

# 1 Variables

## 2 root

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

*Continued on next page*

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

### 3 physical

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

## 4 macroscopic

	var	symbol	documentation	type	units	eqs
159	$\hat{V}_A$	fV	volumetric flow in x-direction	transport	$m^3 s^{-1}$	51
207	$\dot{H}_{zN}^d$	aHnd_z	accumulation of enthalpy due to diffusional mass flow in z-direction	transport	$kg m^2 s^{-3}$	102
209	$\dot{q}_{yN}$	aq_y	accumulation due to heat flow in y-direction	transport	$kg m^2 s^{-3}$	104
205	$\dot{H}_{xN}^d$	aHnd_x	accumulation of enthalpy due to diffusional mass flow in x-direction	transport	$kg m^2 s^{-3}$	100
160	$\hat{n}_{xA,S}^c$	fnc_x	molar convective flow in x-direction	transport	$mol s^{-1}$	52
155	$\hat{n}_{yA,S}^d$	fnd_y	diffusion flow in y-direction	transport	$mol s^{-1}$	47 90
234	$f m_{N,A}$	fm	convective mass flow	transport	$kg s^{-1}$	133
156	$\hat{n}_{zA,S}^d$	fnd_z	diffusion flow in z-direction	transport	$mol s^{-1}$	48 91
210	$\dot{q}_{zN}$	aq_z	accumulation due to heat flow in z-direction	transport	$kg m^2 s^{-3}$	105
194	$\dot{n}_{xN,S}^c$	anc_x	accumulation of molar mass due to convection	transport	$mol s^{-1}$	87
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	$kg m^2 s^{-3}$	103
152	$\dot{q}_{yA}$	fq_y	heat flow in y-direction	transport	$kg m^2 s^{-3}$	44
212	$\dot{n}_{yN,S}^d$	and_y	accumulation due to diffusion in y-direction	transport	$mol s^{-1}$	107
204	$\dot{H}_{xN}^c$	aHnc_x	accumulation of enthalpy due to convective mass flow in x-direction	transport	$kg m^2 s^{-3}$	99
153	$\hat{q}_{zA}$	fq_z	heat flow in z-direction	transport	$kg m^2 s^{-3}$	45
157	$d_A$	d	flow direction of convective flow	transport		49
211	$\hat{w}_A$	fw	a fixed work flow to start with	transport	$kg m^2 s^{-3}$	106
213	$\dot{n}_{zN,S}^d$	and_z	accumulation due to diffusion in z-direction	transport	$mol s^{-1}$	108
206	$\dot{H}_{yN}^d$	aHnd_y	accumulation of enthalpy due to diffusional mass flow in y-direction	transport	$kg m^2 s^{-3}$	101

*Continued on next page*

	var	symbol	documentation	type	units	eqs
214	$\dot{w}_N$	<b>aw</b>	accumulation of enthalpy due to work flow	transport	$kg\,m^2\,s^{-3}$	<b>109</b>
154	$\hat{n}_{x\,A,S}^d$	<b>fnd_x</b>	diffusion flow in x-direction	transport	$mol\,s^{-1}$	<b>46 89</b>
151	$\hat{q}_{xA}$	<b>fq_x</b>	heat flow in x-direction	transport	$kg\,m^2\,s^{-3}$	<b>43</b>
195	$\dot{n}_{x\,N,S}^d$	<b>and_x</b>	accumulation due to diffusion in x-direction	transport	$mol\,s^{-1}$	<b>88</b>
180	$k_{x\,A,S}^d$	<b>kdA_x</b>	diffusivity in arc and x-direction	properties	$kg^{-1}\,m^{-4}\,mol^2\,s$	<b>73</b>
191	$\hat{k}_y^{d,Fick}\,_{A,S}$	<b>kdAFick_y</b>	Fick diffusivity in arc and y-direction	properties	$ms^{-1}$	<b>84</b>
192	$\hat{k}_z^{d,Fick}\,_{A,S}$	<b>kdAFick_z</b>	Fick diffusivity in arc and z-direction	properties	$ms^{-1}$	<b>85</b>
183	$k_{xA}^c$	<b>kcA_x</b>	convective mass conductivity in arc and x diretion	properties	$m^{-1}\,s$	<b>76</b>
188	$k_{zA}^q$	<b>kqA_z</b>	thermal conductivity in arc and z-direction	properties	$kg\,K^{-1}\,s^{-3}$	<b>81</b>
189	$\rho_A$	<b>rhoA</b>	density in arc	properties	$kg\,m^{-3}$	<b>82</b>
193	$h_{A,S}$	<b>hA</b>	partial molar enthalpiies in arc	properties	$kg\,m^2\,mol^{-1}\,s^{-2}$	<b>86</b>
186	$k_{xA}^q$	<b>kqA_x</b>	thermal conductivity in arc and x-direction	properties	$kg\,K^{-1}\,s^{-3}$	<b>79</b>
182	$k_{zA,S}^d$	<b>kdA_z</b>	diffusivity in arc and z-direction	properties	$kg^{-1}\,m^{-4}\,mol^2\,s$	<b>75</b>
181	$k_{yA,S}^d$	<b>kdA_y</b>	diffusivity in arc and y-direction	properties	$kg^{-1}\,m^{-4}\,mol^2\,s$	<b>74</b>
184	$k_{yA}^c$	<b>kcA_y</b>	convective mass conductivity in arc and y-direction	properties	$m^{-1}\,s$	<b>77</b>
190	$\hat{k}_x^{d,Fick}\,_{A,S}$	<b>kdAFick_x</b>	Fick's diffusivity in arc and x-direction	properties	$ms^{-1}$	<b>83</b>
219	$R_N^e$	<b>elResistant</b>	electrical resistant	properties	$kg\,m^2\,A^{-2}\,s^{-3}$	<b>115</b>
185	$k_{zA}^c$	<b>kcA_z</b>	convecive mass conductivity in arc and y-direction	properties	$m^{-1}\,s$	<b>78</b>
187	$k_{yA}^q$	<b>kqA_y</b>	thermal conductivity in arc and y-direction	properties	$kg\,K^{-1}\,s^{-3}$	<b>80</b>
117	$G_N$	<b>G</b>	Gibbs free energy	state	$kg\,m^2\,s^{-2}$	<b>13</b>
203	$n_{N,S}^o$	<b>no</b>	initial mass	state	$mol$	<b>98</b>
216	$H_N^o$	<b>Ho</b>	initial enthalpy	state	$kg\,m^2\,s^{-2}$	<b>111</b>
115	$H_N$	<b>H</b>	Enthalpy	state	$kg\,m^2\,s^{-2}$	<b>11 112</b>
116	$A_N$	<b>A</b>	Helmholtz energy	state	$kg\,m^2\,s^{-2}$	<b>12</b>

Continued on next page

	var	symbol	documentation	type	units	eqs
217	$U^e_N$	Ue	electrical potential – voltage	effort	$kg\,m^2\,A^{-1}\,s^{-3}$	113
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
113	$T_N$	T	temperature	effort	K	9 121
112	$p_N$	p	thermodynamic pressure	effort	$kg\,m^{-1}\,s^{-2}$	8
138	$c_{N,S}$	c	molar concentration	secondaryState	$m^{-3}\,mol$	31
124	$C_{pN}$	Cp	total heat capacity at constant pressure	secondaryState	$kg\,m^2\,K^{-1}\,s^{-2}$	18 117
136	$h_{N,S}$	h	partial molar enthalpies	secondaryState	$kg\,m^2\,mol^{-1}\,s^{-2}$	29
119	$v_{yN}$	v_y	velocity in y-direction	secondaryState	$ms^{-1}$	15
141	$c_{pN}$	cp	specific heat capacity at constant pressure	secondaryState	$m^2\,K^{-1}\,s^{-2}$	34 120
140	$x_{N,S}$	x	mole fraction	secondaryState		33
139	$n^t_N$	nt	total number of moles	secondaryState	mol	32
118	$v_{xN}$	v_x	velocity in x-direction	secondaryState	$ms^{-1}$	14
142	$c_{VN}$	cV	specific heat capacity at constant volume	secondaryState	$m^2\,K^{-1}\,s^{-2}$	35
222	$T^{ref}_N$	T_ref	reference temperature	secondaryState	K	119
120	$v_{zN}$	v_z	velocity in z-direction	secondaryState	$ms^{-1}$	16
125	$C_{VN}$	CV	total heat capacity at constant volume	secondaryState	$kg\,m^2\,K^{-1}\,s^{-2}$	19
202	$\tilde{n}_{N,S}$	np	link variable np to interface macroscopic	conversion	$m^{-3}\,mol\,s^{-1}$	97
196	$\dot{n}_{N,S}$	an	differential mass balance without reaction	diffState	$mol\,s^{-1}$	92
215	$\dot{H}_N$	dH	accumulation of enthalpy	diffState	$kg\,m^2\,s^{-3}$	110
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	internalTransport	A	114
223	$T^n_N$	T_meas_norming	value to norm measurement of temperature	observation	K	122

Continued on next page

	var	symbol	documentation	type	units	eqs
224	$\bar{T}_N$	<b>T_meas</b>	temperature measurement	observation		123

## 5 reactions

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



## 6 control

	var	symbol	documentation	type	units	eqs
239	$y_{ppositive_{N,q}}$	<b>y_p_positive</b>	positive signal only	algebraic		<a href="#">137</a>
226	$\bar{T}_{N,p}$	<b>T_meas</b>	link variable T meas to interface control	algebraic		<a href="#">125</a>
238	$y^p_{N,q}$	<b>y_p_control</b>	output of proportional controller	algebraic		<a href="#">136</a>
231	$e_{N,p}$	<b>control_error</b>	control error in normed temperature	algebraic		<a href="#">130</a>
227	$T_{setpoint_{N,p}}$	<b>T_setpoint</b>	setpoint for temperatue	algebraic		<a href="#">126</a>
237	$p_{N,p,q}$	<b>p</b>	controller gain	algebraic		

## 7 macroscopic-reactions

	var	symbol	documentation	type	units	eqs
166	$_T$	$_T$	link variable T to interface macroscopic »> reactions with source:node	get	$K$	59
164	$_x$	$_x$	link variable x to interface macroscopic »> reactions with source:node	get		57
162	$_c$	$_c$	link variable c to interface macroscopic »> reactions with source:node	get	$m^{-3} mol$	55

## 8 macroscopic-control

	var	symbol	documentation	type	units	eqs
225	<i>_T_meas_I</i>	<b>_T_meas</b>	link variable T meas to interface macroscopic »> control with source:node	get		124

## 9 reactions-macroscopic

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

## 10 Equations

## 11 Generic

no	equation	documentation	layer
1	$0 := \text{Instantiate}(\#, \#)$	numerical value zero	root
2	$1 := \text{Instantiate}(\#, \#)$	numerical value one	root
3	$0.5 := \text{Instantiate}(\#, \#)$	numerical value one half	root
4	$t^o := \text{Instantiate}(t, \#)$	starting time	root
5	$t^e := \text{Instantiate}(t, \#)$	end time	root
6	$\Delta t := \text{Instantiate}(t, \#)$	time interval	root
7	$V_N := r_{xN} \cdot r_{yN} \cdot r_{zN}$	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	$H_N := U_N - p_N \cdot V_N$	Enthalpy	macroscopic
12	$A_N := U_N - T_N \cdot S_N$	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

*Continued on next page*

no	equation	documentation	layer
17	$R := N^A \cdot k^B$	gas constant	physical
18	$C_{pN} := \frac{\partial H_N}{\partial T_N}$	total heat capacity at constant pressure	macroscopic
19	$C_{VN} := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	macroscopic
29	$h_{N,S} := H_N \cdot (n_{N,S})^{-1}$	partial molar enthalpies	macroscopic
30	$m_N := \lambda_S^S \star n_{N,S}$	mass	macroscopic
31	$c_{N,S} := (V_N)^{-1} \cdot n_{N,S}$	molar concentration	macroscopic
32	$n_N^t := \mathbf{reduceSum}(n_{N,S}, S)$	total number of moles	macroscopic
33	$x_{N,S} := (n_N^t)^{-1} \cdot n_{N,S}$	mole fraction	macroscopic
34	$c_{pN} := C_{pN} \cdot (m_N)^{-1}$	specific heat capacity at constant pressure	physical
35	$c_{VN} := C_{VN} \cdot (m_N)^{-1}$	specific heat capacity at constant volume	macroscopic
36	$\rho_N := (V_N)^{-1} \cdot m_N$	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	$\hat{q}_{zA} := k_{zA}^q \cdot A_{xyN} \cdot F_{N,A} \overset{N}{\star} T_N$	heat flow in z-direction	macroscopic

*Continued on next page*

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

*Continued on next page*

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

Continued on next page



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

Continued on next page

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	$H_N^o := \mathbf{Instantiate}(H_N, \#)$	initial enthalpy	macroscopic
112	$H_N := \int_{t^o}^{t^e} \dot{H}_N dt + H_N^o$	Enthalpy	macroscopic
113	$U_N^e := (C_N)^{-1} \cdot U_N$	electrical potential – voltage	macroscopic
114	$I_N^e := \frac{dC_N}{dt}$	current definition	macroscopic
115	$R_N^e := (I_N^e)^{-1} \cdot U_N^e$	electrical resistant	macroscopic
116	$\dot{U}_A^e := F_{N,A} \overset{A}{\star} (R_N^e \cdot I_N^e)$	Kirkhoffs first law	macroscopic
117	$C_{pN} := m_N \cdot c_{pN}$	total heat capacity at constant pressure	macroscopic
119	$T_N^{ref} := \mathbf{Instantiate}(T_N, \#)$	reference temperature	macroscopic
120	$c_{pN} := \mathbf{Instantiate}(c_{pN}, \#)$	constant specific heat capacity at constant pressure	macroscopic
121	$T_N := H_N \cdot (C_{pN})^{-1} + T_N^{ref}$	temperature from constant heat capacity	macroscopic
122	$T_N^n := \mathbf{Instantiate}(T_N, \#)$	value to norm measurement of temperature	macroscopic
123	$\bar{T}_N := T_N \cdot (T_N^n)^{-1}$	temperature measurement	macroscopic
126	$T_{setpointN,p} := \mathbf{Instantiate}(\bar{T}_{N,p}, \#)$	setpoint for temperature	control
130	$e_{N,p} := T_{setpointN,p} - \bar{T}_{N,p}$	control error in normed temperature	control

*Continued on next page*

no	equation	documentation	layer
133	$fm_{N,A} := \hat{V}_A \cdot \rho_N$	convective mass flow	macroscopic
136	$y^p_{N,q} := (-p_{N,p,q}) \overset{p}{\star} e_{N,p}$	output of proportional controller	control
137	$y_{positive_{N,q}} := \mathbf{max}(0 \cdot y^p_{N,q}, y^p_{N,q})$	positive signal only	control

## 12 Interface Link Equation

no	equation	documentation	layer
55	$\_c_{I,S} := F^{source}_{N,I} \star^N c_{N,S}$	interface equation	macroscopic $\rightarrow$ reactions
56	$c_{N,S,p} := (F^{sink}_{N,I} \cdot \_c_{I,S}) \star^I S_{I,p}$	interface equation	reactions
57	$\_x_{I,S} := F^{source}_{N,I} \star^N x_{N,S}$	interface equation	macroscopic $\rightarrow$ reactions
58	$x_{N,S,p} := (F^{sink}_{N,I} \cdot \_x_{I,S}) \star^I S_{I,p}$	interface equation	reactions
59	$\_T_I := F^{source}_{N,I} \star^N T_N$	interface equation	macroscopic $\rightarrow$ reactions
60	$T_{N,p} := (F^{sink}_{N,I} \cdot \_T_I) \star^I S_{I,p}$	interface equation	reactions
96	$\_np_{I,S} := \text{reduceSum} \left( \left( \left( F^{source}_{N,I} \star^N \tilde{n}_{N,S,q} \right) \cdot S_{I,q} \right), q \right)$	interface equation	reactions $\rightarrow$ macroscopic
97	$\tilde{n}_{N,S} := F^{source}_{N,I} \star^I \_np_{I,S}$	interface equation	macroscopic
124	$\_T\_meas_I := F^{source}_{N,I} \star^N \bar{T}_N$	interface equation	macroscopic $\rightarrow$ control
125	$\bar{T}_{N,p} := (F^{sink}_{N,I} \cdot \_T\_meas_I) \star^I S_{I,p}$	interface equation	control