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	$_{ m tokens}$	eqs
141	x_N	х	state	state		[]	
139	$A_{N,D}$	A	dynamic matrix	constant			
140	$B_{A,D}$	В	input gain matrix	constant			

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	$m^{-3} mol s^{-1}$		

	var	symbol	documentation	type	units	tokens	eqs
108	$c^{o}{}_{KS}$	co_KS	standardisation of concentration	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}	Ср	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	$k_{y_N}^q$	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	$k_{y_N}^c$	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
53	k_{xNS}^d	kd_x	diffusional mass conductivity in x-direction	seconaryState	$kg^{-1} m^{-4} mol^2 s$		36
54	$k_{y_{NS}}^d$	kd_y	diffusional mass conductivity in y-direction	seconaryState	$kg^{-1} m^{-4} mol^2 s$		37
55	k_{zNS}^d	kd_z	diffusional mass conductivity in z-direction	seconaryState	$kg^{-1} m^{-4} mol^2 s$		38
56	$k^d{}_{NS}$	kd	Cartesian diffusional mass conductivity vector	seconaryState	$kg^{-1} m^{-4} mol^2 s$		39
60	h_{NS}	h	partial molar enthalpies	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	${ m transport}$	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	$\mod s^{-1}$		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	transport	$kg m^2 s^{-3}$		106
128	\hat{n}_{AS}^d	fnd_AS	diffusional mass transfer in arc	transport	$\mod s^{-1}$		107
129	\hat{n}_{NS}^d	fnd	net diffusional mass transfer	transport	$\mod s^{-1}$		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	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			

	var	symbol	documentation	type	units	tokens	eqs
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	seconaryState	$m^{-3} mol$		62
81	m_N	m	mass in kg	seconaryState	kg		64
82	$ ho_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	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	$ ilde{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	documentation	type	units	tokens	eqs
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9 fluid

	var	symbol	documentation	type	units	tokens	eqs
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10 liquid

	var	symbol	documentation	type	units	tokens	eqs
1	gas						
	var	symbol	documentation	type	units	tokens	eqs
2	control–rea	lphactions					
	var	symbol	documentation	type	units	tokens	eqs
3	m reactions-c	control					
	var	symbol	documentation	type	units	tokens	eqs
4	control–ma	iterial					
	var	symbol	documentation	type	units	tokens	eqs
5	material-c	ontrol					
	var	symbol	documentation	type	units	tokens	eqs

17 macroscopic-control

	var	symbol	documentation	type	units	tokens	eqs
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18 reactions-material

	var	symbol	documentation	type	units	tokens	eqs
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19 material-reactions

	var	symbol	documentation	type	units	tokens	eqs
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${\bf 20} \quad {\bf reactions-macroscopic}$

	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

21 macroscopic-reactions

	var	symbol	documentation	type	units	tokens	eqs
94	T_{NK}	T_NK	temperature of reacive systems	transform	K	[]	77

	var	symbol	documentation	type	units	tokens	eqs
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
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	$k_{y_{NS}}^d$	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	$k^d{}_{NS}$	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	${ m units}$	$_{ m tokens}$	eqs	
25	$_{ m 5}$ gas—solid							
	var	symbol	documentation	type	units	tokens	eqs	
26	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	$p_N := rac{\partial U_N}{\partial V_N}$	thermodynamic pressure	physical
8	$T_N := \frac{\partial U_N}{\partial S_N}$	temperature	physical
9	$\mu_{NS} := rac{\partial U_N}{\partial n_{NS}}$	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	$A_N := U_N - T_N . S_N$	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	$c_{p_S} := C_{p_N} \cdot (\lambda_S)^{-1} \stackrel{N \in NS}{\star} n_{NS}$	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	$k_{y_N}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{y_N}$	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	$\hat{n}^c_{AS} := \hat{V}_A \odot c_{AS}$	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	$c_{KS} := c_{NS} \overset{NS}{\star} P_{NS,KS}$	concentration in the reactive systems	macroscopic
79	$c_{KS} := c_{KS}$	link	macroscopic »> reactions
82	$R_N := A^v{}_N . B_N$	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	$K_{NK} := K^o{}_K \odot exp((-E_{aNK}) \cdot \left(R_N \stackrel{N}{\star} P_{N,NK} \cdot T_{NK}\right)^{-1})$	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	$n_{NS} := \int_{t^o}^{t^e} \dot{n}_{NS} \ dt + n^o{}_{NS}$	$foundation\ state-species\ mass$	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