

# 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		
162	$P_{N,NS}$	P_N_NS	projection of nodes onto the node 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	$mol^{-1}$	
17	$p_N$	p	thermodynamic pressure	effort	$kg\,m^{-1}\,s^{-2}$	6
18	$T_N$	T	temperature	effort	$K$	7

*Continued on next page*

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

## 4 control

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

## 5 reactions

	var	symbol	documentation	type	units	eqs
147	$P_{NK}$	P_NK	reactions per node	projection		
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
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	$c_{NK,KS}$	c	concentration matrix reaction per node and species per reaction	secondaryState	$m^{-3} mol$	123
152	$c^o_{NK,KS}$	co	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
163	$\tilde{n}_{NS}$	nProd	the species production term	secondaryState	$mol s^{-1}$	130

## 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	$\hat{H}_A^d$	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 convectional flow	transport		72
102	$\hat{H}_A^c$	fHc_A	convective enthalpy flow for given stream	transport	$kg m^2 s^{-3}$	77
103	$\hat{H}_N^c$	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	$H_N^o$	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	$\mapsto \xi$	<code>_additive</code>	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	$I_N$	<code>_i</code>	link variable i to interface macroscopic »> control	get	$A$	99
125	$T_N$	<code>_T</code>	link variable T to interface macroscopic »> control	get	$K$	105
142	$Ue_N$	<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	$\tilde{n}_{NS}$	_nProd	link variable nProd to interface reactions »> macroscopic	get	$mol\ s^{-1}$	131

## 30 macroscopic-reactions

	var	symbol	documentation	type	units	eqs
67	$c_{NS}$	<code>_c</code>	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	$C_{vN}^v$	_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	$C_{pN}$	_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	$k^d_{NS}$	<code>_kd</code>	link variable kd to interface material »> macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	66
117	$R^e_N$	<code>_elConductC</code>	link variable elConductC to interface material »> macroscopic	get	$kg^{-1} m^{-2} A^2 s^3$	94
140	$\xi$	<code>_additive</code>	link variable additive to interface material »> macroscopic	get		112

## 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
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
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
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

*Continued on next page*

no	equation	documentation	layer
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
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	$T_{NK} := P_{N,NK} \star^N T_N$	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

Continued on next page

no	equation	documentation	layer
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	$\hat{V}_A := (\rho_N)^{-1} \cdot k_{xN}^c \cdot A_{yzN} \cdot D_{N,A} \star^N p_N$	volumetric flow	macroscopic
68	$\hat{n}_{AS}^d := A_{yzN} \odot (-k_{xNS}^d) \cdot D_{NS,AS} \star^{NS} \mu_{NS}$	diffusional mass flow in a given stream	macroscopic
69	$\hat{n}_{NS}^d := F_{NS,AS} \star^{AS} \hat{n}_{AS}^d$	net diffusional mass flow	macroscopic
70	$\hat{H}_A^d := \left( F_{NS,AS} \star^{NS} h_{NS} \right) \star^{S \in AS} \hat{n}_{AS}^d$	enthalpy flow per diffusional mass stream	macroscopic
71	$\hat{H}_N^d := F_{N,A} \star^A \hat{H}_A^d$	net enthaply stream due to diffusion	macroscopic
72	$d_A := \text{sign} \left( F_{N,A} \star^N p_N \right)$	flow direction of convectional flow	macroscopic
73	$c_{AS} := (0.5 \cdot (F_{NS,AS} - d_A \odot  F_{NS,AS} )) \star^{NS} c_{NS}$	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	$\hat{n}_{NS}^c := F_{NS,AS} \star^{AS} \hat{n}_{AS}^c$	net molar convectional mass flow	macroscopic
76	$\dot{n}_{NS} := \hat{n}_{NS}^c + \hat{n}_{NS}^d + \tilde{n}_{NS}$	differential species balance	macroscopic
77	$\hat{H}_A^c := \left( F_{NS,AS} \star^{NS} h_{NS} \right) \star^{S \in AS} \hat{n}_{AS}^c$	convective enthalpy flow for given stream	macroscopic
78	$\hat{H}_N^c := F_{N,A} \star^A \hat{H}_A^c$	net convectional enthalpy stream	macroscopic
80	$\hat{w}_N := F_{N,A} \star^A \hat{w}_A$	net work stream	macroscopic
81	$\hat{q}_{xA} := A_{yzN} \cdot k_{xN}^q \cdot D_{N,A} \star^N T_N$	heat flow in x-direction for given stream	macroscopic
82	$\hat{q}_N := F_{N,A} \star^A \hat{q}_{xA}$	net heat flow	macroscopic

Continued on next page

no	equation	documentation	layer
83	$\dot{H}_N := \hat{H}^c_N + \hat{H}^d_N + \hat{q}_N + \hat{w}_N$	differential enthalpy balance	macroscopic
86	$n_{NS} := \int_{t^o}^{t^e} \dot{n}_{NS} \, dt$	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
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	$Ue_N := (R^e_N)^{-1} \cdot I_N$	electrical potential – voltage	macroscopic
96	$\dot{U}^e_N := 1 \cdot Ue_N$	Kirkhoff first law	macroscopic
97	$\dot{U}^e_N := \text{Root}(Ue_N)$	Kirkhoff first law	macroscopic
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
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

*Continued on next page*

no	equation	documentation	layer
115	$\check{U}_N^e := U e_N$	measured electrical potential	control
116	$\check{\xi} := \mapsto \xi$	measured additive fraction	control
117	$R_N := (\check{I}_N)^{-1} \cdot \check{U}_N^e$	measured resistance	control
118	$S := \text{MixedStack}(\check{I}_N, \check{U}_N^e, R_N, \check{\xi})$	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	$x_{NK,KS} := (c_{NK,KS}^o)^{-1} \cdot c_{NK,KS}$	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
127	$R := A^v \cdot B$	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	$\tilde{n}_{NS} := V_N \overset{N}{\star} \left( P_{N,NK} \overset{NK}{\star} \left( (K_{NK} \cdot \phi_{NK}) \cdot \left( P_{NS,KS} \overset{KS}{\star} N_{NK,KS} \right) \right) \right)$	the species production term	reactions

## 35 Instantiate

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
41	$E^a_{NK} := \text{Instantiate}(R.T_{NK}, \#)$	Arrhenius activation energy	reactions
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
109	$xo_N := \text{Instantiate}(x_N, \#)$	initial state	control
119	$y^o_A := \text{Instantiate}(y^o_A, \#)$	set point	control

*Continued on next page*



no	equation	documentation	layer
124	$c^o_{NK,KS} := \text{Instantiate}(c_{NK,KS}, \#)$	norming concentration	reactions

## 36 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	$C^{v_N} := C^{v_N}$	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	$CP_N := C_{pN}$	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
66	$k_{NS}^d := k_{NS}^d$	interface equation	material → macroscopic
90	$I_N := I_N$	interface equation	macroscopic → material
94	$R_N^e := k_N^{e,\xi}$	interface equation	material → macroscopic
99	$I_N := I_N$	interface equation	macroscopic → control
104	$\mapsto \xi := \xi$	interface equation	material → control

*Continued on next page*

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