

1 Variables

2 root

	var	symbol	documentation	type	units	eqs
8		F_N_A	fundamental incidence matrix	network		
5		t	time	frame	<i>s</i>	
6		to	starting time	frame	<i>s</i>	4
7		te	end time	frame	<i>s</i>	5
1		value	numerical value	constant		
2		one	numerical value one	constant		1
3		zero	numerical value zero	constant		2
4		onehalf	numerical value one half	constant		3

3 physical

	var	symbol	documentation	type	units	eqs
162		P_N_NS	projection of nodes onto the node species	projection		
32		P_NS_AS	projection node species to arc species	projection		
33		P_K_NK	projection of conversion to node conversion	projection		
34		P_S_NS	projection species to node species	projection		
35		P_N_NK	projection node to node conversion	projection		
36		P_NS_KS	projection node species to conversion species	projection		
37		P_A_NS	projection arc to node species for conductivity	projection		
65		P_NK_KS	projection node conversion to conversion species	projection		
9		P_N_A	projection from node to arc for arc properties	projection		
10		r_x	x-coordinate	frame	m	
11		r_y	y-coordinate	frame	m	
12		r_z	z coordinate	frame	m	
13		U	fundamental state – internal energy	state	$kg\,m^2\,s^{-2}$	
14		S	fundamental state – entropy	state	$kg\,m^2\,K^{-1}\,s^{-2}$	
15		V	fundamental state – volume	state	m^3	
16		n	fundamental state – molar mass	state	mol	86
20		H	enthalpy	state	$kg\,m^2\,s^{-2}$	9 87
21		A	Helmholtz energy	state	$kg\,m^2\,s^{-2}$	10
22		G	Gibbs free energy	state	$kg\,m^2\,s^{-2}$	11
23		charge	fundamental state – charge	state	$A\,s$	
165		boz	Boltzmann constant	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	132
166		R	gas constant	constant	$kg\,m^2\,mol^{-1}\,K^{-1}\,s^{-2}$	133
24		Avogadro	Avogadro number	constant	mol^{-1}	

Continued on next page

	var	symbol	documentation	type	units	eqs
17		p	thermodynamic pressure	effort	$kg\,m^{-1}\,s^{-2}$	6
18		T	temperature	effort	K	7
19		chemPot	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	8 136
27		Ue	electrical potential – voltage	effort	$kg\,m^2\,A^{-1}\,s^{-3}$	14 95
28		v_x	velocity in x-direction	secondaryState	ms^{-1}	15
29		v_y	velocity in y-direction	secondaryState	ms^{-1}	16
30		v_z	velocity in z-direction	secondaryState	ms^{-1}	17

4 control

	var	symbol	documentation	type	units	eqs
136		x	state	state		111
137		xo	initial state	state		109
129		A	dynamic matrix	constant	s^{-1}	
130		B	input matrix	constant	s^{-1}	
131		C	measurement matrix	constant		
132		D	diagonal event matrix (no dimensional problems)	constant		
133		setPoint	set point	constant		119
134		meas	measurements	constant		
135		e	control error	constant		108
139		I_N_D	space transformation D to N	constant		
138		dxdt	differential state (ABCD) model	diffState	s^{-1}	110
141		Imeasured	measured current	algebraic	A	113
143		UeMeasured	measured electrical potential	algebraic	$kg\,m^2\,A^{-1}s^{-3}$	115
144		addMeasured	measured additive fraction	algebraic		116
145		RComputed	measured resistance	algebraic	$kg\,m^2\,A^{-2}s^{-3}$	117
146		store	quantities to be stored	algebraic		118
154		y	output equation	algebraic		126
171		switch	switches at to	algebraic		138

5 reactions

	var	symbol	documentation	type	units	eqs
147		P_NK	reactions per node	projection		
155		Boltzmann	Boltzmann constant	constant	$kg\ m^2\ K^{-1}\ s^{-2}$	
157		GasConstant	gas constant	constant	$kg\ m^2\ mol^{-1}\ K^{-1}\ s^{-2}$	127
158		N_K_KS	stoichiometry	constant		
159		N_NK_KS	extended stoichiometric matrix	constant		128
38		Ko	Arrhenius frequency factor	constant	$m^{-3}\ mol\ s^{-1}$	
62		Ea	Arrhenius activation energy	constant	$kg\ m^2\ mol^{-1}\ s^{-2}$	41
63		K_NK	Arrhenius reaction 'constant'	constant	$m^{-3}\ mol\ s^{-1}$	42
60		T_NK	temperature of the reactive system	effort	K	39
151		c	concentration matrix reaction per node and species per reaction	secondaryState	$m^{-3}\ mol$	123
152		co	norming concentration	secondaryState	$m^{-3}\ mol$	124
153		x	matrix of normed, dimensionless mole fractions	secondaryState		125
160		phi	probability function for reactions	secondaryState		129
163		nProd	the species production term	secondaryState	$mol\ s^{-1}$	130

6 material

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

7 macroscopic

	var	symbol	documentation	type	units	eqs
100		fnc	net molar convectional mass flow	transport	mol s^{-1}	75
102		fHc_A	convective enthalpy flow for given stream	transport	$\text{kg m}^2 \text{s}^{-3}$	77
103		fHc	net convectional enthalpy stream	transport	$\text{kg m}^2 \text{s}^{-3}$	78
104		fw_A	sample work stream	transport	$\text{kg m}^2 \text{s}^{-3}$	79
105		fw	net work stream	transport	$\text{kg m}^2 \text{s}^{-3}$	80
106		fq_A_x	heat flow in x-direction for given stream	transport	$\text{kg m}^2 \text{s}^{-3}$	81
107		fq	net heat flow	transport	$\text{kg m}^2 \text{s}^{-3}$	82
173		fnc_AS_controlled	switched flow	transport	mol s^{-1}	141
92		fV	volumetric flow	transport	$\text{m}^3 \text{s}^{-1}$	67 140
93		fnd_AS	diffusional mass flow in a given stream	transport	mol s^{-1}	68
94		fnd	net diffusional mass flow	transport	mol s^{-1}	69
95		fHd_A	enthalpy flow per diffusional mass stream	transport	$\text{kg m}^2 \text{s}^{-3}$	70
96		fHd	net enthalpy stream due to diffusion	transport	$\text{kg m}^2 \text{s}^{-3}$	71
97		d	flow direction of convectional flow	transport		72
99		fnc_AS	molar convectional mass flow in the given stream	transport	mol s^{-1}	74
71		Ayz	cross sectional area yz	geometry	m^2	48
72		Axz	cross sectional area xz	geometry	m^2	49
73		Axy	cross sectional area xy	geometry	m^2	50
70		F_NS_AS	species related incidence matrix	network		
90		D	difference operator	differenceOperator		
91		D_NS_AS	difference operator for species topology	differenceOperator		
109		Ho	initial enthalpy	state	$\text{kg m}^2 \text{s}^{-2}$	84

Continued on next page

	var	symbol	documentation	type	units	eqs
110		no	initial species	state	<i>mol</i>	85
127		one_S	a vector of ones with the length of the ordinal number of S	constant		
126		intensities	collected intensities	secondaryState		106
128		nTotal	total number of moles	secondaryState	<i>mol</i>	107
168		nt	total number of species in a node	secondaryState	<i>mol</i>	134
169		xi	mole fraction	secondaryState		135
175		gugus		secondaryState	<i>mol</i>	144
57		m	total mass	secondaryState	<i>kg</i>	36
66		c	molar composition	secondaryState	$m^{-3} mol$	44
98		c_AS	concentration in convectonal flow	secondaryState	$m^{-3} mol$	73
170		nProd	production term	conversion	$mol s^{-1}$	137
101		dndt	differential species balance	diffState	$mol s^{-1}$	76 142
108		dHdt	differential enthalpy balance	diffState	$kg m^2 s^{-3}$	83
118		dUedt	Kirkhoffs first law	diffState	$kg m^2 A^{-1} s^{-3}$	96 97 98
113		i	electrical current definition	internalTransport	<i>A</i>	89

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		<code>_additive</code>	link variable additive to interface material » > control	get		104

25 control-macroscopic

	var	symbol	documentation	type	units	eqs
172		<code>_switch</code>	switches at to	get		139

26 macroscopic-control

	var	symbol	documentation	type	units	eqs
119		<code>_i</code>	link variable i to interface macroscopic »> control	get	A	99
125		<code>_T</code>	link variable T to interface macroscopic »> control	get	K	105
142		<code>_Ue</code>	link variable Ue to interface macroscopic »> control	get	$kg\,m^2\,A^{-1}s^{-3}$	114

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
164		<code>_nProd</code>	link variable nProd to interface reactions »> macroscopic	get	mol s^{-1}	131

30 macroscopic-reactions

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

31 material–macroscopic

	var	symbol	documentation	type	units	eqs
117		<code>_elConductC</code>	link variable elConductC to interface material »> macroscopic	get	$kg^{-1} m^{-2} A^2 s^3$	94
140		<code>_additive</code>	link variable additive to interface material »> macroscopic	get		112
41		<code>_Mm</code>	link variable Mm to interface material »> macroscopic	get	$kg mol^{-1}$	20
74		<code>_density</code>	link variable density to interface material »> macroscopic	get	$kg m^{-3}$	51
75		<code>_h</code>	link variable h to interface material »> macroscopic	get	$kg m^2 mol^{-1} s^{-2}$	52
76		<code>_kq_x</code>	link variable kq x to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	53
77		<code>_Cv</code>	link variable Cv to interface material »> macroscopic	get	$kg m^2 K^{-1} s^{-2}$	54
78		<code>_kq_y</code>	link variable kq y to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	55
79		<code>_kq_z</code>	link variable kq z to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	56
80		<code>_kq</code>	link variable kq to interface material »> macroscopic	get	$kg K^{-1} s^{-3}$	57
81		<code>_kc_x</code>	link variable kc x to interface material »> macroscopic	get	$m^{-1} s$	58
82		<code>_Cp</code>	link variable Cp to interface material »> macroscopic	get	$kg m^2 K^{-1} s^{-2}$	59
83		<code>_kc_y</code>	link variable kc y to interface material »> macroscopic	get	$m^{-1} s$	60
84		<code>_kc_z</code>	link variable kc z to interface material »> macroscopic	get	$m^{-1} s$	61
85		<code>_kc</code>	link variable kc to interface material »> macroscopic	get	$m^{-1} s$	62
86		<code>_kd_x</code>	link variable kd x to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	63

Continued on next page

	var	symbol	documentation	type	units	eqs
87		<code>_kd_y</code>	link variable kd y to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	64
88		<code>_kd_z</code>	link variable kd z to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	65
89		<code>_kd</code>	link variable kd to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	66

32 macroscopic-material

	var	symbol	documentation	type	units	eqs
114		<code>_i</code>	link variable i to interface macroscopic »> material	get	<i>A</i>	90
58		<code>_m</code>	link variable m to interface macroscopic »> material	get	<i>kg</i>	37

33 Equations

34 Generic

no	equation	documentation	layer
10	$A_N := U_N - T_N \cdot S_N$	Helmholtz energy	physical
106	$\phi := \text{MixedStack}(p_N, T_N, \mu_{NS}, c_{NS}, Ue_N)$	collected intensities	macroscopic
107	$n^t_N := 1_S \overset{S \in NS}{\star} n_{NS}$	total number of moles	macroscopic
108	$e_A := m_A - y^o_A$	control error	control
11	$G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$	Gibbs free energy	physical
110	$\dot{x}_D := A_{N,D} \overset{N}{\star} x_N + B_{A,D} \overset{A}{\star} e_A$	differential state (ABCD) model	control
111	$x_N := \int_{t^o}^{t^e} 1_{N,D} \overset{D}{\star} \dot{x}_D dt$	state	control
113	$\check{I}_N := I_N$	measured current	control
115	$\check{U}^e_N := Ue_N$	measured electrical potential	control
116	$\check{\xi} := \mapsto \xi$	measured additive fraction	control
117	$R_N := (\check{I}_N)^{-1} \cdot \check{U}^e_N$	measured resistance	control
118	$S := \text{MixedStack}(\check{I}_N, \check{U}^e_N, R_N, \check{\xi})$	quantities to be stored	control
123	$c_{NK,KS} := P_{NK} \cdot (P_{NS,KS} \overset{NS}{\star} c_{NS})$	var doc :	reactions
125	$x_{NK,KS} := (c^o_{NK,KS})^{-1} \cdot c_{NK,KS}$	matrix of normed, dimensionless mole fractions	reactions
126	$y_A := C_{N,A} \overset{N}{\star} x_N + D_A \cdot e_A$	output equation	control

Continued on next page

no	equation	documentation	layer
127	$R := A^v . B$	gas constant	reactions
128	$N_{NK,KS} := P_{K,NK} \overset{K}{\star} N_{K,KS}$	extended stoichiometrix matrix	reactions
129	$\phi_{NK} := \prod_{KS} x_{NK,KS}^{N_{NK,KS}}$	probability function for reactions	reactions
130	$\tilde{n}_{NS} := V_N \overset{N}{\star} \left(P_{N,NK} \overset{NK}{\star} \left((K_{NK} . \phi_{NK}) . \left(P_{NS,KS} \overset{KS}{\star} N_{NK,KS} \right) \right) \right)$	the species production term	reactions
132	$boz_N := \text{Instantiate}(S_N, \#)$	Boltzmann constant	physical
133	$R_N := A^v . boz_N$	gas constant	physical
134	$n_{tN} := 1_S \overset{S \in NS}{\star} n_{NS}$	total number of species in a node	macroscopic
135	$\xi_{NS} := (n_{tN})^{-1} \odot n_{NS}$	mole fraction	macroscopic
136	$\mu_{NS} := (R_N . T_N) \odot \ln(\xi_{NS})$	chemical potential	macroscopic
137	$\tilde{n}_{NS} := \tilde{n}_{NS}$	production term	macroscopic
138	$s := 0.5 . (1 + \text{sign}(t^o))$	switches at to	control
139	$s := s$	switches at to	control \rightarrow macroscopic
14	$Ue_N := (C_N)^{-1} . U_N$	electrical potential – voltage	physical
141	$\hat{n}^{c,controlled}_{AS} := s . \hat{n}^c_{AS}$	switched flow	macroscopic
142	$\dot{n}_{NS} := F_{NS,AS} \overset{AS}{\star} \text{Stack}(\hat{n}^c_{AS}, \hat{n}^{c,controlled}_{AS})$	differential species balance switched	macroscopic
144	$gugus_{NS} := n_{NS} + n_{NS}$		macroscopic
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	$m_N := \lambda_S^{S \in NS} \star n_{NS}$	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
42	$K_{NK} := K^o_K \odot \exp((-E^a_{NK}) \cdot (R \cdot T_{NK})^{-1})$	Arrhenius reaction 'constant'	reactions
44	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar composition	macroscopic
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
6	$p_N := \left(-\frac{\partial U_N}{\partial V_N}\right)$	thermodynamic pressure	physical
67	$\hat{V}_A := (\rho_N)^{-1} \cdot k_{xN}^c \cdot A_{yzN} \cdot D_{N,A} \overset{N}{\star} p_N$	volumetric flow	macroscopic
68	$\hat{n}_{AS}^d := A_{yzN} \odot (-k_{xNS}^d) \cdot D_{NS,AS} \overset{NS}{\star} \mu_{NS}$	diffusional mass flow in a given stream	macroscopic
69	$\hat{n}_{NS}^d := F_{NS,AS} \overset{AS}{\star} \hat{n}_{AS}^d$	net diffusional mass flow	macroscopic
7	$T_N := \frac{\partial U_N}{\partial S_N}$	temperature	physical
70	$\hat{H}_A^d := \left(F_{NS,AS} \overset{NS}{\star} h_{NS}\right) \overset{S \in AS}{\star} \hat{n}_{AS}^d$	enthalpy flow per diffusional mass stream	macroscopic
71	$\hat{H}_N^d := F_{N,A} \overset{A}{\star} \hat{H}_A^d$	net enthaply stream due to diffusion	macroscopic
72	$d_A := \text{sign}\left(F_{N,A} \overset{N}{\star} p_N\right)$	flow direction of convectonal flow	macroscopic
73	$c_{AS} := (0.5 \cdot (F_{NS,AS} - d_A \odot F_{NS,AS})) \overset{NS}{\star} c_{NS}$	concentration in convectonal flow	macroscopic

Continued on next page

no	equation	documentation	layer
74	$\hat{n}_{AS}^c := \hat{V}_A \odot c_{AS}$	molar convetional mass flow in the given stream	macroscopic
75	$\hat{n}_{NS}^c := F_{NS,AS} \overset{AS}{\star} \hat{n}_{AS}^c$	net molar convetional mass flow	macroscopic
76	$\dot{n}_{NS} := \hat{n}_{NS}^c + \hat{n}_{NS}^d + \tilde{n}_{NS}$	differential species balance	macroscopic
77	$\hat{H}_A^c := \left(F_{NS,AS} \overset{NS}{\star} h_{NS} \right) \overset{S \in AS}{\star} \hat{n}_{AS}^c$	convective enthalpy flow for given stream	macroscopic
78	$\hat{H}_N^c := F_{N,A} \overset{A}{\star} \hat{H}_A^c$	net convetional enthalpy stream	macroscopic
8	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	chemical potential	physical
80	$\hat{w}_N := F_{N,A} \overset{A}{\star} \hat{w}_A$	net work stream	macroscopic
81	$\hat{q}_{xA} := A_{yzN} \cdot k_{xN}^q \cdot D_{N,A} \overset{N}{\star} T_N$	heat flow in x-direction for given stream	macroscopic
82	$\hat{q}_N := F_{N,A} \overset{A}{\star} \hat{q}_{xA}$	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
86	$n_{NS} := \int_{t^o}^{t^e} \dot{n}_{NS} dt + n_{NS}^o$	fundamental state – molar mass	macroscopic
87	$H_N := \int_{t^o}^{t^e} \dot{H}_N dt$	enthalpy	macroscopic
89	$I_N := \frac{dC_N}{dt}$	electrical current definition	macroscopic
9	$H_N := U_N - p_N \cdot V_N$	enthalpy	physical
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	$Ue_N := (R_N^e)^{-1} \cdot I_N$	electrical potential – voltage	macroscopic
96	$\dot{U}_N^e := 1 \cdot Ue_N$	Kirkhoff first law	macroscopic

Continued on next page

no	equation	documentation	layer
97	$\dot{U}^e_N := Root(Ue_N)$	Kirkhoff first law	macroscopic

35 Instantiate

no	equation	documentation	layer
1	$1 := \text{Instantiate}(\#, \#)$	numerical value 1	root
109	$x_{oN} := \text{Instantiate}(x_N, \#)$	initial state	control
119	$y^o_A := \text{Instantiate}(y^o_A, \#)$	set point	control
124	$c^o_{NK,KS} := \text{Instantiate}(c_{NK,KS}, \#)$	norming concentration	reactions
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
41	$E^a_{NK} := \text{Instantiate}(R.T_{NK}, \#)$	Arrhenius activation energy	reactions
5	$t^e := \text{Instantiate}(t, \#)$	end time	root
79	$\hat{w}_A := \text{Instantiate}(\hat{H}^c_A, \#)$	sample work stream	macroscopic
84	$H^o_N := \text{Instantiate}(H_N, \#)$	initial enthalpy	macroscopic
85	$n^o_{NS} := \text{Instantiate}(n_{NS}, \#)$	initial species	macroscopic
88	$\xi := \text{Instantiate}(\xi, \#)$	fraction of additives	material
91	$R^e_N := (I_N)^{-1} . Ue_N$	electrical resistant	material
92	$R^e_N := \text{Instantiate}(R^e_N, \#)$	electrical resistant	material
98	$\dot{U}^e_N := \text{Instantiate}(\dot{U}^e_N, 0)$	Kirkhoff first law	macroscopic

36 Instantiation Equation

no	equation	documentation	layer
140	$\hat{V}_A := \text{Instantiate}(\hat{V}_A, \#)$	instantiation equation	macroscopic

37 Interface Link Equation

no	equation	documentation	layer
104	$\mapsto \xi := \xi$	interface equation	material -> control
105	$T_N := T_N$	interface equation	macroscopic -> control
112	$\xi := \xi$	interface equation	material -> macroscopic
114	$Ue_N := Ue_N$	interface equation	macroscopic -> control
131	$\tilde{n}_{NS} := \tilde{n}_{NS}$	interface equation	reactions -> macroscopic
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

Continued on next page

no	equation	documentation	layer
54	$cv_N := C_{VN}$	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
59	$cp_N := C_{pN}$	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

Continued on next page

no	equation	documentation	layer
66	$k_{NS}^d := k_{NS}^d$	interface equation	material \rightarrow macroscopic
90	$I_N := I_N$	interface equation	macroscopic \rightarrow material
94	$R_N^e := k^{e,\xi}_N$	interface equation	material \rightarrow macroscopic
99	$I_N := I_N$	interface equation	macroscopic \rightarrow control