1 Variables

2 root

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

3 physical

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

	var	symbol	documentation	type	units	$_{ m tokens}$	eqs
31	G_N	G	Gibbs energy	state	$kg m^2 s^{-2}$		15
27	B_N	В	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} $ $ kg m^{-1} s^{-2} $		82
22	p_N	p	thermodynamic pressure	effort	$kg m^{-1} s^{-2}$		7
23	T_N	Т	temperature	effort	K		8
24	μ_{NS}	chem_potential	chemical potential	effort	$kg m^2 mol^{-1} s^{-2}$		9
36	v_{xN}	v_x	velocity in x-direction	seconaryState	ms^{-1}		20
37	v_{y_N}	v_y	velocity in y-direction	seconaryState	ms^{-1}		21
38	v_{zN}	v_z	velocity in z-direction	seconaryState	ms^{-1}		22
39	v_N	v	velocity vector	seconaryState	ms^{-1}	[]	23

4 control

	var	symbol	documentation	type	units	tokens	eqs
141	x_N	х	state	state			131
142	xo_N	хо	initial state	state			123
139	$A_{N,D}$	A	dynamic matrix	constant	s^{-1}		
140	$B_{A,D}$	В	input gain matrix	constant	s^{-1}		
156	$I_{N,D}$	I_N_D	map D \rightarrow N – used in integration	constant			
157	u_{sA}	u_s	setpoint in terms of the measurement	constant			
158	T_{IN}	T_I	integrator time constant	constant	s		
155	\dot{x}_D	dxdt	controller dynamics	diffState	s^{-1}		130
153	u_A	u	controller input	input			128

5 reactions

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

6 material

	var	symbol	documentation	type	units	tokens	eqs
40	λ_S	Mm	species molecular masses	constant	$kg mol^{-1}$	[]	
41	C_{p_N}	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_{p_S}	ср	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_{xN}^q	kq_x	thermal conductivity in x-direction	seconaryState	$kg K^{-1} s^{-3}$		28
46	$k^q_{y_N}$	kq_y	thermal conductivity in y-direction	seconaryState	$kg K^{-1} s^{-3}$		29
47	k_{zN}^q	kq_z	thermal conductivity in z-direction	seconaryState	$kg K^{-1} s^{-3}$		30
48	$k^q{}_N$	kq	Carthesian thermal conductivity vector	seconaryState	$kg K^{-1} s^{-3}$		31
49	k_{xN}^c	kc_x	convective mass convectivity in x-direction	seconaryState	$m^{-1} s$		32
50	$k^c_{y_N}$	kc_y	convective mass convectivity in y-direction	seconaryState	$m^{-1} s$		33
51	k_{zN}^c	kc_z	convective mass convectivity in z-direction	seconaryState	$m^{-1} s$		34
52	$k^c{}_N$	kc	Cartesian convective mass convectivity vector	seconaryState	$m^{-1} s$		35

	var	symbol	documentation	type	units	tokens	eqs
53	k_{xNS}^d	kd_x	diffusional mass conductivity in x-direction	seconaryState	$kg^{-1} m^{-4} mol^2 s$		36
54	$k^d_{y_{NS}}$	kd_y	diffusional mass conductivity in y-direction	${\bf seconary State}$	$kg^{-1} m^{-4} mol^2 s$		37
55	k_{zNS}^d	kd_z	diffusional mass conductivity in z-direction	${\bf seconary State}$	$kg^{-1} m^{-4} mol^2 s$		38
56	k^d_{NS}	kd	Cartesian diffusional mass conductivity vector	${\rm seconaryState}$	$kg^{-1} m^{-4} mol^2 s$		39
60	h_{NS}	h	partial molar enthalpies	${\bf seconaryState}$	$kg m^2 mol^{-1} s^{-2}$		43

7 macroscopic

	var	symbol	documentation	type	units	tokens	eqs
78	d_A	d	direction of convective flow	transport			61
80	A_{y,z_N}	Ayz	cross sectional area in x-direction	$\operatorname{transport}$	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	${ m transport}$	$m^{-3} mol$		67
85	\hat{n}_{AS}^c	fnc_AS	convective mass flow by stream	transport	$\mod s^{-1}$		68
86	\hat{n}_{NS}^c	fnc	net convective mass flow	transport	$\mod s^{-1}$		69
115	\hat{m}_A	fm_A	mass flow in arc	transport	$kg s^{-1}$		94
125	\hat{H}^c_A	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	${ m transport}$	$kg m^2 s^{-3}$		106
128	\hat{n}_{AS}^d	fnd_AS	diffusional mass transfer in arc	${ m transport}$	$\mod s^{-1}$		107
129	\hat{n}_{NS}^d	fnd	net diffusional mass transfer	transport	$\mod s^{-1}$		108
130	\hat{H}^d_A	fHd_A	enthalpy flow due to mass diffusion	${ m transport}$	$kg m^2 s^{-3}$		109
131	\hat{H}_N^d	fHd	net enthalpy flow due to diffusion	${ m transport}$	$kg m^2 s^{-3}$		110
135	\hat{w}_A	fw_A	example of work flow	${ m transport}$	$kg m^2 s^{-3}$		114
136	\hat{w}_N	fw	net work flow	${ m transport}$	$kg m^2 s^{-3}$	[]	115

	var	symbol	documentation	type	units	tokens	eqs
10	$F_{NS,AS}$	F_NS_AS	blick incidence matrix of directed species graph	network			6
9	$P_{NS,AS}$	P_NS_AS	node species to arc species projection	projection			
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	$H^o{}_N$	Но	initial condition for enthalpy	state	$kg m^2 s^{-2}$		120
92	1_{NK}	one_NK	one with energy	effort			75
79	c_{NS}	С	molar concentration	${\rm seconaryState}$	$m^{-3} mol$		62
81	m_N	m	mass in kg	${\rm seconaryState}$	kg		64
82	$ ho_N$	density	density	${\rm seconaryState}$	$kg m^{-3}$		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	ξ_{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	$\mod s^{-1}$		93
132	\dot{n}_{NS}	dndt	species mass accumulation	diffState	$\mod s^{-1}$		111
133	\dot{H}_N	dHdt	differential enthalpy balance	diffState	$kg m^2 s^{-3}$	[]	116

8 solid

var	symbol	${ m documentation}$	type	units	tokens	eqs					
uid											
var	symbol	documentation	type	units	tokens	eqs					
10 liquid											
var	symbol	documentation	type	${ m units}$	tokens	eqs					
$11 { m gas}$											
var	symbol	documentation	type	units	tokens	eqs					
control-reactio	ons										
var	symbol	documentation	type	units	tokens	eqs					
13 reactions-control											
var	symbol	documentation	type	units	tokens	eqs					
	iquid var gas var control—reaction var reactions—control	var symbol var symbol gas var symbol control—reactions var symbol eactions—control	var symbol documentation iquid var symbol documentation gas var symbol documentation control—reactions var symbol documentation ceactions—control	raid var symbol documentation type iquid var symbol documentation type gas var symbol documentation type control—reactions var symbol documentation type control—reactions	var symbol documentation type units iquid var symbol documentation type units gas var symbol documentation type units control-reactions var symbol documentation type units control-reactions	raid var symbol documentation type units tokens iquid var symbol documentation type units tokens gas var symbol documentation type units tokens control-reactions var symbol documentation type units tokens control-reactions var symbol documentation type units tokens					

14 control-material

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

15 material-control

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

$16 \quad control-macroscopic$

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

17 macroscopic-control

	var	symbol	documentation	type	units	tokens	eqs
143	$T^n{}_N$	T_n	norming temperature	constant	K	[]	
144	$p^n{}_N$	p_n	norming pressure	constant	$kg m^{-1} s^{-2}$		
145	$c^n{}_{NS}$	c_n	norming concentration	constant	$m^{-3} mol$		
146	$F_{N,A}$	F_N_A	projection N -> A	constant			
151	$F_{A,NS}$	F_A_NS	${\rm projection~NS} \mathrel{->} {\rm A}$	constant		[]	
148	s_{TA}	s_T	normed temperature signal	${ m transform}$			125
149	s_{p_A}	s_p	normed pressure signal	${ m transform}$			126
152	s_{cA}	s_c	noremed concentration signal vector	${ m transform}$			127

18 reactions-material

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

19 material-reactions

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

${\bf 20} \quad {\bf reactions-macroscopic}$

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

${\bf 21} \quad {\bf macroscopic-reactions}$

	var	symbol	documentation	type	units	tokens	eqs
94	T_{NK}	T_NK	temperature of reacive 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

${\bf 22} \quad {\bf material-macroscopic}$

	var	symbol	documentation	type	units	tokens	eqs
61	λ_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

	var	symbol	documentation	type	units	tokens	eqs
63	$k_{y_N}^q$	kq_y	link	transform	$kg K^{-1} s^{-3}$		46
64	k_{zN}^q	kq_z	link	transform	$kg K^{-1} s^{-3}$		47
65	$k^q{}_N$	kq	link	transform	$kg K^{-1} s^{-3}$		48
66	k_{xN}^c	kc_x	link	transform	$m^{-1} s$		49
67	$k_{y_N}^c$	kc_y	link	transform	$m^{-1} s$		50
68	k_{zN}^c	kc_z	link	transform	$m^{-1} s$		51
69	$k^c{}_N$	kc	link	transform	$m^{-1} s$		52
70	k_{xNS}^d	kd_x	link	transform	$kg^{-1} m^{-4} mol^2 s$		53
73	$k_{y}^{d}_{NS}$	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^d_{NS}	kd	link	transform	$kg^{-1} m^{-4} mol^2 s$		58
76	c_{p_S}	ср	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

${\bf 23} \quad {\bf macroscopic-material}$

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

24 gas-liquid

_							
	var	symbol	documentation	type	units	$_{ m tokens}$	eas
	rai	SJ III S SI	a o c a i i c i i c i c i c i c i c i c i c	of be	dillos	Concin	040

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	$v_{y_N} := \frac{\partial r_{y_N}}{\partial t}$	velocity in y-direction	physical
22	$v_{zN} := \frac{\partial r_{zN}}{\partial t}$	velocity in z-direction	physical
23	$v_N := Stack\left(v_{xN}, v_{y_N}, v_{z_N}\right)$	velocity vector	physical

no	equation	documentation	layer
24	$C_{p_N} := \frac{\partial H_N}{\partial T_N}$	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	$c_{p_S} := C_{p_N} \cdot (\lambda_S)^{-1} \overset{N \in NS}{\star} n_{NS}$	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	$k_{y_N}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{y_N}$	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	$k^{q}{}_{N} := Stack \left(k^{q}_{xN}, k^{q}_{yN}, k^{q}_{zN}\right)$	Carthesian thermal conductivity vector	material
32	$k_{xN}^c := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass convectivity in x-direction	material
33	$k_{y_N}^c := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{y_N}$	convective mass convectivity in y-direction	material
34	$k_{zN}^c := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convective mass convectivity in z-direction	material
35	$k^{c}{}_{N} := Stack\left(k^{c}_{xN}, k^{c}_{yN}, k^{c}_{zN}\right)$	Cartesian convective mass convectivity 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	$k_{y_{NS}}^d := (\mu_{NS})^{-1} \cdot \left(v_{y_N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in y- direction	material

no	equation	documentation	layer
	$k_{zNS}^d := (\mu_{NS})^{-1} \cdot \left(v_{zN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in z-direction	material
39	${k^d}_{NS} := Stack\left(k^d_{xNS}, k^d_{yNS}, k^d_{zNS}\right)$	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	$h_{NS} := H_N \odot \left(n_{NS} \right)^{-1}$	partial molar enthalpies	material
44	$\lambda_S := \lambda_S$	link to molar masses	material »> macro- scopic
45	$k_{xN}^q := k_{xN}^q$	link	material »> macro- scopic
46	$k_{y_N}^q := k_{y_N}^q$	link	material »> macro- scopic
47	$k_{zN}^q:=k_{zN}^q$	link	material »> macro- scopic
48	$k^q{}_N := k^q{}_N$	link	material »> macro- scopic
49	$k_{xN}^c := k_{xN}^c$	link	material »> macro- scopic
50	$k_{y_N}^c := k_{y_N}^c$	link	material »> macro- scopic
51	$k_{zN}^c := k_{zN}^c$	link	material »> macro- scopic

no	equation	documentation	layer
52	$k^c{}_N := k^c{}_N$	link	material »> macro- scopic
53	$k_{xNS}^d := k_{xNS}^d$	link	material »> macro- scopic
56	$k_{y_{NS}}^d := k_{y_{NS}}^d$	link	material »> macro- scopic
57	$k_{zNS}^d := k_{zNS}^d$	link	material »> macro- scopic
58	$k^d{}_{NS} := k^d{}_{NS}$	link	material »> macro- scopic
59	$c_{p_S} := c_{p_S}$	link	material »> macro- scopic
60	$c_{vS} := c_{vS}$	link	material »> macro- scopic
61	$d_A := \operatorname{sign}\left(F_{N,A} \stackrel{N}{\star} p_N\right)$	direction of convective flow	macroscopic
62	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar concentration	macroscopic
63	$A_{y,z_N} := r_{y_N} \cdot r_{z_N}$	cross sectional area in x-direction	macroscopic
64	$m_N := \lambda_S \overset{S \in NS}{\star} n_{NS}$	mass in kg	macroscopic
65	$\rho_N := \left(V_N\right)^{-1} . m_N$	density	macroscopic
66	$\hat{V}_A := (\rho_N)^{-1} \cdot k_{xN}^c \cdot A_{y,z_N} \cdot F_{N,A} \overset{N}{\star} p_N$	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

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

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

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

no	equation	documentation	layer
130	$\dot{x}_D := A_{N,D} \overset{N}{\star} x_N + B_{A,D} \overset{A}{\star} u_A$	controller dynamics	control
131	$x_N := \int_{t^o}^{t^e} I_{N,D} \stackrel{D}{\star} \dot{x}_D \ dt$	state	control