## 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	$\mid m \mid$	
11	$r_{yN}$	r_y	y-coordinate	frame	$\mid m \mid$	
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	$H_N$	Н	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	As	
24	$A^v$	Avogadro	Avogadro number	constant	$mol^{-1}$	
17	$p_N$	p	thermodynamic pressure	effort	$kg  m^{-1}  s^{-2}$	6
18	$T_N$	Т	temperature	effort	K	7
19	$\mu_{NS}$	chemPot	chemical potential	effort	$kg  m^2  mol^{-1}  s^{-2}$	8

	var	symbol	documentation	type	units	eqs
27	$Ue_N$	Ue	electrical potential – voltage	effort	$kg  m^2  A^{-1} s^{-3}$	14 95
28	$v_{xN}$	v_x	velocitiy in x-direction	secondaryState	$ms^{-1}$	15
29	$v_{yN}$	v_y	velocity in y-direction	secondaryState	$ms^{-1}$	16
30	$v_{zN}$	V_Z	velocity in z-direction	secondaryState	$ms^{-1}$	17

### 4 control

	var	symbol	documentation	type	units	eqs
136	$x_N$	х	state	state		111
137	$xo_N$	xo	initial state	state		109
129	$A_{N,D}$	A	dynamic matrix	constant	$s^{-1}$	
130	$B_{A,D}$	В	input matrix	constant	$s^{-1}$	
131	$C_{N,A}$	C	measurement matrix	constant		
132	$D_A$	D	diagonal event matrix (no dimensional problems)	constant		
133	$y^o{}_A$	setPoint	set point	constant		119
134	$m_A$	meas	measurements	constant		
135	$e_A$	е	control error	constant		108
139	$1_{N,D}$	I_N_D	space transformation D to N	constant		
138	$\dot{x}_D$	dxdt	differential state (ABCD) model	diffState	$s^{-1}$	110
141	$\check{I}_N$	Imeasured	measured current	algebraic	A	113
143	$\check{U}^e{}_N$	UeMeasured	measured electrical potential	algebraic	$kg m^2 A^{-1} s^{-3}$	115
144	$\check{\xi}$	addMeasured	measured additive fraction	algebraic		116
145	$RComputed_N$	RComputed	measured resistance	algebraic	$kg m^2 A^{-2} s^{-3}$	117
146	store	store	quantities to be stored	algebraic		118
154	$y_A$	у	output equation	algebraic		126

### 5 reactions

	var	symbol	documentation	type	units	eqs
147	$P_{NK}$	P_NK	reactions per node	projection		
38	$K^o{}_K$	Ко	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
155	B	Boltzmann	Boltzmann constant	constant	$kg  m^2  K^{-1}  s^{-2}$	
157	R	GasConstant	gas constant	constant	$kg  m^2  mol^{-1}  K^{-1}  s^{-2}$	127
158	$N_{K,KS}$	N_K_KS	stoichiometry	constant		
159	$N_{NK,KS}$	N_NK_KS	extended stoichiometrix matrix	constant		128
60	$T_{NK}$	T_NK	temperature of the reactive system	effort	K	39
151	$c_{NK,KS}$	С	concentration matrix reaction per node and species per reaction	secondaryState	$m^{-3}  mol$	123
152	$c^{o}{}_{NK,KS}$	со	norming concentration	secondaryState	$m^{-3}  mol$	124
153	$x_{NK,KS}$	x	matrix of normed, dimensionless mole fractions	secondaryState		125
160	$\phi_{NK}$	phi	probability function for reactions	secondaryState		129

### 6 material

	var	symbol	documentation	type	units	eqs
40	$\lambda_S$	Mm	species molecular mass	constant	$kg  mol^{-1}$	
112	ξ	additive	fraction of additives	constant		88
42	$C_{pN}$	Ср	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	$k^q{}_N$	kq	thermal conductivity	property	$kg K^{-1} s^{-3}$	26
48	$k_{xN}^c$	kc_x	convecitve mass conductivity in x-direction	property	$m^{-1} s$	27
49	$k_{yN}^c$	kc_y	convecitve mass conductivity in y-direction	property	$m^{-1} s$	28
50	$k_{zN}^c$	kc_z	convecitve mass conductivity in z-direction	property	$m^{-1} s$	29
51	$k^c{}_N$	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	$k^d_{NS}$	kd	diffusional mass condctivity	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	$ ho_N$	density	density	property	$kg m^{-3}$	38
115	$R^e{}_N$	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	$\hat{n}^d{}_{AS}$	fnd_AS	diffusional mass flow in a given stream	transport	$mol  s^{-1}$	68
94	$\hat{n}^d{}_{NS}$	fnd	net diffusional mass flow	transport	$mol  s^{-1}$	69
95	$\hat{H}^d{}_A$	fHd_A	enthalpy flow per diffusional mass stream	transport	$kg m^2 s^{-3}$	70
96	$\hat{H}^d{}_N$	fHd	net enthaply stream due to diffusion	transport	$kg m^2 s^{-3}$	71
97	$d_A$	d	flow direction of convectional flow	transport		72
102	$\hat{H}^{c}{}_{A}$	fHc_A	convective enthalpy flow for given stream	transport	$kg m^2 s^{-3}$	77
103	$\hat{H}^c{}_N$	fHc	net convectional 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	$H^o{}_N$	Но	initial enthalpy	state	$kg m^2 s^{-2}$	84
110	$n^o{}_{NS}$	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

	var	symbol	documentation	type	units	eqs
66	$c_{NS}$	С	molar composition	secondaryState	$m^{-3}  mol$	44
98	$c_{AS}$	c_AS	concentration in convectional flow	secondaryState	$m^{-3}  mol$	73
99	$\hat{n}^c{}_{AS}$	fnc_AS	molar convetional mass flow in the given stream	secondaryState	$mol  s^{-1}$	74
100	$\hat{n}^c{}_{NS}$	fnc	net molar convectional mass flow	secondaryState	$mol  s^{-1}$	75
126	$\phi$	intensities	collected intensities	secondaryState		106
128	$n^t{}_N$	nTotal	total number of moles	secondaryState	mol	107
101	$\dot{n}_{NS}$	dndt	differential species balance	diffState	$mol  s^{-1}$	76
108	$\dot{H}_N$	dHdt	differential enthalpy balance	diffState	$kgm^2s^{-3}$	83
118	$\dot{U}^e{}_N$	dUedt	Kirkhoff first law	diffState	$kg m^2 A^{-1} s^{-3}$	96 97
						98
113	$I_N$	i	electrical current definition	internalTransport	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	ξ	_additive	link variable additive to interface material $\gg > { m control}$	get		104

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

	var	symbol	documentation	type	units	eqs
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### 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
142	$Ue_N$	_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
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## macroscopic-reactions

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

### material-macroscopic

	var	symbol	documentation	type	units	eqs
41	$\lambda_S$	_Mm	link variable Mm to interface material »> macroscopic	get	$kgmol^{-1}$	20
74	$ ho_N$	_density	link variable density to interface material $\gg >$ 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	$\begin{array}{ c c c c c c } link \ variable \ kq \ x \ to \ interface \ material \ >> \ macroscopic \\ \end{array}$	get	$kg K^{-1} s^{-3}$	53
77	$Cv_N$	_Cv	$\begin{tabular}{ll} link variable Cv to interface material $> $ macroscopic \\ \end{tabular}$	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	$k^q{}_N$	_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	$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	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	$k^c{}_N$	_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 $\gg$ 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 $\gg >$ macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	65

	var	symbol	documentation	type	units	eqs
89	$k^d_{NS}$	_kd	link variable kd to interface material $\gg$ macroscopic	get	$kg^{-1}  m^{-4}  mol^2  s$	66
117	$R^e{}_N$	_elConductC	link variable elConductC to interface material »> macroscopic	get	$kg^{-1} m^{-2} A^2 s^3$	94
140	additive	_additive	$\begin{array}{c} \mbox{link variable additive to interface material } > \mbox{macroscopic} \\ \mbox{scopic} \end{array}$	get		112

### 32 macroscopic-material

	var	symbol	documentation	type	units	eqs
58	$m_N$	_m	link variable m to interface macroscopic $\gg >$ material	get	kg	37
114	$i_N$	_i	link variable i to interface macroscopic »> material	$\operatorname{get}$	A	90

# 33 Equations

### 34 Generic

no	equation	documentation	layer
1	1 := Instantiate(#, #)	numerical value 1	root
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
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	$\mu_{NS} := rac{\partial  U_N}{\partial  n_{NS}}$	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
14	$Ue_N := (C_N)^{-1} \cdot U_N$	electrical potential – voltage	physical
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	physical
21	$C_{pN} := \frac{\partial H_N}{\partial T_N}$	total heat capacity at constant pressure	material

no	equation	documentation	layer
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	$k^q{}_N := \operatorname{Stack}\left(k^q_{xN}, k^q_{yN}, k^q_{zN}\right)$	thermal conductivity	material
27	$k_{xN}^c := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convecitve mass conductivity in x-direction	material
28	$k_{yN}^c := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$	convecitve mass conductivity in y-direction	material
29	$k_{zN}^c := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convecitve mass conductivity in z-direction	material
30	$k^c{}_N := \operatorname{Stack}\left(k^c_{xN}, k^c_{yN}, k^c_{zN}\right)$	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
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

no	equation	documentation	layer
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
41	$E^a{}_{NK} := \text{Instantiate}(R . T_{NK}, \#)$	Arrhenius activation energy	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	$A_{yzN} := r_{yN} . r_{zN}$	cross sectional area yz	macroscopic
49	$A_{xzN} := r_{xN} \cdot r_{zN}$	cross sectional area xz	macroscopic
50	$A_{xyN} := r_{xN} . r_{yN}$	cross sectional area xy	macroscopic
67	$\hat{V}_A := \left(\rho_N\right)^{-1} \cdot k_{xN}^c \cdot A_{yzN} \cdot D_{N,A} \stackrel{N}{\star} p_N$	volumetric flow	macroscopic
68	$\hat{n}^d{}_{AS} := A_{yzN} \odot \left( -k^d_{xNS} \right) . D_{NS,AS} \overset{NS}{\star} \mu_{NS}$	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
70	$\hat{H}^d{}_A := \left(F_{NS,AS} \overset{NS}{\star} h_{NS}\right) \overset{S \in AS}{\star} \hat{n}^d{}_{AS}$	enthalpy flow per diffusional mass stream	macroscopic
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	$c_{AS} := (0.5 \cdot (F_{NS,AS} - d_A \odot  F_{NS,AS} )) \stackrel{NS}{\star} c_{NS}$	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

no	equation	documentation	layer
76	$\dot{n}_{NS} := \hat{n}^c{}_{NS} + \hat{n}^d{}_{NS}$	differential species balance	macroscopic
77	$\hat{H}^c{}_A := \left(F_{NS,AS} \overset{NS}{\star} h_{NS}\right) \overset{S \in AS}{\star} \hat{n}^c{}_{AS}$	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
79	$\hat{w}_A := \text{Instantiate}(\hat{H}^c{}_A, \#)$	sample work stream	macroscopic
80	$\hat{w}_N := F_{N,A} \overset{A}{\star} \hat{w}_A$	net work stream	macroscopic
81	$\hat{q}_{xA} := A_{yzN} \cdot k_{xN}^q \cdot D_{N,A} \stackrel{N}{\star} T_N$	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
84	$H^o{}_N := \text{Instantiate}(H_N, \#)$	initial enthalpy	macroscopic
85	$n^o{}_{NS} := \text{Instantiate}(n_{NS}, \#)$	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	$\xi := \operatorname{Instantiate}(\xi, \#)$	fraction of additives	material
89	$I_N := rac{d  C_N}{d  t}$	electrical current definition	macroscopic
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
93	$k^{e,\xi}{}_N := (R^e{}_N)^{-1} \cdot \xi$	simple model for the electrical conductivity as a function of the additive	material

no	equation	documentation	layer
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
98	$\dot{U}^e{}_N := \operatorname{Instantiate}(\dot{U}^e{}_N, 0)$	Kirkhoff first law	macroscopic
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
109	$xo_N := \text{Instantiate}(x_N, \#)$	initial state	control
	$\dot{x}_D := A_{N,D} \overset{N}{\star} x_N + B_{A,D} \overset{A}{\star} e_A$	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	$\check{\xi} := \xi$	measured additive fraction	control

no	equation	documentation	layer
117	$RComputed_N := (\check{I}_N)^{-1} . \check{U}^e{}_N$	measured resistance	control
118	$store := \operatorname{MixedStack}\left(\check{I}_N, \check{U}^e{}_N, RComputed_N, \check{\xi} \right)$	quantities to be stored	control
119	$y^o{}_A := \text{Instantiate}(y^o{}_A, \#)$	set point	control
123	$c_{NK,KS} := P_{NK} \cdot \left( P_{NS,KS} \overset{NS}{\star} c_{NS} \right)$	var doc :	reactions
124	$c^{o}_{NK,KS} := \text{Instantiate}(c_{NK,KS}, \#)$	norming concentration	reactions
125	$x_{NK,KS} := (c^o_{NK,KS})^{-1} \cdot c_{NK,KS}$	matrix of normed, dimensionless mole fractions	reactions
126	$y_A := C_{N,A} \stackrel{N}{\star} x_N + D_A \cdot e_A$	output equation	control
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

## 35 Interface Link Equation

no	equation	documentation	layer
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
54	$Cv_N := C_{VN}$	interface equation	material -> macro- scopic
55	$egin{aligned} k_{yN}^q := k_{yN}^q \end{aligned}$	interface equation	material -> macro- scopic
56	$k_{zN}^q := k_{zN}^q$	interface equation	material -> macro- scopic
57	$\left  \begin{array}{c} k^q{}_N := k^q{}_N \end{array} \right $	interface equation	material -> macro- scopic
58	$k_{xN}^c := k_{xN}^c$	interface equation	material -> macro- scopic

no	equation	documentation	layer
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
	$k_{xNS}^d := k_{xNS}^d$	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
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
104	$\xi := \xi$	interface equation	material -> control

no	equation	documentation	layer
105	$T_N := T_N$	interface equation	macroscopic -> control
112	$additive := \xi$	interface equation	material -> macro- scopic
114	$Ue_N := Ue_N$	interface equation	macroscopic -> control