1 Variables

2 root

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

Continued on next page

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

3 physical

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

4 macroscopic

	var	symbol	documentation	type	units	eqs
156	$\hat{n}^d_{z\,A,S}$	fnd_z	diffusion flow in z-direction	transport	$mol\, s^{-1}$	48 91
157	d_A	d	flow direction of convective flow	transport		49
194	$\dot{n}_{N,S}$	anc	accumulation of molar mass due to convection	transport	$mol\, s^{-1}$	87
152	$\hat{q}_{y\,A}$	fq_y	heat flow in y-direction	transport	$kg\, m^2\, s^{-3}$	44
153	$\hat{q}_{z\,A}$	fq_z	heat flow in z-direction	transport	$kg\, m^2\, s^{-3}$	45
154	$\hat{n}^d_{x\,A,S}$	fnd_x	diffusion flow in x-direction	transport	$mol\, s^{-1}$	46 89
155	$\hat{n}^d_{y\,A,S}$	fnd_y	diffusion flow in y-direction	transport	$mol\, s^{-1}$	47 90
195	$\dot{n}^d{}_{N,S}$	and_x	accumulation due to diffusion in x-direction	transport	$mol\, s^{-1}$	88
159	$\hat{V}_A$	fV	volumetric flow in x-direction	transport	$m^3\, s^{-1}$	51
160	$\hat{n}^c_{x\,A,S}$	fnc_x	molar convective flow in x-direction	transport	$mol\, s^{-1}$	52
151	$\hat{q}_{x\,A}$	fq_x	heat flow in x-direction	transport	$kg\, m^2\, s^{-3}$	43
158	$c_{A,S}$	c_AS	concentration in convective event-dynamic flow	transport	$m^{-3}\, mol$	50
184	$k^c_{y\,A}$	kcA_y	convective mass conductivity in arc and y-direction	properties	$m^{-1}\, s$	77
186	$k^q_{x\,A}$	kqA_x	thermal conductivity in arc and x-direction	properties	$kg\, K^{-1}\, s^{-3}$	79
193	$h_{A,S}$	hA	partial molar enthalpiies in arc	properties	$kg\, m^2\, mol^{-1}\, s^{-2}$	86
185	$k^c_{z\,A}$	kcA_z	convecive mass conductivity in arc and y-direction	properties	$m^{-1}\, s$	78
190	$\hat{k}^{d,Fick}_x{}_{A,S}$	kdAFick_x	Fick's diffusivity in arc and x-direction	properties	ms^{-1}	83
192	$\hat{k}^{d,Fick}_z{}_{A,S}$	kdAFick_z	Fick diffusivity in arc and z-direction	properties	ms^{-1}	85
180	$k^d_{x\,A,S}$	kdA_x	diffusivity in arc and x-direction	properties	$kg^{-1}\, m^{-4}\, mol^2\, s$	73
187	$k^q_{y\,A}$	kqA_y	thermal conductivity in arc and y-direction	properties	$kg\, K^{-1}\, s^{-3}$	80
183	$k^c_{x\,A}$	kcA_x	convective mass conductivity in arc and x diretion	properties	$m^{-1}\, s$	76
191	$\hat{k}^{d,Fick}_y{}_{A,S}$	kdAFick_y	Fick diffusivity in arc and y-direction	properties	ms^{-1}	84
188	$k^q_{z\,A}$	kqA_z	thermal conductivity in arc and z-direction	properties	$kg\, K^{-1}\, s^{-3}$	81

Continued on next page

	var	symbol	documentation	type	units	eqs
189	ρ_A	`rhoA`	density in arc	properties	$kg\, m^{-3}$	82
182	$k^d_z{}_{A,S}$	`kdA_z`	diffusivity in arc and z-direction	properties	$kg^{-1}\, m^{-4}\, mol^2\, s$	75
181	$k^d_y{}_{A,S}$	`kdA_y`	diffusivity in arc and y-direction	properties	$kg^{-1}\, m^{-4}\, mol^2\, s$	74
117	G_N	`G`	Gibbs free energy	state	$kg\, m^2\, s^{-2}$	13
115	H_N	`H`	Enthalpy	state	$kg\, m^2\, s^{-2}$	11
116	A_N	`A`	Helmholtz energy	state	$kg\, m^2\, s^{-2}$	12
113	T_N	`T`	temperature	effort	K	9
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
112	p_N	`p`	thermodynamic pressure	effort	$kg\, m^{-1}\, s^{-2}$	8
125	CV_N	`CV`	total heat capacity at constant volume	secondaryState	$kg\, m^2\, K^{-1}\, s^{-2}$	19
136	$h_{N,S}$	`h`	partial molar enthalpies	secondaryState	$kg\, m^2\, mol^{-1}\, s^{-2}$	29
120	$v_z{}_N$	`v_z`	velocity in z-direction	secondaryState	ms^{-1}	16
138	$c_{N,S}$	`c`	molar concentration	secondaryState	$m^{-3}\, mol$	31
142	$c_V{}_N$	`cV`	specific heat capacity at constant volume	secondaryState	$m^2\, K^{-1}\, s^{-2}$	35
140	$x_{N,S}$	`x`	mole fraction	secondaryState		33
118	$v_x{}_N$	`v_x`	velocity in x-direction	secondaryState	ms^{-1}	14
139	$n^t{}_N$	`nt`	total number of moles	secondaryState	mol	32
141	$c_p{}_N$	`cp`	specific heat capacity at constant pressure	secondaryState	$m^2\, K^{-1}\, s^{-2}$	34
124	Cp_N	`Cp`	total heat capacity at constant pressure	secondaryState	$kg\, m^2\, K^{-1}\, s^{-2}$	18
119	$v_y{}_N$	`v_y`	velocity in y-direction	secondaryState	ms^{-1}	15
196	$\dot{n}_{N,S}$	`an`	differential mass balance without reaction	diffState	$mol\, s^{-1}$	92

5 reactions

	var	symbol	documentation	type	units	eqs
26	$N_{S,K}$	`N`	stoichiometric matrix	constant		
167	$T_{N,p}$	`T`	link variable T to interface reactions	effort	K	60
165	$x_{N,S,p}$	`x`	link variable x to interface reactions	secondaryState		58
171	$V_{N,p}$	`V`	link variable V to interface reactions	secondaryState	m^3	64
163	$c_{N,S,p}$	`c`	link variable c to interface reactions	secondaryState	$m^{-3}\,mol$	56
169	$\xi_{N,K,p}$	`probability`	probability of reaction to take place	conversion		62
168	$f_{N,S,K,p}$	`factor`	factor for probability computation	conversion		61

6 macroscopic–reactions

	var	symbol	documentation	type	units	eqs
164	$\_x_{I,S}$	`_x`	link variable x to interface macroscopic »> reactions with source:node	get		57
166	$\_T_{I}$	`_T`	link variable T to interface macroscopic »> reactions with source:node	get	K	59
162	$\_c_{I,S}$	`_c`	link variable c to interface macroscopic »> reactions with source:node	get	$m^{-3}\,mol$	55
170	$\_V_{I}$	`_V`	link variable V to interface macroscopic »> reactions with source:node	get	m^{3}	63

7 Equations

8 Generic

no	equation	documentation	layer
1	$0 := \textbf{Instantiate}(\#, \#)$	numerical value zero	root
2	$1 := \textbf{Instantiate}(\#, \#)$	numerical value one	root
3	$0.5 := \textbf{Instantiate}(\#, \#)$	numerical value one half	root
4	$t^o := \textbf{Instantiate}(t, \#)$	starting time	root
5	$t^e := \textbf{Instantiate}(t, \#)$	end time	root
6	$\Delta t := \textbf{Instantiate}(t, \#)$	time interval	root
7	$V_N := r_{xN} \,.\, r_{yN} \,.\, r_{zN}$	volume	physical
8	$p_N := \frac{\partial U_N}{\partial V_N}$	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	$H_N := U_N - p_N \,.\, V_N$	Enthalpy	macroscopic
12	$A_N := U_N - T_N \,.\, S_N$	Helmholtz energy	macroscopic
13	$G_N := U_N + p_N \,.\, V_N - T_N \,.\, S_N$	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

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

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no	equation	documentation	layer
46	$\hat{n}^{d}_{x}{}_{A,S} := \hat{k}^{d,Fick}_{x}{}_{A,S} \,.\, A_{yz}{}_{N} \,.\, F_{N,A} \overset{N}{\star} c_{N,S}$	Fick diffusion flow in x-direction	macroscopic
47	$\hat{n}^{d}_{y}{}_{A,S} := \hat{k}^{d,Fick}_{y}{}_{A,S} \,.\, A_{xz}{}_{N} \,.\, F_{N,A} \overset{N}{\star} c_{N,S}$	Fick diffusion flow in y-direction	macroscopic
48	$\hat{n}^{d}_{z}{}_{A,S} := \hat{k}^{d,Fick}_{z}{}_{A,S} \,.\, (A_{xy}{}_{N} \,.\, F_{N,A}) \overset{N}{\star} c_{N,S}$	Fick diffusion flow in z-direction	macroscopic
49	$d_{A} := \mathbf{sign}\left(F_{N,A} \overset{N}{\star} p_{N}\right)$	flow direction of convective flow	macroscopic
50	$c_{A,S} := (0.5 \,.\, (F_{N,A} - d_{A} \,.\, \lvert F_{N,A}\rvert)) \overset{N}{\star} c_{N,S}$	concentration in convective event-dynamic flow	macroscopic
51	$\hat{V}_{A} := (\rho_{A})^{-1} \,.\, k^{c}_{x}{}_{A} \,.\, A_{yz}{}_{N} \,.\, F_{N,A} \overset{N}{\star} p_{N}$	volumetric flow in x-direction	macroscopic
52	$\hat{n}^{c}_{x}{}_{A,S} := \hat{V}_{A} \,.\, c_{A,S}$	molar convective flow in x-direction	macroscopic
53	$\mu^{o}{}_{N,S} := \mathbf{Instantiate}(\mu_{N,S}, \#)$	instantiating standard chemical potential	macroscopic
54	$\mu_{N,S} := \mu^{o}{}_{N,S} + R \,.\, T_{N} \,.\, \mathbf{ln}\left(x_{N,S}\right)$	chemical potential standard model with mole fraction	macroscopic
61	$f_{N,S,K,p} := x_{N,S,p}{}^{((\lvert N_{S,K}\rvert))}$	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	$k^{d}_{x}{}_{A,S} := I_{N,A} \overset{N}{\star} \left((\mu_{N,S})^{-1} \,.\, \left(v_{x}{}_{N} \,.\, \left((V_{N})^{-1} \,.\, \frac{\partial U_{N}}{\partial \mu_{N,S}}\right)\right)\right)$	diffusivity in arc and x-direction	macroscopic
74	$k^{d}_{y}{}_{A,S} := I_{N,A} \overset{N}{\star} \left((\mu_{N,S})^{-1} \,.\, \left(v_{y}{}_{N} \,.\, \left((V_{N})^{-1} \,.\, \frac{\partial U_{N}}{\partial \mu_{N,S}}\right)\right)\right)$	diffusivity in arc and y-direction	macroscopic
75	$k^{d}_{z}{}_{A,S} := I_{N,A} \overset{N}{\star} \left((\mu_{N,S})^{-1} \,.\, \left(v_{z}{}_{N} \,.\, \left((V_{N})^{-1} \,.\, \frac{\partial U_{N}}{\partial \mu_{N,S}}\right)\right)\right)$	diffusivity in arc and z-direction	macroscopic
76	$k^{c}_{x}{}_{A} := I_{N,A} \overset{N}{\star} \left(\left(\lambda_{S} \overset{S}{\star} (\mu_{N,S})^{-1}\right) \,.\, (V_{N})^{-1} \,.\, \frac{\partial U_{N}}{\partial p_{N}} \,.\, v_{x}{}_{N}\right)$	convective mass conductivity in arc and x diretion	macroscopic
77	$k^{c}_{y}{}_{A} := I_{N,A} \overset{N}{\star} \left(\left(\lambda_{S} \overset{S}{\star} (\mu_{N,S})^{-1}\right) \,.\, (V_{N})^{-1} \,.\, \frac{\partial U_{N}}{\partial p_{N}} \,.\, v_{y}{}_{N}\right)$	convective mass conductivity in arc and y-direction	macroscopic

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no	equation	documentation	layer
78	$k^c_{z\,A} := I_{N,A} \overset{N}{\star} \left(\left(\lambda_S \overset{S}{\star} (\mu_{N,S})^{-1} \right) . (V_N)^{-1} . \frac{\partial U_N}{\partial p_N} . v_{z\,N} \right)$	convecive mass conductivity in arc and y-direction	macroscopic
79	$k^q_{x\,A} := I_{N,A} \overset{N}{\star} \left((V_N)^{-1} . Cp_N . v_{x\,N} \right)$	thermal conductivity in arc and x-direction	macroscopic
80	$k^q_{y\,A} := I_{N,A} \overset{N}{\star} \left((V_N)^{-1} . Cp_N . v_{y\,N} \right)$	thermal conductivity in arc and y-direction	macroscopic
81	$k^q_{z\,A} := I_{N,A} \overset{N}{\star} \left((V_N)^{-1} . Cp_N . v_{z\,N} \right)$	thermal conductivity in arc and z-direction	macroscopic
82	$\rho_A := I_{N,A} \overset{N}{\star} \rho_N$	density in arc	macroscopic
83	$\hat{k}^{d,Fick}_{x}{}_{A,S} := I_{N,A} \overset{N}{\star} \left(v_{x\,N} . \frac{\partial U_N}{\partial \mu_{N,S}} . (n_{N,S})^{-1} \right)$	Fick's diffusivity in arc and x-direction	macroscopic
84	$\hat{k}^{d,Fick}_{y}{}_{A,S} := I_{N,A} \overset{N}{\star} \left(v_{y\,N} . \frac{\partial U_N}{\partial \mu_{N,S}} . (n_{N,S})^{-1} \right)$	Fick diffusivity in arc and y-direction	macroscopic
85	$\hat{k}^{d,Fick}_{z}{}_{A,S} := I_{N,A} \overset{N}{\star} \left(v_{z\,N} . \frac{\partial U_N}{\partial \mu_{N,S}} . (n_{N,S})^{-1} \right)$	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	$\dot{n}_{N,S} := F_{N,A} \overset{A}{\star} \hat{n}^c_{x\,A,S}$	accumulation of molar mass due to convection	macroscopic
88	$\dot{n}^d{}_{N,S} := F_{N,A} \overset{A}{\star} \hat{n}^d_{x\,A,S}$	accumulation due to diffusion in x-direction	macroscopic
89	$\hat{n}^d_{x\,A,S} := k^d_{x\,A,S} . (A_{yz\,N} . F_{N,A}) \overset{N}{\star} \mu_{N,S}$	Fick diffusion flow in x-direction	macroscopic
90	$\hat{n}^d_{y\,A,S} := k^d_{y\,A,S} . (A_{yz\,N} . F_{N,A}) \overset{N}{\star} \mu_{N,S}$	Fick diffusion flow in y-direction	macroscopic
91	$\hat{n}^d_{z\,A,S} := k^d_{z\,A,S} . (A_{xy\,N} . F_{N,A}) \overset{N}{\star} \mu_{N,S}$	mass diffusion flow in z-direction	macroscopic
92	$\dot{n}_{N,S} := \dot{n}_{N,S} + \dot{n}^d{}_{N,S}$	differential mass balance without reaction	macroscopic

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no	equation	documentation	layer
93	$n_{N,S} := \int_{t^o}^{t^e} \dot{n}_{N,S} \; d\,t$	fundamental state – molar mass	macroscopic

9 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 –> reactions
58	$x_{N,S,p} := \left({F^{sink}}_{N,I} \cdot \_x_{I,S}\right) \overset{I}{\star} S_{I,p}$	interface equation	reactions
59	$\_T_{I} := {F^{source}}_{N,I} \overset{N}{\star} T_{N}$	interface equation	macroscopic –> reactions
60	$T_{N,p} := \left({F^{sink}}_{N,I} \cdot \_T_{I}\right) \overset{I}{\star} S_{I,p}$	interface equation	reactions
63	$\_V_{I} := {F^{source}}_{N,I} \overset{N}{\star} V_{N}$	interface equation	macroscopic –> reactions
64	$V_{N,p} := \left({F^{sink}}_{N,I} \cdot \_V_{I}\right) \overset{I}{\star} S_{I,p}$	interface equation	reactions