

# 1 Variables

## 2 root

	var	symbol	documentation	type	units	tokens	eqs
1	$F_{N,A}$	<b>F</b>	incidence matrix of directed graph	network		[]	
2	$t$	<b>t</b>	time	frame	$s$	[]	
3	$\#$	<b>value</b>	numerical value	constant		[]	
4	1	<b>one</b>	numerical value 1	constant		[]	1
5	0	<b>zero</b>	numerical value 0	constant		[]	2
6	1/2	<b>onehalf</b>	numerical value 1/2	constant		[]	3
58	$t^o$	<b>to</b>	starting time	constant	$s$	[]	41
59	$t^e$	<b>te</b>	end time	constant	$s$	[]	42

## 3 physical

	var	symbol	documentation	type	units	tokens	eqs
15	$r_{xN}$	<b>r_x</b>	x-coordinate	frame	$m$	[]	
16	$r_{yN}$	<b>r_y</b>	y-coordinate	frame	$m$	[]	
17	$r_{zN}$	<b>r_z</b>	z-coordinate	frame	$m$	[]	
18	$n_{NS}$	<b>n</b>	foundation state – species mass	state	$mol$	[]	119
19	$U_N$	<b>U</b>	foundation state – internal energy	state	$kg\,m^2\,s^{-2}$	[]	
20	$S_N$	<b>S</b>	foundation state – entropy	state	$kg\,m^2\,K^{-1}\,s^{-2}$	[]	
21	$V_N$	<b>V</b>	foundation state – volume	state	$m^3$	[]	
29	$H_N$	<b>H</b>	enthalpy	state	$kg\,m^2\,s^{-2}$	[]	13 122
30	$A_N$	<b>A</b>	Helmholtz energy	state	$kg\,m^2\,s^{-2}$	[]	14

*Continued on next page*

	var	symbol	documentation	type	units	tokens	eqs
31	$G_N$	G	Gibbs energy	state	$kg\,m^2\,s^{-2}$	[]	15
27	$B_N$	B	Boltzmann constant	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	[]	11
101	$A^v_N$	Av	Avogadro number	constant	$mol^{-1}$	[]	
102	$R_N$	R	Gas constant	constant	$kg\,m^2\,mol^{-1}\,K^{-1}\,s^{-2}$	[]	82
22	$p_N$	p	thermodynamic pressure	effort	$kg\,m^{-1}\,s^{-2}$	[]	7
23	$T_N$	T	temperature	effort	$K$	[]	8
24	$\mu_{NS}$	chem_potential	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	[]	9
36	$v_{xN}$	v_x	velocity in x-direction	secondaryState	$ms^{-1}$	[]	20
37	$v_{yN}$	v_y	velocity in y-direction	secondaryState	$ms^{-1}$	[]	21
38	$v_{zN}$	v_z	velocity in z-direction	secondaryState	$ms^{-1}$	[]	22
39	$v_N$	v	velocity vector	secondaryState	$ms^{-1}$	[]	23

## 4 control

	var	symbol	documentation	type	units	tokens	eqs
141	$x_N$	x	state	state		[]	131
142	$x_{oN}$	xo	initial state	state		[]	123
153	$u_A$	u	controller input	state		[]	128
139	$A_{N,D}$	A	dynamic matrix	constant	$s^{-1}$	[]	
140	$B_{A,D}$	B	input gain matrix	constant	$s^{-1}$	[]	
156	$I_{NDN,D}$	I_N_D	map D $\rightarrow$ N – used in integration	constant		[]	
155	$dxdt_D$	dxdt	controller dynamics	diffState	$s^{-1}$	[]	130

## 5 reactions

	var	symbol	documentation	type	units	tokens	eqs
98	$N_{S,K}$	N	stoichiometric matrix	constant		[]	
104	$E_{a,NK}$	Ea	Arrhenius's activation energy	constant	$kg\ m^2\ mol^{-1}\ s^{-2}$	[]	84
105	$K^o_K$	Ko	Arrhenius's frequency factor	constant	$m^{-3}\ mol\ s^{-1}$	[]	
108	$c^o_{KS}$	co_KS	standardisation of concentration	constant	$m^{-3}\ mol$	[]	87
106	$K_{NK}$	K_NK	Arrhenius reaction constants	secondaryState	$m^{-3}\ mol\ s^{-1}$	[]	85
109	$\phi_{KS}$	phi_KS	propabilities to meet	secondaryState		[]	88

## 6 material

	var	symbol	documentation	type	units	tokens	eqs
40	$\lambda_S$	Mm	species molecular masses	constant	$kg\ mol^{-1}$	[]	
41	$C_{pN}$	Cp	total heat capacity at constant pressure	constant	$kg\ m^2\ K^{-1}\ s^{-2}$	[]	24
42	$C_{vN}$	Cv	total heat capacity at constant volume	constant	$kg\ m^2\ K^{-1}\ s^{-2}$	[]	25
43	$c_{pS}$	cp	specific heat capacity at constant pressure	constant	$m^2\ mol^2\ K^{-1}\ s^{-2}$	[]	26
44	$c_{vS}$	cv	specific heat capacity at constant volume	constant	$m^2\ mol^2\ K^{-1}\ s^{-2}$	[]	27
45	$k^q_{xN}$	kq_x	thermal conductivity in x-direction	secondaryState	$kg\ K^{-1}\ s^{-3}$	[]	28
46	$k^q_{yN}$	kq_y	thermal conductivity in y-direction	secondaryState	$kg\ K^{-1}\ s^{-3}$	[]	29
47	$k^q_{zN}$	kq_z	thermal conductivity in z-direction	secondaryState	$kg\ K^{-1}\ s^{-3}$	[]	30
48	$k^q_N$	kq	Cartesian thermal conductivity vector	secondaryState	$kg\ K^{-1}\ s^{-3}$	[]	31
49	$k^c_{xN}$	kc_x	convective mass convectivity in x-direction	secondaryState	$m^{-1}\ s$	[]	32
50	$k^c_{yN}$	kc_y	convective mass convectivity in y-direction	secondaryState	$m^{-1}\ s$	[]	33
51	$k^c_{zN}$	kc_z	convective mass convectivity in z-direction	secondaryState	$m^{-1}\ s$	[]	34
52	$k^c_N$	kc	Cartesian convective mass convectivity vector	secondaryState	$m^{-1}\ s$	[]	35
53	$k^d_{xNS}$	kd_x	diffusional mass conductivity in x-direction	secondaryState	$kg^{-1}\ m^{-4}\ mol^2\ s$	[]	36
54	$k^d_{yNS}$	kd_y	diffusional mass conductivity in y-direction	secondaryState	$kg^{-1}\ m^{-4}\ mol^2\ s$	[]	37

*Continued on next page*

	var	symbol	documentation	type	units	tokens	eqs
55	$k_{zNS}^d$	kd_z	diffusional mass conductivity in z-direction	secondaryState	$kg^{-1} m^{-4} mol^2 s$	[]	38
56	$k_{NS}^d$	kd	Cartesian diffusional mass conductivity vector	secondaryState	$kg^{-1} m^{-4} mol^2 s$	[]	39
60	$h_{NS}$	h	partial molar enthalpies	secondaryState	$kg m^2 mol^{-1} s^{-2}$	[]	43

## 7 macroscopic

	var	symbol	documentation	type	units	tokens	eqs
78	$d_A$	d	direction of convective flow	transport		[]	61
80	$A_{y,zN}$	Ayz	cross sectional area in x-direction	transport	$m^2$	[]	63
83	$\hat{V}_A$	fV	convective volumetric flow	transport	$m^3 s^{-1}$	[]	66
84	$c_{AS}$	c_AS	molar species concentration in convective flow	transport	$m^{-3} mol$	[]	67
85	$\hat{n}_{AS}^c$	fnc_AS	convective mass flow by stream	transport	$mol s^{-1}$	[]	68
86	$\hat{n}_{NS}^c$	fnc	net convective mass flow	transport	$mol s^{-1}$	[]	69
115	$\hat{m}_A$	fm_A	mass flow in arc	transport	$kg s^{-1}$	[]	94
125	$\hat{H}_A^c$	fHc_A	enthalpy flow due to convection	transport	$kg m^2 s^{-3}$	[]	104
127	$\hat{H}_N^c$	fHc	net enthalpy flow due to convection	transport	$kg m^2 s^{-3}$	[]	106
128	$\hat{n}_{AS}^d$	fnd_AS	diffusional mass transfer in arc	transport	$mol s^{-1}$	[]	107
129	$\hat{n}_{NS}^d$	fnd	net diffusional mass transfer	transport	$mol s^{-1}$	[]	108
130	$\hat{H}_A^d$	fHd_A	enthalpy flow due to mass diffusion	transport	$kg m^2 s^{-3}$	[]	109
131	$\hat{H}_N^d$	fHd	net enthalpy flow due to diffusion	transport	$kg m^2 s^{-3}$	[]	110
135	$\hat{w}_A$	fw_A	example of work flow	transport	$kg m^2 s^{-3}$	[]	114
136	$\hat{w}_N$	fw	net work flow	transport	$kg m^2 s^{-3}$	[]	115
10	$F_{NS,AS}$	F_NS_AS	block incidence matrix of directed species graph	network		[]	6
9	$P_{NS,AS}$	P_NS_AS	node species to arc species projection	projection		[]	

*Continued on next page*

	var	symbol	documentation	type	units	tokens	eqs
11	$P_{K,NK}$	P_K_NK	projection of conversion to node x conversion	projection		[]	
12	$P_{S,NS}$	P_S_NS	projection species to conversion x species	projection		[]	
13	$P_{N,NK}$	P_N_NK	projection node to node x conversion	projection		[]	
14	$P_{NK,KS}$	P_NK_KS	projection node x conversion to conversion x species	projection		[]	
95	$P_{NS,KS}$	P_NS_KS	projection node x species to conversion x species	projection		[]	
137	$n^o_{NS}$	no	initial condition for species mass	state	$mol$	[]	118
138	$H^o_N$	Ho	initial condition for enthalpy	state	$kg\ m^2\ s^{-2}$	[]	120
92	$1_{NK}$	one_NK	one with energy	effort		[]	75
79	$c_{NS}$	c	molar concentration	seconaryState	$m^{-3}\ mol$	[]	62
81	$m_N$	m	mass in kg	seconaryState	$kg$	[]	64
82	$\rho_N$	density	density	seconaryState	$kg\ m^{-3}$	[]	65
91	$T_{NK}$	T_NK	temperature in reactive systems	conversion	$K$	[]	74
96	$c_{KS}$	c_KS	concentration in the reactive systems	conversion	$m^{-3}\ mol$	[]	78
112	$\xi_{NK}$	xi	extent of reaction	conversion	$m^{-3}\ mol\ s^{-1}$	[]	91
113	$N_{NS,NK}$	N_NS_NK	extended stoichiometry	conversion		[]	92
114	$\tilde{n}_{NS}$	pn	production term	conversion	$mol\ s^{-1}$	[]	93
132	$\dot{n}_{NS}$	dndt	species mass accumulation	diffState	$mol\ s^{-1}$	[]	111
133	$\dot{H}_N$	dHdt	differential enthalpy balance	diffState	$kg\ m^2\ s^{-3}$	[]	116

## 8 solid

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

## 9 fluid

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

## 10 liquid

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

## 11 gas

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

## 12 control-reactions

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

## 13 reactions-control

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

## 14 control-material

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

## 15 material-control

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

## 16 control–macroscopic

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

## 17 macroscopic–control

	var	symbol	documentation	type	units	tokens	eqs
143	$T_{nN}$	T_n	norming temperature	constant	$K$	[]	
144	$p_{nN}$	p_n	norming pressure	constant	$kg\ m^{-1}\ s^{-2}$	[]	
145	$c_{nNS}$	c_n	norming concentration	constant	$m^{-3}\ mol$	[]	
146	$F_{NAN,A}$	F_N_A	projection N → A	constant		[]	
151	$F_{ANS_{A,NS}}$	F_A_NS	projection NS → A	constant		[]	
148	$s_{TA}$	s_T	normed temperature signal	transform		[]	125
149	$s_{pA}$	s_p	normed pressure signal	transform		[]	126
152	$s_{cA}$	s_c	normed concentration signal vector	transform		[]	127

## 18 reactions–material

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

## 19 material–reactions

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

## 20 reactions–macroscopic

	var	symbol	documentation	type	units	tokens	eqs
107	$K_{NK}$	K_NK	link	transform	$m^{-3} mol s^{-1}$	[]	86
110	$\phi_{KS}$	phi_KS	link	transform		[]	89
111	$N_{S,K}$	N	link	transform		[]	90

## 21 macroscopic–reactions

	var	symbol	documentation	type	units	tokens	eqs
94	$T_{NK}$	T_NK	temperature of reactive systems	transform	$K$	[]	77
97	$c_{KS}$	c_KS	link	transform	$m^{-3} mol$	[]	79
103	$P_{N,NK}$	P_N_NK	link	transform		[]	83

## 22 material–macroscopic

	var	symbol	documentation	type	units	tokens	eqs
61	$\lambda_S$	Mm	link to molar masses	transform	$kg mol^{-1}$	[]	44
62	$k_{xN}^q$	kq_x	link	transform	$kg K^{-1} s^{-3}$	[]	45
63	$k_{yN}^q$	kq_y	link	transform		[]	46
64	$k_{zN}^q$	kq_z	link	transform		[]	47
65	$k_N^q$	kq	link	transform	$kg K^{-1} s^{-3}$	[]	48
66	$k_{xN}^c$	kc_x	link	transform		[]	49

Continued on next page



	var	symbol	documentation	type	units	tokens	eqs
67	$k_{yN}^c$	kc_y	link	transform	$m^{-1} s$	[]	50
68	$k_{zN}^c$	kc_z	link	transform	$m^{-1} s$	[]	51
69	$k_N^c$	kc	link	transform	$m^{-1} s$	[]	52
70	$k_{xNS}^d$	kd_x	link	transform	$kg^{-1} m^{-4} mol^2 s$	[]	53
73	$k_{yNS}^d$	kd_y	link	transform	$kg^{-1} m^{-4} mol^2 s$	[]	56
74	$k_{zNS}^d$	kd_z	link	transform	$kg^{-1} m^{-4} mol^2 s$	[]	57
75	$k_{NS}^d$	kd	link	transform	$kg^{-1} m^{-4} mol^2 s$	[]	58
76	$c_{pS}$	cp	link	transform	$m^2 mol^2 K^{-1} s^{-2}$	[]	59
77	$c_{vS}$	cv	link	transform	$m^2 mol^2 K^{-1} s^{-2}$	[]	60
119	$h_{NS}$	h	link	transform	$kg m^2 mol^{-1} s^{-2}$	[]	98

## 23 macroscopic–material

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

## 24 gas–liquid

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

## 25 gas–solid

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

## 26 liquid–solid

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

## 27 Equations

### 27.1 Model equations

no	equation	documentation	layer
1	$1 := Set(\#, \#)$	numerical value 1	root
2	$0 := Set(\#, \#)$	numerical value 1	root
3	$1/2 := Set(\#, \#)$	numerical value 1/2	root
6	$F_{NS,AS} := F_{N,A} \odot P_{NS,AS}$	blick incidence matrix of directed species graph	physical
7	$p_N := \frac{\partial U_N}{\partial V_N}$	thermodynamic pressure	physical
8	$T_N := \frac{\partial U_N}{\partial S_N}$	temperature	physical
9	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	chemical potential	physical
11	$B_N := Set(S_N, \#)$	Boltzmann constant	physical
13	$H_N := U_N + p_N \cdot V_N$	enthalpy	physical
14	$A_N := U_N - T_N \cdot S_N$	Helmholtz energy	physical
15	$G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$	Gibbs energy	physical
20	$v_{xN} := \frac{\partial r_{xN}}{\partial t}$	velocity in x-direction	physical
21	$v_{yN} := \frac{\partial r_{yN}}{\partial t}$	velocity in y-direction	physical
22	$v_{zN} := \frac{\partial r_{zN}}{\partial t}$	velocity in z-direction	physical
23	$v_N := Stack(v_{xN}, v_{yN}, v_{zN})$	velocity vector	physical

*Continued on next page*

no	equation	documentation	layer
24	$C_{pN} := \frac{\partial H_N}{\partial T_N}$	total heat capacity at constant pressure	material
25	$C_{vN} := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	material
26	$c_{pS} := C_{pN} \cdot (\lambda_S)^{-1} \stackrel{N \in NS}{\star} n_{NS}$	specific heat capacity at constant pressure	material
27	$c_{vS} := C_{vN} \cdot (\lambda_S)^{-1} \stackrel{N \in NS}{\star} n_{NS}$	specific heat capacity at constant volume	material
28	$k_{xN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}$	thermal conductivity in x-direction	material
29	$k_{yN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{yN}$	thermal conductivity in y-direction	material
30	$k_{zN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{zN}$	thermal conductivity in z-direction	material
31	$k_N^q := Stack(k_{xN}^q, k_{yN}^q, k_{zN}^q)$	Cartesian thermal conductivity vector	material
32	$k_{xN}^c := \left( \lambda_S \stackrel{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass conductivity in x-direction	material
33	$k_{yN}^c := \left( \lambda_S \stackrel{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$	convective mass conductivity in y-direction	material
34	$k_{zN}^c := \left( \lambda_S \stackrel{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convective mass conductivity in z-direction	material
35	$k_N^c := Stack(k_{xN}^c, k_{yN}^c, k_{zN}^c)$	Cartesian convective mass conductivity vector	material
36	$k_{xNS}^d := (\mu_{NS})^{-1} \cdot \left( v_{xN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in x-direction	material
37	$k_{yNS}^d := (\mu_{NS})^{-1} \cdot \left( v_{yN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in y-direction	material

Continued on next page

no	equation	documentation	layer
38	$k_{zNS}^d := (\mu_{NS})^{-1} \cdot \left( v_{zN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in z-direction	material
39	$k_{NS}^d := Stack \left( k_{xNS}^d, k_{yNS}^d, k_{zNS}^d \right)$	Cartesian diffusional mass conductivity vector	material
41	$t^o := Set(t, t)$	starting time	root
42	$t^e := Set(t, t)$	end time	root
43	$h_{NS} := H_N \odot (n_{NS})^{-1}$	partial molar enthalpies	material
44	$\lambda_S := \lambda_S$	link to molar masses	material » > macroscopic
45	$k_{xN}^q := k_{xN}^q$	link	material » > macroscopic
46	$k_{yN}^q := k_{yN}^q$	link	material » > macroscopic
47	$k_{zN}^q := k_{zN}^q$	link	material » > macroscopic
48	$k_N^q := k_N^q$	link	material » > macroscopic
49	$k_{xN}^c := k_{xN}^c$	link	material » > macroscopic
50	$k_{yN}^c := k_{yN}^c$	link	material » > macroscopic
51	$k_{zN}^c := k_{zN}^c$	link	material » > macroscopic

*Continued on next page*

no	equation	documentation	layer
52	$k_N^c := k_N^c$	link	material » macroscopic
53	$k_{xNS}^d := k_{xNS}^d$	link	material » macroscopic
56	$k_{yNS}^d := k_{yNS}^d$	link	material » macroscopic
57	$k_{zNS}^d := k_{zNS}^d$	link	material » macroscopic
58	$k_{NS}^d := k_{NS}^d$	link	material » macroscopic
59	$c_{pS} := c_{pS}$	link	material » macroscopic
60	$c_{vS} := c_{vS}$	link	material » macroscopic
61	$d_A := \text{sign} \left( F_{N,A} \overset{N}{\star} p_N \right)$	direction of convective flow	macroscopic
62	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar concentration	macroscopic
63	$A_{y,zN} := r_{yN} \cdot r_{zN}$	cross sectional area in x-direction	macroscopic
64	$m_N := \lambda_S \overset{S \in NS}{\star} n_{NS}$	mass in kg	macroscopic
65	$\rho_N := (V_N)^{-1} \cdot m_N$	density	macroscopic
66	$\hat{V}_A := (\rho_N)^{-1} \cdot k_{xN}^c \cdot A_{y,zN} \cdot F_{N,A} \overset{N}{\star} p_N$	convective volumetric flow	macroscopic
67	$c_{AS} := (1/2 \cdot (F_{NS,AS} - d_A \odot  F_{NS,AS} )) \overset{NS}{\star} c_{NS}$	molar species concentration in convective flow	macroscopic

*Continued on next page*

no	equation	documentation	layer
68	$\hat{n}_{AS}^c := \hat{V}_A \odot c_{AS}$	convective mass flow by stream	macroscopic
69	$\hat{n}_{NS}^c := F_{NS,AS} \overset{AS}{\star} \hat{n}_{AS}^c$	net convective mass flow	macroscopic
74	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature in reactive systems	macroscopic
75	$1_{NK} := (T_{NK})^{-1} \cdot T_{NK}$	one with energy	macroscopic
77	$T_{NK} := T_{NK}$	temperature of reactive systems	macroscopic » > reactions
78	$c_{KS} := c_{NS} \overset{NS}{\star} P_{NS,KS}$	concentration in the reactive systems	macroscopic
79	$c_{KS} := c_{KS}$	link	macroscopic » > reactions
82	$R_N := A^v_N \cdot B_N$	Gas constant	physical
83	$P_{N,NK} := P_{N,NK}$	link	macroscopic » > reactions
84	$E_{a_{NK}} := Set(P_{N,NK} \overset{N}{\star} R_N \cdot T_{NK}, \#)$	Arrhenius's activation energy	reactions
85	$K_{NK} := K^o_K \odot exp((-E_{a_{NK}}) \cdot (R_N \overset{N}{\star} P_{N,NK} \cdot T_{NK})^{-1})$	Arrhenius reaction constants	reactions
86	$K_{NK} := K_{NK}$	link	reactions » > macroscopic
87	$c^o_{KS} := Set(c_{KS}, \#)$	standardisation of concentration	reactions
88	$\phi_{KS} := \prod (c_{KS} \cdot (c^o_{KS})^{-1})$	propabilities to meet	reactions
89	$\phi_{KS} := \phi_{KS}$	link	reactions » > macroscopic

*Continued on next page*

no	equation	documentation	layer
90	$N_{S,K} := N_{S,K}$	link	reactions »> macroscopic
91	$\xi_{NK} := K_{NK} \cdot P_{NK,KS} \star^{KS} \phi_{KS}$	extent of reaction	macroscopic
92	$N_{NS,NK} := P_{S,NS} \star^S \left( \left( P_{K,NK} \cdot T_{NK} \cdot (T_{NK})^{-1} \right) \star^K N_{S,K} \right)$	extended stoichiometry	macroscopic
93	$\tilde{n}_{NS} := V_N \odot \left( N_{NS,NK} \star^{NK} \xi_{NK} \right)$	production term	macroscopic
94	$\hat{m}_A := \lambda_S \star^{S \in AS} \hat{n}_{AS}^c$	mass flow in arc	macroscopic
98	$h_{NS} := h_{NS}$	link	material »> macroscopic
104	$\hat{H}_A^c := \left( F_{NS,AS} \star^{NS} h_{NS} \right) \star^{S \in AS} \hat{n}_{AS}^c$	enthalpy flow due to convection	macroscopic
106	$\hat{H}_N^c := F_{N,A} \star^A \hat{H}_A^c$	net enthalpy flow due to convection	macroscopic
107	$\hat{n}_{AS}^d := A_{y,z_N} \odot \left( -k_{xNS}^d \right) \cdot F_{NS,AS} \star^{NS} \mu_{NS}$	diffusional mass transfer in arc	macroscopic
108	$\hat{n}_{NS}^d := F_{NS,AS} \star^{AS} \hat{n}_{AS}^d$	net diffusional mass transfer	macroscopic
109	$\hat{H}_A^d := \left( F_{NS,AS} \star^{NS} h_{NS} \right) \star^{S \in AS} \hat{n}_{AS}^d$	enthalpy flow due to mass diffusion	macroscopic
110	$\hat{H}_N^d := F_{N,A} \star^A \hat{H}_A^d$	net enthalpy flow due to diffusion	macroscopic
111	$\dot{n}_{NS} := \hat{n}_{NS}^c + \hat{n}_{NS}^d + \tilde{n}_{NS}$	species mass accumulation	macroscopic

Continued on next page



no	equation	documentation	layer
114	$\hat{w}_A := Set(\hat{H}_A^c, \#)$	example of work flow	macroscopic
115	$\hat{w}_N := F_{N,A} \overset{A}{\star} \hat{w}_A$	net work flow	macroscopic
116	$\dot{H}_N := \hat{H}_N^c + \hat{H}_N^d + \hat{w}_N$	differential enthalpy balance	macroscopic
118	$n_{NS}^o := Set(n_{NS}, \#)$	initial condition for species mass	macroscopic
119	$n_{NS} := \int_{t^o}^{t^e} \dot{n}_{NS} dt + n_{NS}^o$	foundation state – species mass	macroscopic
120	$H_N^o := Set(H_N, \#)$	initial condition for enthalpy	macroscopic
122	$H_N := \int_{t^o}^{t^e} \dot{H}_N dt + H_N^o$	enthalpy	macroscopic
123	$xo_N := Set(x_N, \#)$	initial state	control
125	$s_{TA} := F_{NAN,A} \overset{N}{\star} \left( T_N \cdot (T_{nN})^{-1} \right)$	normed temperature signal	macroscopic control » >
126	$s_{pA} := F_{NAN,A} \overset{N}{\star} \left( p_N \cdot (p_{nN})^{-1} \right)$	normed pressure signal	macroscopic control » >
127	$s_{cA} := F_{ANS,A,NS} \overset{NS}{\star} \left( c_{NS} \cdot (c_{nNS})^{-1} \right)$	normed concentration signal vector	macroscopic control » >
128	$u_A := Stack(s_{TA}, s_{pA}, s_{cA})$	controller input	control

*Continued on next page*

no	equation	documentation	layer
130	$dxdt_D := A_{N,D} \overset{N}{\star} x_N + B_{A,D} \overset{A}{\star} u_A$	controller dynamics	control
131	$x_N := \int_{t_o}^{t_e} I_{NDN,D} \overset{D}{\star} dxdt_D \, dt$	state	control