## 1 Variables

## 2 root

	var	symbol	documentation	type	units	eqs
8		F_N_A	fundamental incidence matrix	network		
5		t	time	frame	s	
6		to	starting time	frame	s	4
7		te	end time	frame	s	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	$kgm^2s^{-2}$	
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		н	enthalpy	state	$kgm^2s^{-2}$	9 87
21		A	Helmholtz energy	state	$kgm^2s^{-2}$	10
22		G	Gibbs free energy	state	$kgm^2s^{-2}$	11
23		charge	fundamental state – charge	state	As	
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	$mol^{-1}$	

	var	symbol	documentation	type	units	eqs
17		р	thermodynamic pressure	effort	$kg  m^{-1}  s^{-2}$	6
18		Т	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		_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		х	state	state		111
137		xo	initial state	state		109
129		A	dynamic matrix	constant	$s^{-1}$	
130		В	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		е	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		у	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	$ \begin{vmatrix} kg  m^2  K^{-1}  s^{-2} \\ kg  m^2  mol^{-1}  K^{-1}  s^{-2} \end{vmatrix} $	
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		Ко	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		С	concentration matrix reaction per node and species per reaction	secondaryState	$m^{-3}  mol$	123
152		со	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		Ср	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	$kg^{-1}m^{-4}mol^2s$	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	$kg m^2 s^{-3}$	77
103		fHc	net convectional enthalpy stream	transport	$kg m^2 s^{-3}$	78
104		fw_A	sample work stream	transport	$kg m^2 s^{-3}$	79
105		fw	net work stream	transport	$kg m^2 s^{-3}$	80
106		fq_A_x	heat flow in x-direction for given stream	transport	$kgm^2s^{-3}$	81
107		fq	net heat flow	transport	$kg m^2 s^{-3}$	82
173		fnc_AS_controlled	switched flow	transport	$mol  s^{-1}$	141
92		fV	volumetric flow	transport	$m^3 s^{-1}$	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	$kg m^2 s^{-3}$	70
96		fHd	net enthalpy stream due to diffusion	transport	$kg m^2 s^{-3}$	71
97		d	flow direction of convectional flow	transport		72
99		fnc_AS	molar convectional mass flow in the given stream	transport	$\mod s^{-1}$	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	${\it difference Operator}$		
109		Но	initial enthalpy	state	$kgm^2s^{-2}$	84

	var	symbol	documentation	type	units	eqs
110		no	initial species	state	mol	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	mol	107
168		nt	total number of species in a node	secondaryState	mol	134
169		xi	mole fraction	secondaryState		135
175		gugus		secondaryState	mol	144
176		g		secondaryState	mol	145
57		m	total mass	secondaryState	kg	36
66		С	molar composition	secondaryState	$m^{-3}  mol$	44
98		c_AS	concentration in convectional flow	secondaryState	$m^{-3}  mol$	73
177		gugu		secondaryState	mol	146
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	$kgm^2s^{-3}$	83
118		dUedt	Kirkhoffs first law	diffState	$kg  m^2  A^{-1} s^{-3}$	96 97 98
113		i	electrical current definition	${\it internal Transport}$	A	89

## 8 solid

	var	symbol	documentation	type	units	eqs
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## 9 fluid

	var	symbol	documentation	type	units	eqs
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# 10 liquid

	var	symbol	documentation	type	units	eqs
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# 11 gas

	var	symbol	documentation	type	units	eqs
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#### 12 control-control

var symbol documentation type units eqs			symbol	documentation	type	units	eqs
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# 13 gas-liquid

	var	symbol	documentation	type	units	eqs
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## 14 gas-gas

	var	symbol	documentation	type	units	eqs
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# 15 liquid-liquid

	var	symbol	documentation	type	units	eqs
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# 16 gas-solid

	var	symbol	documentation	type	units	eqs
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# 17 solid-solid

	var	symbol	documentation	type	units	eqs
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# 18 liquid-solid

	var	symbol	documentation	type	units	eqs
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### 19 material-material

	var	symbol	documentation	type	units	eqs
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#### 20 reactions—reactions

	var	symbol	documentation	type	units	eqs
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### 21 control-reactions

	var	symbol	documentation	type	units	eqs
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#### 22 reactions-control

	var	symbol	documentation	type	units	eqs
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#### 23 control-material

	var	symbol	documentation	type	units	eqs
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## 24 material-control

	var	symbol	documentation	type	units	eqs
124		_additive	link variable additive to interface material $\gg > { m control}$	get		104

## ${\bf 25} \quad {\bf control-macroscopic}$

	var	symbol	documentation	type	units	eqs
172		_switch	switches at to	get		139

### 26 macroscopic-control

	var	symbol	documentation	type	units	eqs
119		_i	link variable i to interface macroscopic $\gg>$ control	get	A	99
125		_T	link variable T to interface macroscopic $\gg>$ control	get	K	105
142		_Ue	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	
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### 28 material-reactions

	var	symbol	documentation	type	units	eqs
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### 29 reactions-macroscopic

	var	symbol	documentation	type	units	eqs
164		_nProd	link variable nProd to interface reactions $\gg$ macroscopic	get	$mol  s^{-1}$	131

## macroscopic-reactions

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

### material-macroscopic

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

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

### 32 macroscopic-material

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

# 33 Equations

### 34 Generic

no	equation	documentation	layer
10	$A_N := U_N - T_N \cdot S_N$	Helmholtz energy	physical
106	$\phi := \operatorname{MixedStack}(p_N, T_N, \mu_{NS}, c_{NS}, Ue_N)$	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	$x_N := \int_{t^o}^{t^e} 1_{N,D} \stackrel{D}{\star} \dot{x}_D \ dt$	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	$S := \operatorname{MixedStack}\left(\check{I}_N, \check{U}^e{}_N, R_N, \check{\xi} ight)$	quantities to be stored	control
123	$c_{NK,KS} := P_{NK} \cdot \left( P_{NS,KS} \overset{NS}{\star} c_{NS} \right)$	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

no	equation	documentation	layer
127	$R := A^v \cdot B$	gas constant	reactions
128	$N_{NK,KS} := P_{K,NK} \stackrel{K}{\star} N_{K,KS}$	extended stoichiometrix matrix	reactions
129	$\phi_{NK} := \prod_{KS} x_{NK,KS}^{N_{NK,KS}}$	probability function for reactions	reactions
130	$\tilde{n}_{NS} := V_N \overset{N}{\star} \left( P_{N,NK} \overset{NK}{\star} \left( \left( K_{NK} . \phi_{NK} \right) . \left( P_{NS,KS} \overset{KS}{\star} N_{NK,KS} \right) \right) \right)$	the species production term	reactions
132	$boz_N := \text{Instantiate}(S_N, \#)$	Boltzmann constant	physical
133	$R_N := A^v \cdot boz_N$	gas constant	physical
134	$n_{tN} := 1_S \overset{S \in NS}{\star} n_{NS}$	total number of species in a node	macroscopic
135	$\xi_{NS} := \left(n_{tN}\right)^{-1} \odot n_{NS}$	mole fraction	macroscopic
136	$\mu_{NS} := (R_N . T_N) \odot ln(\xi_{NS})$	chemical potential	macroscopic
137	$ ilde{n}_{NS} :=  ilde{n}_{NS}$	production term	macroscopic
138	$s := 0.5 \cdot (1 + \text{sign}(t^o))$	switches at to	control
139	s := s	switches at to	control -> macro- scopic
14	$Ue_N := (C_N)^{-1} \cdot U_N$	electrical potential – voltage	physical
141	$\hat{n}^{c,controlled}_{AS} := s \cdot \hat{n}^c{}_{AS}$	switched flow	macroscopic
142	$\dot{n}_{NS} := F_{NS,AS} \overset{AS}{\star} \operatorname{Stack} \left( \hat{n}^{c}{}_{AS}, \hat{n}^{c,controlled}{}_{AS} \right)$	differential species balance switched	macroscopic
144	$gugus_{NS} := n_{NS} + n_{NS}$		macroscopic
145	$g_{NS} := n_{NS} + n_{NS}$		macroscopic
146	$gugu_{NS} := n_{NS} + n_{NS}$		macroscopic

no	equation	documentation	layer
15	$v_{xN} := \frac{\partial  r_{xN}}{\partial  t}$	velocitiy in x-direction	physical
16	$v_{yN} := \frac{\partial r_{yN}}{\partial t}$	velocity in y direction	physical
17	$v_{zN} := \frac{\partial r_{zN}}{\partial t}$	velocity in z-direction	macroscopic
21	$C_{pN} := rac{\partial  H_N}{\partial  T_N}$	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	$k_x^q N := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}$	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	$\left  \begin{array}{l} k^q{}_N := \operatorname{Stack} \left( k^q_{xN}, k^q_{yN}, k^q_{zN} \right) \end{array} \right.$	thermal conductivity	material
27	$k_{xN}^c := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass conductivity in x-direction	material
28	$k_{yN}^c := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$	convective mass conductivity in y-direction	material
29	$k_{zN}^c := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convective mass conductivity in z-direction	material
30	$k^{c}_{N} := \operatorname{Stack}\left(k_{xN}^{c}, k_{yN}^{c}, k_{zN}^{c}\right)$	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

no	equation	documentation	layer
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	$k^d_{NS} := \operatorname{Stack}\left(k^d_{xNS}, k^d_{yNS}, k^d_{zNS}\right)$	diffusional mass condctivity	material
35	$h_{NS} := H_N \odot \left( n_{NS} \right)^{-1}$	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	$T_{NK} := P_{N,NK} \stackrel{N}{\star} T_N$	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	$\hat{V}_A := (\rho_N)^{-1} \cdot k_{xN}^c \cdot A_{yzN} \cdot D_{N,A} \stackrel{N}{\star} p_N$	volumetric flow	macroscopic
68	$\hat{n}^d{}_{AS} := A_{yzN} \odot \left( -k_{xNS}^d \right) . D_{NS,AS} \overset{NS}{\star} \mu_{NS}$	diffusional mass flow in a given stream	macroscopic
69	$\hat{n}^d{}_{NS} := F_{NS,AS} \stackrel{AS}{\star} \hat{n}^d{}_{AS}$	net diffusional mass flow	macroscopic
7	$T_N := \frac{\partial U_N}{\partial S_N}$	temperature	physical
70	$\hat{H}^d{}_A := \left(F_{NS,AS} \overset{NS}{\star}{}_{hNS}\right) \overset{S \in AS}{\star} \hat{n}^d{}_{AS}$	enthalpy flow per diffusional mass stream	macroscopic

no	equation	${f documentation}$	layer
71	$\hat{H}^d{}_N := F_{N,A} \stackrel{A}{\star} \hat{H}^d{}_A$	net enthaply stream due to diffusion	macroscopic
72	$d_A := \operatorname{sign}\left(F_{N,A} \stackrel{N}{\star} p_N\right)$	flow direction of convectional flow	macroscopic
73	$c_{AS} := (0.5 \cdot (F_{NS,AS} - d_A \odot  F_{NS,AS} )) \overset{NS}{\star} c_{NS}$	concentration in convectional flow	macroscopic
74	$\hat{n}^c{}_{AS} := \hat{V}_A \odot c_{AS}$	molar convetional mass flow in the given stream	macroscopic
75	$\hat{n}^c{}_{NS} := F_{NS,AS} \stackrel{AS}{\star} \hat{n}^c{}_{AS}$	net molar convectional mass flow	macroscopic
76	$\dot{n}_{NS} := \hat{n}^c{}_{NS} + \hat{n}^d{}_{NS} + \tilde{n}_{NS}$	differential species balance	macroscopic
77	$\hat{H}^{c}{}_{A} := \left(F_{NS,AS} \overset{NS}{\star}{}_{hNS}\right) \overset{S \in AS}{\star} \hat{n}^{c}{}_{AS}$	convective enthalpy flow for given stream	macroscopic
78	$\hat{H}^c{}_N := F_{N,A} \stackrel{A}{\star} \hat{H}^c{}_A$	net convectional enthalpy stream	macroscopic
8	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	chemical potential	physical
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	$\dot{H}_N := \hat{H}^c{}_N + \hat{H}^d{}_N + \hat{q}_N + \hat{w}_N$	differential enthalpy balance	macroscopic
86	$n_{NS} := \int_{t^o}^{t^e}  \dot{n}_{NS}  \; dt + n^o{}_{NS}$	fundamental state – molar mass	macroscopic
87	$H_N := \int_{t^o}^{t^e} \dot{H}_N \ dt$	enthalpy	macroscopic
89	$I_N := \frac{d  C_N}{d  t}$	electrical current definition	macroscopic
9	$H_N := U_N - p_N . V_N$	enthalpy	physical

no	equation	documentation	layer
93	$k^{e,\xi}{}_N := (R^e{}_N)^{-1} \cdot \xi$	simple model for the electrical conductivity as a function of the additive	material
95	$Ue_N := (R^e{}_N)^{-1} . I_N$	electrical potential – voltage	macroscopic
96	$\dot{U}^e{}_N := 1 . Ue_N$	Kirkhoff first law	macroscopic
97	$\dot{U}^e{}_N := Root\left(Ue_N\right)$	Kirkhoff first law	macroscopic

#### 35 Instantiate

no	equation	documentation	layer
1	1 := 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 := Instantiate(#, #)	numerical value zero	root
3	0.5 := 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	$H^o{}_N := \operatorname{Instantiate}(H_N, \#)$	initial enthalpy	macroscopic
85	$n^o{}_{NS} := \operatorname{Instantiate}(n_{NS}, \#)$	initial species	macroscopic
88	$\xi := \operatorname{Instantiate}(\xi, \#)$	fraction of additives	material
91	$R^e{}_N := (I_N)^{-1} \cdot Ue_N$	electrical resistant	material
92	$R^e{}_N := \operatorname{Instantiate}(R^e{}_N, \#)$	electrical resistant	material
98	$\dot{U}^e{}_N := \operatorname{Instantiate}(\dot{U}^e{}_N, 0)$	Kirkhoff first law	macroscopic

# 36 Instantiation Equation

no	equation	documentation	layer
140	$\hat{V}_A := \operatorname{Instantiate}(\hat{V}_A, \#)$	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 -> macro- scopic
114	$Ue_N:=Ue_N$	interface equation	macroscopic -> control
131	$ ilde{n}_{NS} :=  ilde{n}_{NS}$	interface equation	reactions -> macroscopic
20	$\lambda_S := \lambda_S$	interface equation	material -> macro- scopic
37	$m_N := m_N$	interface equation	macroscopic -> material
45	$c_{NS} := c_{NS}$	interface equation	macroscopic -> reactions
51	$ ho_N :=  ho_N$	interface equation	material -> macro- scopic
52	$h_{NS} := h_{NS}$	interface equation	material -> macro- scopic
53	$k_{xN}^q := k_{xN}^q$	interface equation	material -> macro- scopic

no	equation	documentation	layer
54	$_{C}v_{N}:=C_{VN}$	interface equation	material -> macro- scopic
55	$k_{yN}^q := k_y^q {}_N$	interface equation	material -> macro- scopic
56	$k_{zN}^q := k_{zN}^q$	interface equation	material -> macro- scopic
57	$k^q{}_N := k^q{}_N$	interface equation	material -> macro- scopic
58	$k_{xN}^c := k_{xN}^c$	interface equation	material -> macro- scopic
59	$_Cp_N:=C_{pN}$	interface equation	material -> macro- scopic
60	$k_{yN}^c := k_{yN}^c$	interface equation	material -> macro- scopic
61	$k_{zN}^c := k_{zN}^c$	interface equation	material -> macro- scopic
62	$k^c{}_N := k^c{}_N$	interface equation	material -> macro- scopic
63	$k_{xNS}^d := k_{xNS}^d$	interface equation	material -> macro- scopic
64	$k_{yNS}^d := k_{yNS}^d$	interface equation	material -> macro- scopic
65	$k_{zNS}^d := k_{zNS}^d$	interface equation	material -> macro- scopic

no	equation	documentation	layer
66	$k^d{}_{NS} := k^d{}_{NS}$	interface equation	material -> macro- scopic
90	$I_N := I_N$	interface equation	macroscopic -> material
94	$R^e{}_N := k^{e,\xi}{}_N$	interface equation	material -> macro- scopic
99	$I_N:=I_N$	interface equation	macroscopic -> control