

## 1 Variables

### 2 root

	var	symbol	documentation	type	units	eqs
8	$F_{N,A}$	F_N_A	fudamental incidence matrix	network		
5	$t$	t	time	frame	s	
6	$t^o$	to	starting time	frame	s	4
7	$t^e$	te	end time	frame	s	5
1	#	value	numerical value	constant		
2	1	one	numerical value one	constant		1
3	0	zero	numerical value zero	constant		2
4	0.5	onehalf	numerical value one half	constant		3

### 3 physical

	var	symbol	documentation	type	units	eqs
9	$P_{N,A}$	P_N_A	projection from node to arc for arc properties	projection		
32	$P_{NS,AS}$	P_NS_AS	projection node species to arc species	projection		
33	$P_{K,NK}$	P_K_NK	projection of conversion to node conversion	projection		
34	$P_{S,NS}$	P_S_NS	projection species to node species	projection		
35	$P_{N,NK}$	P_N_NK	projection node to node conversion	projection		
36	$P_{NS,KS}$	P_NS_KS	projection node species to conversion species	projection		
37	$P_{A,NS}$	P_A_NS	projection arc to node species for conductivity	projection		
65	$P_{NK,KS}$	P_NK_KS	projection node conversion to conversion species	projection		
10	$r_{xN}$	r_x	x-coordinate	frame	$m$	
11	$r_{yN}$	r_y	y-coordinate	frame	$m$	
12	$r_{zN}$	r_z	z coordinate	frame	$m$	
13	$U_N$	U	fundamental state – internal energy	state	$kg\,m^2\,s^{-2}$	
14	$S_N$	S	fundamental state – entropy	state	$kg\,m^2\,K^{-1}\,s^{-2}$	
15	$V_N$	V	fundamental state – volume	state	$m^3$	
16	$n_{NS}$	n	fundamental state – molar mass	state	$mol$	86
20	$H_N$	H	enthalpy	state	$kg\,m^2\,s^{-2}$	9 87
21	$A_N$	A	Helmholtz energy	state	$kg\,m^2\,s^{-2}$	10
22	$G_N$	G	Gibbs free energy	state	$kg\,m^2\,s^{-2}$	11
23	$C_N$	charge	fundamental state – charge	state	$A\,s$	
24	$A^v$	Avogadro	Avogadro number	constant	$mol^{-1}$	
25	$k^B_N$	Boltzmann	Boltzmann constant	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	12
26	$R_N$	GasConstant	gas constant	constant	$kg\,m^2\,mol^{-1}\,K^{-1}\,s^{-2}$	13
17	$p_N$	p	thermodynamic pressure	effort	$kg\,m^{-1}\,s^{-2}$	6

Continued on next page

	var	symbol	documentation	type	units	eqs
18	$T_N$	<b>T</b>	temperature	effort	$K$	<b>7</b>
19	$\mu_{NS}$	<b>chemPot</b>	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	<b>8</b>
27	$Ue_N$	<b>Ue</b>	electrical potential – voltage	effort	$kg\,m^2\,A^{-1}\,s^{-3}$	<b>14 95</b>
28	$v_{xN}$	<b>v_x</b>	velocity in x-direction	secondaryState	$ms^{-1}$	<b>15</b>
29	$v_{yN}$	<b>v_y</b>	velocity in y-direction	secondaryState	$ms^{-1}$	<b>16</b>
30	$v_{zN}$	<b>v_z</b>	velocity in z-direction	secondaryState	$ms^{-1}$	<b>17</b>

## 4 control

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 5 reactions

	var	symbol	documentation	type	units	eqs
38	$K^o_K$	Ko	Arrhenius frequency factor	constant	$m^{-3} mol s^{-1}$	
62	$E^a_{NK}$	Ea	Arrhenius activation energy	constant	$kg m^2 mol^{-1} s^{-2}$	41
63	$K_{NK}$	K_NK	Arrhenius reaction 'constant'	constant	$m^{-3} mol s^{-1}$	42
60	$T_{NK}$	T_NK	temperature of the reactive system	effort	$K$	39
68	$c_{KS}$	c_KS	concentrations associated with reactions	secondaryState	$m^{-3} mol$	46
69	$c^o_{KS}$	co_KS	norming concentrations	secondaryState	$m^{-3} mol$	47

## 6 material

	var	symbol	documentation	type	units	eqs
40	$\lambda_S$	Mm	species molecular mass	constant	$kg\ mol^{-1}$	
112	$\xi$	additive	fraction of additives	constant		88
42	$C_{pN}$	Cp	total heat capacity at constant pressure	property	$kg\ m^2\ K^{-1}\ s^{-2}$	21
43	$C_{VN}$	Cv	total heat capacity at constant volume	property	$kg\ m^2\ K^{-1}\ s^{-2}$	22
44	$k_{xN}^q$	kq_x	thermal conductivity in x-direction	property	$kg\ K^{-1}\ s^{-3}$	23
45	$k_{yN}^q$	kq_y	thermal conductivity in y-direction	property	$kg\ K^{-1}\ s^{-3}$	24
46	$k_{zN}^q$	kq_z	thermal conductivity in z-direction'	property	$kg\ K^{-1}\ s^{-3}$	25
47	$k_N^q$	kq	thermal conductivity	property	$kg\ K^{-1}\ s^{-3}$	26
48	$k_{xN}^c$	kc_x	convective mass conductivity in x-direction	property	$m^{-1}\ s$	27
49	$k_{yN}^c$	kc_y	convective mass conductivity in y-direction	property	$m^{-1}\ s$	28
50	$k_{zN}^c$	kc_z	convective mass conductivity in z-direction	property	$m^{-1}\ s$	29
51	$k_N^c$	kc	convective mass conductivity	property	$m^{-1}\ s$	30
52	$k_{xNS}^d$	kd_x	diffusional mass conductivity in x-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	31
53	$k_{yNS}^d$	kd_y	diffusional mass conductivity in y-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	32
54	$k_{zNS}^d$	kd_z	diffusional mass conductivity in z-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	33
55	$k_{NS}^d$	kd	diffusional mass conductivity	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	34
56	$h_{NS}$	h	partial molar enthalpies	property	$kg\ m^2\ mol^{-1}\ s^{-2}$	35
59	$\rho_N$	density	density	property	$kg\ m^{-3}$	38
115	$R_N^e$	elResist	electrical resistant	property	$kg\ m^2\ A^{-2}\ s^{-3}$	91 92
116	$k^{e,\xi}_N$	elConductC	simple model for the electrical conductivity as a function of the additive	property	$kg^{-1}\ m^{-2}\ A^2\ s^3$	93

## 7 macroscopic

	var	symbol	documentation	type	units	eqs
92	$\hat{V}_A$	fV	volumetric flow	transport	$m^3 s^{-1}$	67
93	$\hat{n}_{AS}^d$	fnd_AS	diffusional mass flow in a given stream	transport	$mol s^{-1}$	68
94	$\hat{n}_{NS}^d$	fnd	net diffusional mass flow	transport	$mol s^{-1}$	69
95	$\hat{H}_{AS}^d$	fHd_A	enthalpy flow per diffusional mass stream	transport	$kg m^2 s^{-3}$	70
96	$\hat{H}_N^d$	fHd	net enthaply stream due to diffusion	transport	$kg m^2 s^{-3}$	71
97	$d_A$	d	flow direction of convectioal flow	transport		72
102	$\hat{H}_{AS}^c$	fHc_A	convective enthalpy flow for given stream	transport	$kg m^2 s^{-3}$	77
103	$\hat{H}_N^c$	fHc	net convectioal enthalpy stream	transport	$kg m^2 s^{-3}$	78
104	$\hat{w}_A$	fw_A	sample work stream	transport	$kg m^2 s^{-3}$	79
105	$\hat{w}_N$	fw	net work stream	transport	$kg m^2 s^{-3}$	80
106	$\hat{q}_{xA}$	fq_A_x	heat flow in x-direction for given stream	transport	$kg m^2 s^{-3}$	81
107	$\hat{q}_N$	fq	net heat flow	transport	$kg m^2 s^{-3}$	82
71	$A_{yzN}$	Ayz	cross sectional area yz	geometry	$m^2$	48
72	$A_{xzN}$	Axz	cross sectional area xz	geometry	$m^2$	49
73	$A_{xyN}$	Axy	cross sectional area xy	geometry	$m^2$	50
70	$F_{NS,AS}$	F_NS_AS	species related incidence matrix	network		
90	$D_{N,A}$	D	difference operator	differenceOperator		
91	$D_{NS,AS}$	D_NS_AS	difference operator for species topology	differenceOperator		
109	$H_N^o$	Ho	initial enthalpy	state	$kg m^2 s^{-2}$	84
110	$n_{NS}^o$	no	initial species	state	$mol$	85
127	$1_S$	one_S	a vector of ones with the length of the ordinal number of S	constant		
57	$m_N$	m	total mass	secondaryState	$kg$	36

Continued on next page

	var	symbol	documentation	type	units	eqs
66	$c_{NS}$	<b>c</b>	molar composition	secondaryState	$m^{-3} mol$	<a href="#">44</a>
98	$c_{AS}$	<b>c_AS</b>	concentration in convectional flow	secondaryState	$m^{-3} mol$	<a href="#">73</a>
99	$\hat{n}_{AS}^c$	<b>fnc_AS</b>	molar convetional mass flow in the given stream	secondaryState	$mol s^{-1}$	<a href="#">74</a>
100	$\hat{n}_{NS}^c$	<b>fnc</b>	net molar convectional mass flow	secondaryState	$mol s^{-1}$	<a href="#">75</a>
126	$\phi$	<b>intensities</b>	collected intensities	secondaryState		<a href="#">106</a>
128	$n_N^t$	<b>nTotal</b>	total number of moles	secondaryState	$mol$	<a href="#">107</a>
101	$\dot{n}_{NS}$	<b>dndt</b>	differential species balance	diffState	$mol s^{-1}$	<a href="#">76</a>
108	$\dot{H}_N$	<b>dHdt</b>	differential enthalpy balance	diffState	$kg m^2 s^{-3}$	<a href="#">83</a>
118	$\dot{U}_N^e$	<b>dUedt</b>	Kirkhoff first law	diffState	$kg m^2 A^{-1} s^{-3}$	<a href="#">96</a> <a href="#">97</a> <a href="#">98</a>
113	$I_N$	<b>i</b>	electrical current definition	internalTransport	$A$	<a href="#">89</a>



## 8 solid

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 9 fluid

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 10 liquid

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 11 gas

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 12 control-control

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 13 gas–liquid

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 14 gas–gas

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 15 liquid–liquid

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----



## 16 gas–solid

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 17    solid–solid

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 18 liquid–solid

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 19 material–material

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 20 reactions-reactions

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 21 control-reactions

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 22 reactions-control

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 23 control-material

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----



## 24 material-control

	var	symbol	documentation	type	units	eqs
124	$\xi$	additive	link variable additive to interface material » > control	get		104

## 25 control-macroscopic

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 26 macroscopic-control

	var	symbol	documentation	type	units	eqs
119	$I_N$	i	link variable i to interface macroscopic »> control	get	$A$	99
125	$T_N$	T	link variable T to interface macroscopic »> control	get	$K$	105

## 27 reactions-material

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 28 material-reactions

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 29 reactions-macroscopic

	var	symbol	documentation	type	units	eqs
--	-----	--------	---------------	------	-------	-----

## 30 macroscopic-reactions

	var	symbol	documentation	type	units	eqs
67	$c_{NS}$	<b>c</b>	link variable c to interface macroscopic »> reactions	get	$m^{-3} mol$	45

### 31 material–macroscopic

	var	symbol	documentation	type	units	eqs
41	$\lambda_S$	Mm	link variable Mm to interface material »> macroscopic	get	$kg\,mol^{-1}$	20
74	$\rho_N$	density	link variable density to interface material »> macroscopic	get	$kg\,m^{-3}$	51
75	$h_{NS}$	h	link variable h to interface material »> macroscopic	get	$kg\,m^2\,mol^{-1}\,s^{-2}$	52
76	$k_{xN}^q$	kq_x	link variable kq x to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	53
77	$Cv_N$	Cv	link variable Cv to interface material »> macroscopic	get	$kg\,m^2\,K^{-1}\,s^{-2}$	54
78	$k_{yN}^q$	kq_y	link variable kq y to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	55
79	$k_{zN}^q$	kq_z	link variable kq z to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	56
80	$k_N^q$	kq	link variable kq to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	57
81	$k_{xN}^c$	kc_x	link variable kc x to interface material »> macroscopic	get	$m^{-1}\,s$	58
82	$Cp_N$	Cp	link variable Cp to interface material »> macroscopic	get	$kg\,m^2\,K^{-1}\,s^{-2}$	59
83	$k_{yN}^c$	kc_y	link variable kc y to interface material »> macroscopic	get	$m^{-1}\,s$	60
84	$k_{zN}^c$	kc_z	link variable kc z to interface material »> macroscopic	get	$m^{-1}\,s$	61
85	$k_N^c$	kc	link variable kc to interface material »> macroscopic	get	$m^{-1}\,s$	62
86	$k_{xNS}^d$	kd_x	link variable kd x to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	63
87	$k_{yNS}^d$	kd_y	link variable kd y to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	64
88	$k_{zNS}^d$	kd_z	link variable kd z to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	65

*Continued on next page*



	var	symbol	documentation	type	units	eqs
89	$k^d_{NS}$	<b>kd</b>	link variable kd to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	<b>66</b>
117	$R^e_N$	<b>elConductC</b>	link variable elConductC to interface material »> macroscopic	get	$kg^{-1} m^{-2} A^2 s^3$	<b>94</b>

## 32 macroscopic-material

	var	symbol	documentation	type	units	eqs
58	$m_N$	m	link variable m to interface macroscopic »> material	get	$kg$	37
114	$i_N$	i	link variable i to interface macroscopic »> material	get	$A$	90

### 33 Equations

### 34 Generic

no	equation	documentation	layer
1	$1 := \text{Instantiate}(\#, \#)$	numerical value 1	root
2	$0 := \text{Instantiate}(\#, \#)$	numerical value zero	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	$p_N := \left(-\frac{\partial U_N}{\partial V_N}\right)$	thermodynamic pressure	physical
7	$T_N := \frac{\partial U_N}{\partial S_N}$	temperature	physical
8	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	chemical potential	physical
9	$H_N := U_N - p_N \cdot V_N$	enthalpy	physical
10	$A_N := U_N - T_N \cdot S_N$	Helmholtz energy	physical
11	$G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$	Gibbs free energy	physical
12	$k^B_N := \text{Instantiate}(S_N, \#)$	Boltzmann constant	physical
13	$R_N := A^v \cdot k^B_N$	gas constant	physical
14	$Ue_N := (C_N)^{-1} \cdot U_N$	electrical potential – voltage	physical
15	$v_{xN} := \frac{\partial r_{xN}}{\partial t}$	velocity in x-direction	physical
16	$v_{yN} := \frac{\partial r_{yN}}{\partial t}$	velocity in y direction	physical

*Continued on next page*

no	equation	documentation	layer
17	$v_{zN} := \frac{\partial r_{zN}}{\partial t}$	velocity in z-direction	physical
21	$C_{pN} := \frac{\partial H_N}{\partial T_N}$	total heat capacity at constant pressure	material
22	$C_{VN} := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	material
23	$k_{xN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}$	thermal conductivity in x-direction	material
24	$k_{yN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{yN}$	thermal conductivity in y-direction	material
25	$k_{zN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{zN}$	thermal conductivity in z-direction'	material
26	$k_N^q := \text{Stack}(k_{xN}^q, k_{yN}^q, k_{zN}^q)$	thermal conductivity	material
27	$k_{xN}^c := \left( \lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass conductivity in x-direction	material
28	$k_{yN}^c := \left( \lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$	convective mass conductivity in y-direction	material
29	$k_{zN}^c := \left( \lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convective mass conductivity in z-direction	material
30	$k_N^c := \text{Stack}(k_{xN}^c, k_{yN}^c, k_{zN}^c)$	convective mass conductivity	material
31	$k_{xNS}^d := (\mu_{NS})^{-1} \cdot \left( v_{xN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in x-direction	material
32	$k_{yNS}^d := (\mu_{NS})^{-1} \cdot \left( v_{yN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in y-direction	material
33	$k_{zNS}^d := (\mu_{NS})^{-1} \cdot \left( v_{zN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in z-direction	material
34	$k_{NS}^d := \text{Stack}(k_{xNS}^d, k_{yNS}^d, k_{zNS}^d)$	diffusional mass conductivity	material

*Continued on next page*

no	equation	documentation	layer
35	$h_{NS} := H_N \odot (n_{NS})^{-1}$	partial molar enthalpies	material
36	$m_N := \lambda_S \overset{S \in NS}{\star} n_{NS}$	total mass	macroscopic
38	$\rho_N := m_N \cdot (V_N)^{-1}$	density	material
39	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature of the reactive system	reactions
41	$E^a_{NK} := \text{Instantiate}(P_{N,NK} \overset{N}{\star} R_N \cdot T_{NK}, \#)$	Arrhenius activation energy	reactions
42	$K_{NK} := K^o_K \odot \exp((-E^a_{NK}) \cdot (R_N \overset{N}{\star} P_{N,NK} \cdot T_{NK})^{-1})$	Arrhenius reaction 'constant'	reactions
44	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar composition	macroscopic
46	$c_{KS} := c_{NS} \overset{NS}{\star} P_{NS,KS}$	concentrations associated with reactions	reactions
47	$c^o_{KS} := \text{Instantiate}(c_{KS}, \#)$	norming concentrations	reactions
48	$A_{yzN} := r_{yN} \cdot r_{zN}$	cross sectional area yz	macroscopic
49	$A_{xzN} := r_{xN} \cdot r_{zN}$	cross sectional area xz	macroscopic
50	$A_{xyN} := r_{xN} \cdot r_{yN}$	cross sectional area xy	macroscopic
67	$\hat{V}_A := (\rho_N)^{-1} \cdot k^c_{xN} \cdot A_{yzN} \cdot D_{N,A} \overset{N}{\star} p_N$	volumetric flow	macroscopic
68	$\hat{n}^d_{AS} := A_{yzN} \odot (-k^d_{xNS}) \cdot D_{NS,AS} \overset{NS}{\star} \mu_{NS}$	diffusional mass flow in a given stream	macroscopic
69	$\hat{n}^d_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^d_{AS}$	net diffusional mass flow	macroscopic
70	$\hat{H}^d_A := (F_{NS,AS} \overset{NS}{\star} h_{NS}) \overset{S \in AS}{\star} \hat{n}^d_{AS}$	enthalpy flow per diffusional mass stream	macroscopic
71	$\hat{H}^d_N := F_{N,A} \overset{A}{\star} \hat{H}^d_A$	net enthaply stream due to diffusion	macroscopic

Continued on next page

no	equation	documentation	layer
72	$d_A := \text{sign} \left( F_{N,A} \stackrel{N}{\star} p_N \right)$	flow direction of convectional flow	macroscopic
73	$c_{AS} := (0.5 \cdot (F_{NS,AS} - d_A \odot  F_{NS,AS} )) \stackrel{NS}{\star} c_{NS}$	concentration in convectional flow	macroscopic
74	$\hat{n}_{AS}^c := \hat{V}_A \odot c_{AS}$	molar convetional mass flow in the given stream	macroscopic
75	$\hat{n}_{NS}^c := F_{NS,AS} \stackrel{AS}{\star} \hat{n}_{AS}^c$	net molar convectional mass flow	macroscopic
76	$\dot{n}_{NS} := \hat{n}_{NS}^c + \hat{n}_{NS}^d$	differential species balance	macroscopic
77	$\hat{H}_A^c := \left( F_{NS,AS} \stackrel{NS}{\star} h_{NS} \right) \stackrel{S \in AS}{\star} \hat{n}_{AS}^c$	convective enthalpy flow for given stream	macroscopic
78	$\hat{H}_N^c := F_{N,A} \stackrel{A}{\star} \hat{H}_A^c$	net convectional enthalpy stream	macroscopic
79	$\hat{w}_A := \text{Instantiate}(\hat{H}_A^c, \#)$	sample work stream	macroscopic
80	$\hat{w}_N := F_{N,A} \stackrel{A}{\star} \hat{w}_A$	net work stream	macroscopic
81	$\hat{q}_{xA} := A_{yzN} \cdot k_{xN}^q \cdot D_{N,A} \stackrel{N}{\star} T_N$	heat flow in x-direction for given stream	macroscopic
82	$\hat{q}_N := F_{N,A} \stackrel{A}{\star} \hat{q}_{xA}$	net heat flow	macroscopic
83	$\dot{H}_N := \hat{H}_N^c + \hat{H}_N^d + \hat{q}_N + \hat{w}_N$	differential enthalpy balance	macroscopic
84	$H_N^o := \text{Instantiate}(H_N, \#)$	initial enthalpy	macroscopic
85	$n_{NS}^o := \text{Instantiate}(n_{NS}, \#)$	initial species	macroscopic
86	$n_{NS} := \int_{t^o}^{t^e} \dot{n}_{NS} dt$	fundamental state – molar mass	macroscopic
87	$H_N := \int_{t^o}^{t^e} \dot{H}_N dt$	enthalpy	macroscopic
88	$\xi := \text{Instantiate}(\xi, \#)$	fraction of additives	material

*Continued on next page*

no	equation	documentation	layer
89	$I_N := \frac{dC_N}{dt}$	electrical current definition	macroscopic
91	$R_N^e := (i_N)^{-1} \cdot U_{eN}$	electrical resistant	material
92	$R_N^e := \text{Instantiate}(R_N^e, \#)$	electrical resistant	material
93	$k^{e,\xi}_N := (R_N^e)^{-1} \cdot \xi$	simple model for the electrical conductivity as a function of the additive	material
95	$U_{eN} := (R_N^e)^{-1} \cdot I_N$	electrical potential – voltage	macroscopic
96	$\dot{U}_N^e := 1 \cdot U_{eN}$	Kirkhoff first law	macroscopic
97	$\dot{U}_N^e := \text{Root}(U_{eN})$	Kirkhoff first law	macroscopic
98	$\dot{U}_N^e := \text{Instantiate}(\dot{U}_N^e, 0)$	Kirkhoff first law	macroscopic
106	$\phi := \text{MixedStack}(p_N, T_N, \mu_{NS}, c_{NS}, U_{eN})$	collected intensities	macroscopic
107	$n_N^t := 1_S \overset{S \in NS}{\star} n_{NS}$	total number of moles	macroscopic

## 35 Interface Link Equation

no	equation	documentation	layer
20	$\lambda_S := \lambda_S$	interface equation	material → macroscopic
37	$m_N := m_N$	interface equation	macroscopic → material
45	$c_{NS} := c_{NS}$	interface equation	macroscopic → reactions
51	$\rho_N := \rho_N$	interface equation	material → macroscopic
52	$h_{NS} := h_{NS}$	interface equation	material → macroscopic
53	$k_{xN}^q := k_{xN}^q$	interface equation	material → macroscopic
54	$Cv_N := Cv_N$	interface equation	material → macroscopic
55	$k_{yN}^q := k_{yN}^q$	interface equation	material → macroscopic
56	$k_{zN}^q := k_{zN}^q$	interface equation	material → macroscopic
57	$k_N^q := k_N^q$	interface equation	material → macroscopic
58	$k_{xN}^c := k_{xN}^c$	interface equation	material → macroscopic

*Continued on next page*



no	equation	documentation	layer
59	$Cp_N := Cp_N$	interface equation	material → macroscopic
60	$k_{yN}^c := k_{yN}^c$	interface equation	material → macroscopic
61	$k_{zN}^c := k_{zN}^c$	interface equation	material → macroscopic
62	$k_N^c := k_N^c$	interface equation	material → macroscopic
63	$k_{xNS}^d := k_{xNS}^d$	interface equation	material → macroscopic
64	$k_{yNS}^d := k_{yNS}^d$	interface equation	material → macroscopic
65	$k_{zNS}^d := k_{zNS}^d$	interface equation	material → macroscopic
66	$k_{NS}^d := k_{NS}^d$	interface equation	material → macroscopic
90	$i_N := i_N$	interface equation	macroscopic → material
94	$R_N^e := R_N^e$	interface equation	material → macroscopic
99	$I_N := I_N$	interface equation	macroscopic → control
104	$\xi := \xi$	interface equation	material → control

*Continued on next page*

no	equation	documentation	layer
105	$T_N := T_N$	interface equation	macroscopic control →