53
142	$c_{VN}$	cV	specific heat capacity at constant volume	secondaryState	$m^2 K^{-1} s^{-2}$	35
138	$c_{N,S}$	С	molar concentration	secondaryState	$m^{-3}  mol$	31
125	$CV_N$	CV	total heat capacity at constant volume	secondaryState	$kg  m^2  K^{-1}  s^{-2}$	19
124	$Cp_N$	Ср	total heat capacity at constant pressure	secondaryState	$kg  m^2  K^{-1}  s^{-2}$	18
118	$v_{xN}$	v_x	velocity in x-direction	secondaryState	$ms^{-1}$	14
136	$h_{N,S}$	h	partial molar enthalpies	secondaryState	$kg  m^2  mol^{-1}  s^{-2}$	29
141	$c_{pN}$	ср	specific heat capacity at constant pressure	secondaryState	$m^2 K^{-1} s^{-2}$	34
120	$v_{zN}$	v_z	velocity in z-direction	secondaryState	$ms^{-1}$	16
139	$n^t_N$	nt	total number of moles	secondaryState	mol	32
119	$v_{yN}$	v_y	velocity in y-direction	secondaryState	$ms^{-1}$	15
140	$x_{N,S}$	x	mole fraction	secondaryState		33
202	$ ilde{n}_{N,S}$	np	link variable np to interface macroscopic	conversion	$m^{-3}  mol  s^{-1}$	97
215	$\dot{H}_N$	dH	accumulation of enthalpy	diffState	$kgm^2s^{-3}$	110
196	$\dot{n}_{N,S}$	an	differential mass balance without reaction	diffState	$mol  s^{-1}$	92
220	$\dot{U}^e{}_A$	dUe	Kirkhoffs first law	diffState	$kg  m^2  A^{-1} s^{-3}$	116
218	$I^e{}_N$	current	current definition	internal Transport	A	114

#### 5 reactions

	var	symbol	documentation	type	units	eqs
198	$K^o{}_K$	Ко	Arrhenius frequency factor	constant	$m^{-3}  mol  s^{-1}$	
197	$E^a{}_K$	Ea	Arrhenius activation energy	constant	$kg  m^2  mol^{-1}  s^{-2}$	
26	$N_{S,K}$	N	stoichiometric matrix	constant		
167	$T_{N,p}$	Т	link variable T to interface reactions	effort	K	60
163	$c_{N,S,p}$	С	link variable c to interface reactions	secondaryState	$m^{-3}  mol$	56
165	$x_{N,S,p}$	x	link variable x to interface reactions	secondaryState		58
200	$ ilde{n}_{N,S,q}$	np	production from reaction set	conversion	$m^{-3}  mol  s^{-1}$	95
199	$K_{N,K,p}$	K	Arrhenius reaction "constant"	conversion	$m^{-3}  mol  s^{-1}$	94
168	$f_{N,S,K,p}$	factor	factor for probability computation	conversion		61
169	$\xi_{N,K,p}$	probability	probability of reaction to take place	conversion		62

### macroscopic-reactions

	var	symbol	documentation	type	units	eqs
166	$\_T_I$	_Т	link variable T to interface macroscopic $\gg>$ reactions with source:node	get	K	59
164	$\_x_{I,S}$	_x	$\begin{array}{c} \mbox{link variable x to interface macroscopic } > \mbox{reactions} \\ \mbox{with source:node} \end{array}$	get		57
162	$\_c_{I,S}$	_c	link variable c to interface macroscopic »> reactions with source:node	get	$m^{-3}  mol$	55

# 7 reactions-macroscopic

	var	symbol	documentation	type	${ m units}$	eqs
201	$\_np_{I,S}$	_np	link variable np to interface reactions »> macroscopic with source:node	get	$m^{-3}  mol  s^{-1}$	96

# 8 Equations

### 9 Generic

no	equation	documentation	layer
1	$0 := \mathbf{Instantiate}(\#, \#)$	numerical value zero	root
2	$1 := \mathbf{Instantiate}(\#, \#)$	numerical value one	root
3	$0.5 := \mathbf{Instantiate}(\#, \#)$	numerical value one half	root
4	$t^o := \mathbf{Instantiate}(t, \#)$	starting time	root
5	$t^e := \mathbf{Instantiate}(t, \#)$	end time	root
6	$\Delta t := \mathbf{Instantiate}(t,\#)$	time interval	root
7	$V_N := r_{xN} \cdot r_{yN} \cdot r_{zN}$	volume	physical
8	$p_N := rac{\partial U_N}{\partial V_N}$	thermodynamic pressure	physical
9	$T_N := \frac{\partial U_N}{\partial S_N}$	temperature	macroscopic
10	$\mu_{N,S} := \frac{\partial U_N}{\partial n_{N,S}}$	chemical potential	macroscopic
11	$H_N := U_N - p_N \cdot V_N$	Enthalpy	macroscopic
12	$A_N := U_N - T_N . S_N$	Helmholtz energy	macroscopic
13	$G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$	Gibbs free energy	macroscopic
14	$v_{xN} := \frac{\partial r_{xN}}{\partial t}$	velocity in x-direction	macroscopic
15	$v_{yN} := \frac{\partial r_{yN}}{\partial t}$	velocity in y-direction	macroscopic
16	$v_{zN} := \frac{\partial r_{zN}}{\partial t}$	velocity in z-direction	macroscopic

no	equation	documentation	layer
17	$R := N^A \cdot k^B$	gas constant	physical
18	$Cp_N := rac{\partial H_N}{\partial T_N}$	total heat capacity at constant pressure	macroscopic
19	$CV_N := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	macroscopic
29	$h_{N,S} := H_N \cdot (n_{N,S})^{-1}$	partial molar enthalpies	macroscopic
30	$m_N := \lambda_S \stackrel{S}{\star} n_{N,S}$	mass	macroscopic
31	$c_{N,S} := (V_N)^{-1} \cdot n_{N,S}$	molar concentration	macroscopic
32	$n^{t}{}_{N} := \mathbf{reduceSum}\left(n_{N,S},S ight)$	total number of moles	macroscopic
33	$x_{N,S} := \left(n^t{}_N\right)^{-1} \cdot n_{N,S}$	mole fraction	macroscopic
34	$c_{pN} := Cp_N \cdot (m_N)^{-1}$	specific heat capacity at constant pressure	physical
35	$c_{VN} := CV_N \cdot \left(m_N\right)^{-1}$	specific heat capacity at constant volume	macroscopic
36	$\rho_N := \left(V_N\right)^{-1} . m_N$	density	physical
40	$A_{xyN} := r_{xN} \cdot r_{yN}$	cross sectional area xy	physical
41	$A_{xzN} := r_{xN} \cdot r_{zN}$	cross sectional are xz	physical
42	$A_{yzN} := r_{yN} \cdot r_{zN}$	cross sectional area yz	physical
43	$\hat{q}_{xA} := k_{xA}^q \cdot A_{yzN} \cdot F_{N,A} \overset{N}{\star} T_N$	heat flow in x-direction	macroscopic
44	$\hat{q}_{yA} := k_{yA}^q \cdot A_{xzN} \cdot F_{N,A} \overset{N}{\star} T_N$	heat flow in y-direction	macroscopic
45	$\hat{q}_{zA} := k_{zA}^q \cdot A_{xyN} \cdot F_{N,A} \stackrel{N}{\star} T_N$	heat flow in z-direction	macroscopic

no	equation	documentation	layer
46	$\hat{n}_{xA,S}^d := \hat{k}_x^{d,Fick}{}_{A,S} \cdot A_{yzN} \cdot F_{N,A} \overset{N}{\star} c_{N,S}$	Fick diffusion flow in x-direction	macroscopic
47	$\hat{n}_{yA,S}^d := \hat{k}_y^{d,Fick}{}_{A,S} \cdot A_{xzN} \cdot F_{N,A} \stackrel{N}{\star} c_{N,S}$	Fick diffusion flow in y-direction	macroscopic
48	$\hat{n}_{zA,S}^d := \hat{k}_z^{d,Fick}{}_{A,S} \cdot (A_{xyN} \cdot F_{N,A}) \stackrel{N}{\star} c_{N,S}$	Fick diffusion flow in z-direction	macroscopic
49	$d_A := \mathbf{sign}\left(F_{N,A} \stackrel{N}{\star} p_N ight)$	flow direction of convective flow	macroscopic
50	$c_{A,S} := (0.5 \cdot (F_{N,A} - d_A \cdot  F_{N,A} )) \stackrel{N}{\star} c_{N,S}$	concentration in convective event- dynamic flow	macroscopic
51	$\hat{V}_A := (\rho_A)^{-1} \cdot k_{xA}^c \cdot A_{yzN} \cdot F_{N,A} \stackrel{N}{\star} p_N$	volumetric flow in x-direction	macroscopic
52	$\hat{n}_{xA,S}^c := \hat{V}_A \cdot c_{A,S}$	molar convective flow in x-direction	macroscopic
53	$\mu^o{}_{N,S} := \mathbf{Instantiate}(\mu_{N,S},\#)$	instantiating standard chemical potential	macroscopic
54	$\mu_{N,S} := \mu^o{}_{N,S} + R \cdot T_N \cdot \ln\left(x_{N,S}\right)$	chemical potential standard model with mole fraction	macroscopic
61	$f_{N,S,K,p} := x_{N,S,p}(( N_{S,K} ))$	factor for probability computation	reactions
62	$\xi_{N,K,p} := \prod_S f_{N,S,K,p}$	probability of reaction to take place	reactions
73	$k_{xA,S}^d := I_{N,A} * \left( \left( \mu_{N,S} \right)^{-1} \cdot \left( v_{xN} \cdot \left( \left( V_N \right)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \right) \right) \right)$	diffusivity in arc and x-direction	macroscopic
74	$k_{yA,S}^d := I_{N,A} * \left( \left( \mu_{N,S} \right)^{-1} \cdot \left( v_{yN} \cdot \left( \left( V_N \right)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \right) \right) \right)$	diffusivity in arc and y-direction	macroscopic
75	$k_{zA,S}^d := I_{N,A} * \left( (\mu_{N,S})^{-1} \cdot \left( v_{zN} \cdot \left( (V_N)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \right) \right) \right)$	diffusivity in arc and z-direction	macroscopic
76	$k_{xA}^c := I_{N,A} \stackrel{N}{\star} \left( \left( \lambda_S \stackrel{S}{\star} (\mu_{N,S})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN} \right)$	convective mass conductivity in arc and x diretion	macroscopic
77	$k_{yA}^c := I_{N,A} * \left( \left( \lambda_S * (\mu_{N,S})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN} \right)$	convective mass conductivity in arc and y-direction	macroscopic

no	equation	documentation	layer
78	$k_{zA}^c := I_{N,A} * \left( \left( \lambda_S * (\mu_{N,S})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN} \right)$	convecive mass conductivity in arc and y-direction	macroscopic
79	$k_{xA}^q := I_{N,A} \stackrel{N}{\star} \left( (V_N)^{-1} \cdot Cp_N \cdot v_{xN} \right)$	thermal conductivity in arc and x-direction	macroscopic
80	$k_{yA}^{q} := I_{N,A} * \left( (V_{N})^{-1} . Cp_{N} . v_{yN} \right)$	thermal conductivity in arc and y-direction	macroscopic
81	$k_{zA}^q := I_{N,A} * \left( (V_N)^{-1} \cdot Cp_N \cdot v_{zN} \right)$	thermal conductivity in arc and z-direction	macroscopic
82	$ ho_A := I_{N,A} \stackrel{N}{\star}  ho_N$	density in arc	macroscopic
83	$\hat{k}_x^{d,Fick}{}_{A,S} := I_{N,A} \stackrel{N}{\star} \left( v_{xN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$	Fick's diffusivity in arc and x-direction	macroscopic
84	$\hat{k}_{y}^{d,Fick}{}_{A,S} := I_{N,A} \stackrel{N}{\star} \left( v_{yN} \cdot \frac{\partial U_{N}}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$	Fick diffusivity in arc and y-direction	macroscopic
85	$\hat{k}_z^{d,Fick}{}_{A,S} := I_{N,A} \stackrel{N}{\star} \left( v_{zN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$	Fick diffusivity in arc and z-direction	macroscopic
86	$h_{A,S} := I_{N,A} \overset{N}{\star} h_{N,S}$	partial molar enthalpiies in arc	macroscopic
87	$anc_{xN,S} := F_{N,A} \stackrel{A}{\star} \hat{n}_{xA,S}^c$	accumulation of molar mass due to convection	macroscopic
88	$\dot{n}_{xN,S}^d := F_{N,A} \stackrel{A}{\star} \hat{n}_{xA,S}^d$	accumulation due to diffusion in x-direction	macroscopic
89	$\hat{n}_{xA,S}^d := k_{xA,S}^d \cdot (A_{yzN} \cdot F_{N,A}) \stackrel{N}{\star} \mu_{N,S}$	Fick diffusion flow in x-direction	macroscopic
90	$\hat{n}_{yA,S}^d := k_{yA,S}^d \cdot (A_{yzN} \cdot F_{N,A}) *^{N}_{\star} \mu_{N,S}$	Fick diffusion flow in y-direction	macroscopic
91	$\hat{n}_{zA,S}^d := k_{zA,S}^d \cdot (A_{xyN} \cdot F_{N,A}) \overset{N}{\star} \mu_{N,S}$	mass diffusion flow in z-direction	macroscopic
92	$\dot{n}_{N,S} := anc_{xN,S} + \dot{n}_{xN,S}^d + V_N \cdot \tilde{n}_{N,S}$	differential mass balance without reaction	macroscopic

no	equation	documentation	layer
93	$n_{N,S} := \int_{t^o}^{t^e} \dot{n}_{N,S} \ dt + n^o{}_{N,S}$	fundamental state – molar mass	macroscopic
94	$K_{N,K,p} := K^o{}_K \cdot \exp\left((-E^a{}_K) \cdot (R \cdot T_{N,p})^{-1}\right)$	Arrhenius reaction "constant"	reactions
95	$\tilde{n}_{N,S,q} := A_{N,p,q} \stackrel{p}{\star} \left( N_{S,K} \stackrel{K}{\star} \left( K_{N,K,p} \cdot \xi_{N,K,p} \right) \right)$	production from reaction set	reactions
98	$n^o{}_{N,S} := \mathbf{Instantiate}(n_{N,S},\#)$	initial mass	macroscopic
99	$\dot{H}_{xN}^c := F_{N,A} \stackrel{A}{\star} \left( \hat{n}_{xA,S}^c \stackrel{S}{\star} h_{N,S} \right)$	enthalpy accumulation due to convective flow in x-direction	macroscopic
100	$\dot{H}_{xN}^d := F_{N,A} \stackrel{A}{\star} \left( \hat{n}_{xA,S}^d \stackrel{S}{\star} h_{N,S} \right)$	accumulation of enthalpy due to diffusional mass flow in x-direction	macroscopic
101	$\dot{H}_{yN}^d := F_{N,A} \stackrel{A}{\star} \left( \hat{n}_{yA,S}^d \stackrel{S}{\star} h_{N,S} \right)$	accumulation of enthalpy due to diffusional mass flow in y-direction	macroscopic
102	$\dot{H}_{zN}^d := F_{N,A} \stackrel{A}{\star} \left( \hat{n}_{zA,S}^d \stackrel{S}{\star} h_{N,S} \right)$	accumulation of enthalpy due to diffusional mass flow in z-direction	macroscopic
103	$\dot{q}_{xN} := F_{N,A} \overset{A}{\star} \hat{q}_{xA}$	accumulation due to heat flow in x-direction	macroscopic
104	$\dot{q}_{yN} := F_{N,A} \stackrel{A}{\star} \hat{q}_{yA}$	accumulation due to heat flow in y-direction	macroscopic
105	$\dot{q}_{zN} := F_{N,A} \overset{A}{\star} \hat{q}_{zA}$	accumulation due to heat flow in z-direction	macroscopic
106	$\hat{w}_A := \mathbf{Instantiate}(\hat{q}_{xA}, \#)$	a fixed work flow to start with	macroscopic
107	$\dot{n}^d_{yN,S} := F_{N,A} \star \hat{n}^d_{yA,S}$	accumulation due to diffusion in y-direction	macroscopic
108	$\dot{n}_{zN,S}^d := F_{N,A} \star \hat{n}_{zA,S}^d$	accumulation due to diffusion in z-direction	macroscopic

no	equation	documentation	layer
109	$\dot{w}_N := F_{N,A} \overset{A}{\star} \hat{w}_A$	accumulation of enthalpy due to work flow	macroscopic
110	$\dot{H}_N := \dot{H}_{xN}^c + \dot{H}_{xN}^d + \dot{H}_{yN}^d + \dot{H}_{zN}^d + \dot{q}_{xN} + \dot{q}_{yN} + \dot{q}_{zN} + \dot{w}_N$	accumulation of enthalpy	macroscopic
111	$H^o{}_N := \mathbf{Instantiate}(H_N,\#)$	initial enthalpy	macroscopic
112	$H_N := \int_{t^o}^{t^e} \dot{H}_N \ dt + H^o{}_N$	Enthalpy	macroscopic
113	$U^e_N := (C_N)^{-1} \cdot U_N$	electrical potential – voltage	macroscopic
114	$I^e{}_N := rac{dC_N}{dt}$	current definition	macroscopic
115	$R^e{}_N := (I^e{}_N)^{-1} . U^e{}_N$	electrical resistant	macroscopic
116	$\dot{U}^e{}_A := F_{N,A} \stackrel{A}{\star} (R^e{}_N . I^e{}_N)$	Kirkhoffs first law	macroscopic

# 10 Interface Link Equation

no	equation	documentation	layer
55	$\_c_{I,S} := F^{source}{}_{N,I} \overset{N}{\star} c_{N,S}$	interface equation	macroscopic -> reactions
56	$c_{N,S,p} := \left(F^{sink}_{N,I} \cdot \_c_{I,S}\right) \overset{I}{\star} S_{I,p}$	interface equation	reactions
57	$x_{I,S} := F^{source}_{N,I} \overset{N}{\star} x_{N,S}$	interface equation	macroscopic -> re- actions
58	$x_{N,S,p} := (F^{sink}_{N,I} \cdot \_x_{I,S}) \overset{I}{\star} S_{I,p}$	interface equation	reactions
59		interface equation	macroscopic -> re- actions
60	$T_{N,p} := (F^{sink}_{N,I} \cdot \_T_I) \overset{I}{\star} S_{I,p}$	interface equation	reactions
96	$\_np_{I,S} := \mathbf{reduceSum}\left(\left(\left(F^{source}_{N,I} \overset{N}{\star} \tilde{n}_{N,S,q}\right).S_{I,q}\right), q\right)$	interface equation	reactions -> macroscopic
97	$\tilde{n}_{N,S} := F^{source}{}_{N,I} \overset{I}{\star} \_np_{I,S}$	interface equation	macroscopic