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	$r_{x\,N}$	`r_x`	x-coordinate	frame	m	[]	
16	$r_{y\,N}$	`r_y`	y-coordinate	frame	m	[]	
17	$r_{z\,N}$	`r_z`	z-coordinate	frame	m	[]	
18	$n_{N\,S}$	`n`	foundation state – species mass	state	mol	[]	119
19	U_N	`U`	foundation state – internal energy	state	$kg\,m^2\,s^{-2}$	[]	
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	`H`	enthalpy	state	$kg\,m^2\,s^{-2}$	[]	13 122
30	A_N	`A`	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	μ_{NS}	`chem_pot`	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	[]	9
36	${v_x}_N$	`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	${v_z}_N$	`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	`x`	state	state		[]	131
142	xo_N	`xo`	initial state	state		[]	123
139	$A_{N,D}$	`A`	dynamic matrix	constant	s^{-1}	[]	
140	$B_{A,D}$	`B`	input gain matrix	constant	s^{-1}	[]	
156	$I_{N,D}$	`I_N_D`	map D –> N – used in integration	constant		[]	
157	${u_s}_A$	`u_s`	setpoint in terms of the measurement	constant		[]	
158	${T_I}_N$	`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	$E_{a\,NK}$	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	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	$C_{v\,N}$	Cv	total heat capacity at constant volume	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	[]	25
43	$c_{p\,S}$	cp	specific heat capacity at constant pressure	constant	$m^2\,mol^2\,K^{-1}\,s^{-2}$	[]	26 133
44	$c_{v\,S}$	cv	specific heat capacity at constant volume	constant	$m^2\,mol^2\,K^{-1}\,s^{-2}$	[]	27 134
45	${k^q_x}_N$	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	${k^q_z}_N$	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	${k^c_x}_N$	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	${k^c_z}_N$	kc_z	convective mass convectivity in z-direction	seconaryState	$m^{-1}\,s$	[]	34

Continued on next page

	var	symbol	documentation	type	units	tokens	eqs
52	${k^c}_N$	kc	Cartesian convective mass convectivity vector	seconaryState	$m^{-1}\,s$	[]	35
53	$k^d_{x\,NS}$	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	seconaryState	$kg^{-1}\,m^{-4}\,mol^2\,s$	[]	37
55	$k^d_{z\,NS}$	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	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	$\hat{n}^c_{AS}$	fnc_AS	convective mass flow by stream	transport	$mol\,s^{-1}$	[]	68
86	$\hat{n}^c_{NS}$	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	$\hat{H}^c_A$	fHc_A	enthalpy flow due to convection	transport	$kg\,m^2\,s^{-3}$	[]	104
127	$\hat{H}^c_N$	fHc	net enthalpy flow due to convection	transport	$kg\,m^2\,s^{-3}$	[]	106
128	$\hat{n}^d_{AS}$	fnd_AS	diffusional mass transfer in arc	transport	$mol\,s^{-1}$	[]	107
129	$\hat{n}^d_{NS}$	fnd	net diffusional mass transfer	transport	$mol\,s^{-1}$	[]	108
130	$\hat{H}^d_A$	fHd_A	enthalpy flow due to mass diffusion	transport	$kg\,m^2\,s^{-3}$	[]	109
131	$\hat{H}^d_N$	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

Continued on next page

	var	symbol	documentation	type	units	tokens	eqs
176	$fq_{A x A}$	fq_A_x	conductive heat transfer in x-direction	transport	$kg\, m^2\, s^{-3}$	[]	162
177	$fq_{x N}$	fq_x	net convective heat transfer in x-direction	transport	$kg\, m^2\, s^{-3}$	[]	163
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	${H^o}_N$	Ho	initial condition for enthalpy	state	$kg\, m^2\, s^{-2}$	[]	120
159	X	X	state for nodes with mass and energy	state		[]	132
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	ρ_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	$\tilde{n}_{NS}$	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	$kg\, m^2\, s^{-3}$	[]	164

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	${T^n}_N$	`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`	projection NS –> A	constant		[]	
148	${s_T}_A$	`s_T`	normed temperature signal	transform		[]	125
149	${s_p}_A$	`s_p`	normed pressure signal	transform		[]	126
152	${s_c}_A$	`s_c`	noremed 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	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
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	λ_S	Mm	link to molar masses	transform	$kg\, mol^{-1}$	[]	44
62	$k^q_{x\,N}$	kq_x	link	transform	$kg\, K^{-1}\, s^{-3}$	[]	45

Continued on next page

	var	symbol	documentation	type	units	tokens	eqs
63	$k^q_{y\,N}$	kq_y	link	transform	$kg\,K^{-1}\,s^{-3}$	[]	46
64	$k^q_{z\,N}$	kq_z	link	transform	$kg\,K^{-1}\,s^{-3}$	[]	47
65	$k^q{}_N$	kq	link	transform	$kg\,K^{-1}\,s^{-3}$	[]	48
66	$k^c_{x\,N}$	kc_x	link	transform	$m^{-1}\,s$	[]	49
67	$k^c_{y\,N}$	kc_y	link	transform	$m^{-1}\,s$	[]	50
68	$k^c_{z\,N}$	kc_z	link	transform	$m^{-1}\,s$	[]	51
69	$k^c{}_N$	kc	link	transform	$m^{-1}\,s$	[]	52
70	$k^d_{x\,NS}$	kd_x	link	transform	$kg^{-1}\,m^{-4}\,mol^2\,s$	[]	53
73	$k^d_{y\,NS}$	kd_y	link	transform	$kg^{-1}\,m^{-4}\,mol^2\,s$	[]	56
74	$k^d_{z\,NS}$	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	$c_{p\,S}$	cp	link	transform	$m^2\,mol^2\,K^{-1}\,s^{-2}$	[]	59
77	$c_{v\,S}$	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
160	$\mu^\alpha{}_{NS}$	chem_pot_left	left chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	[]	135 137

Continued on next page

	var	symbol	documentation	type	units	tokens	eqs
161	${\mu^{\beta}}_{NS}$	chem_pot_right	right chemical potential	effort	$kg\,m^{2}\,mol^{-1}\,s^{-2}$	[]	136 138
164	${T^{-\epsilon}}_{N}$	T_left	temparture left	effort	K	[]	143 145
165	${T^{+\epsilon}}_{N}$	T_right	right temperature	effort	K	[]	144 146
166	${p^{-\epsilon}}_{N}$	p_left	left pressure	effort	$kg\,m^{-1}\,s^{-2}$	[]	147 151
167	${p^{+\epsilon}}_{N}$	p_right	right pressure	effort	$kg\,m^{-1}\,s^{-2}$	[]	148 150
162	$\hat{q}^{-\epsilon}_{AS}$	fnd_AS_left	left diffusional mass flow	transport	$mol\,s^{-1}$	[]	139 141
163	$\hat{q}^{+\epsilon}_{AS}$	fnd_AS_right	right diffusional mass flow	transport	$mol\,s^{-1}$	[]	140 142
168	${\hat{n}^{c-\epsilon}}_{AS}$	fnc_AS_left	left convective mass flow	transport	$mol\,s^{-1}$	[]	152 154
169	${\hat{n}^{c+\epsilon}}_{AS}$	fnc_AS_right	right convective mass flow	transport	$mol\,s^{-1}$	[]	153 155

25 gas–gas

	var	symbol	documentation	type	units	tokens	eqs

26 liquid–liquid

	var	symbol	documentation	type	units	tokens	eqs

27 gas–solid

	var	symbol	documentation	type	units	tokens	eqs

28 solid–solid

	var	symbol	documentation	type	units	tokens	eqs

29 liquid–solid

	var	symbol	documentation	type	units	tokens	eqs

30 Equations

30.1 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	$H_N := U_N + p_N \,.\, V_N$	enthalpy	physical
14	$A_N := U_N - T_N \,.\, S_N$	Helmholtz energy	physical
15	$G_N := U_N + p_N \,.\, V_N - T_N \,.\, S_N$	Gibbs energy	physical
20	$v_{x\,N} := \frac{\partial r_{x\,N}}{\partial t}$	velocity in x-direction	physical
21	$v_{y\,N} := \frac{\partial r_{y\,N}}{\partial t}$	velocity in y-direction	physical
22	$v_{z\,N} := \frac{\partial r_{z\,N}}{\partial t}$	velocity in z-direction	physical
23	$v_N := Stack\left(v_{x\,N}, v_{y\,N}, v_{z\,N}\right)$	velocity vector	physical

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no	equation	documentation	layer
24	$C_{p\,N} := \frac{\partial\, H_N}{\partial\, T_N}$	total heat capacity at constant pressure	material
25	$C_{v\,N} := \frac{\partial\, U_N}{\partial\, T_N}$	total heat capacity at constant volume	material
26	$c_{p\,S} := C_{p\,N} \,.\, (\lambda_S)^{-1} \overset{N \in NS}{\star} n_{NS}$	specific heat capacity at constant pressure	material
27	$c_{v\,S} := C_{v\,N} \,.\, (\lambda_S)^{-1} \overset{N \in NS}{\star} n_{NS}$	specific heat capacity at constant volume	material
28	$k^q_{x\,N} := (V_N)^{-1} \,.\, \frac{\partial\, U_N}{\partial\, T_N} \,.\, v_{x\,N}$	thermal conductivity in x-direction	material
29	$k^q_{y\,N} := (V_N)^{-1} \,.\, \frac{\partial\, U_N}{\partial\, T_N} \,.\, v_{y\,N}$	thermal conductivity in y-direction	material
30	$k^q_{z\,N} := (V_N)^{-1} \,.\, \frac{\partial\, U_N}{\partial\, T_N} \,.\, v_{z\,N}$	thermal conductivity in z-direction	material
31	$k^q{}_N := Stack\left(k^q_{x\,N}, k^q_{y\,N}, k^q_{z\,N}\right)$	Carthesian thermal conductivity vector	material
32	$k^c_{x\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \,.\, (V_N)^{-1} \,.\, \frac{\partial\, U_N}{\partial\, p_N} \,.\, v_{x\,N}$	convective mass convectivity in x-direction	material
33	$k^c_{y\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \,.\, (V_N)^{-1} \,.\, \frac{\partial\, U_N}{\partial\, p_N} \,.\, v_{y\,N}$	convective mass convectivity in y-direction	material
34	$k^c_{z\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \,.\, (V_N)^{-1} \,.\, \frac{\partial\, U_N}{\partial\, p_N} \,.\, v_{z\,N}$	convective mass convectivity in z-direction	material
35	$k^c{}_N := Stack\left(k^c_{x\,N}, k^c_{y\,N}, k^c_{z\,N}\right)$	Cartesian convective mass convectivity vector	material
36	$k^d_{x\,NS} := (\mu_{NS})^{-1} \,.\, \left(v_{x\,N} \odot \left((V_N)^{-1} \odot \frac{\partial\, U_N}{\partial\, \mu_{NS}}\right)\right)$	diffusional mass conductivity in x-direction	material
37	$k^d_{y\,NS} := (\mu_{NS})^{-1} \,.\, \left(v_{y\,N} \odot \left((V_N)^{-1} \odot \frac{\partial\, U_N}{\partial\, \mu_{NS}}\right)\right)$	diffusional mass conductivity in y-direction	material

Continued on next page

no	equation	documentation	layer
38	$k^{d}_{z\,NS} := (\mu_{NS})^{-1} \cdot \left(v_{z\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in z-direction	material
39	$k^{d}{}_{NS} := Stack\left(k^{d}_{x\,NS}, k^{d}_{y\,NS}, k^{d}_{z\,NS}\right)$	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	$k^{q}_{x\,N} := k^{q}_{x\,N}$	link	material »> macroscopic
46	$k^{q}_{y\,N} := k^{q}_{y\,N}$	link	material »> macroscopic
47	$k^{q}_{z\,N} := k^{q}_{z\,N}$	link	material »> macroscopic
48	$k^{q}{}_{N} := k^{q}{}_{N}$	link	material »> macroscopic
49	$k^{c}_{x\,N} := k^{c}_{x\,N}$	link	material »> macroscopic
50	$k^{c}_{y\,N} := k^{c}_{y\,N}$	link	material »> macroscopic
51	$k^{c}_{z\,N} := k^{c}_{z\,N}$	link	material »> macroscopic

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no	equation	documentation	layer
52	${k^c}_N := {k^c}_N$	link	material »> macroscopic
53	${k^d_x}_{NS} := {k^d_x}_{NS}$	link	material »> macroscopic
56	${k^d_y}_{NS} := {k^d_y}_{NS}$	link	material »> macroscopic
57	${k^d_z}_{NS} := {k^d_z}_{NS}$	link	material »> macroscopic
58	${k^d}_{NS} := {k^d}_{NS}$	link	material »> macroscopic
59	${c_p}_S := {c_p}_S$	link	material »> macroscopic
60	${c_v}_S := {c_v}_S$	link	material »> macroscopic
61	$d_A := \mathrm{sign}\left(F_{N,A} \overset{N}{\star} p_N\right)$	direction of convective flow	macroscopic
62	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar concentration	macroscopic
63	${A_{y,z}}_N := {r_y}_N \,.\, {r_z}_N$	cross sectional area in x-direction	macroscopic
64	$m_N := \lambda_S \overset{S \in NS}{\star} n_{NS}$	mass in kg	macroscopic
65	$\rho_N := (V_N)^{-1} \,.\, m_N$	density	macroscopic
66	$\hat{V}_A := (\rho_N)^{-1} \,.\, {k^c_x}_N \,.\, {A_{y,z}}_N \,.\, F_{N,A} \overset{N}{\star} p_N$	convective volumetric flow	macroscopic
67	$c_{AS} := (1/2 \,.\, (F_{NS,AS} - d_A \odot \lvert F_{NS,AS} \rvert)) \overset{NS}{\star} c_{NS}$	molar species concentration in convective flow	macroscopic

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

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no	equation	documentation	layer
90	$N_{S,K} := N_{S,K}$	link	reactions »> macroscopic
91	$\xi_{NK} := K_{NK} \,.\, P_{NK,KS} \overset{KS}{\star} \phi_{KS}$	extent of reaction	macroscopic
92	$N_{NS,NK} := P_{S,NS} \overset{S}{\star} \left(\left(P_{K,NK} \,.\, T_{NK} \,.\, (T_{NK})^{-1}\right) \overset{K}{\star} N_{S,K}\right)$	extended stoichiometry	macroscopic
93	$\tilde{n}_{NS} := V_N \odot \left(N_{NS,NK} \overset{NK}{\star} \xi_{NK}\right)$	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	$\hat{H}^c_A := \left(F_{NS,AS} \overset{NS}{\star} h_{NS}\right) \overset{S \in AS}{\star} \hat{n}^c_{AS}$	enthalpy flow due to convection	macroscopic
106	$\hat{H}^c_N := F_{N,A} \overset{A}{\star} \hat{H}^c_A$	net enthalpy flow due to convection	macroscopic
107	$\hat{n}^d_{AS} := A_{y,z\,N} \odot \left(-k^d_{x\,NS}\right) \,.\, F_{NS,AS} \overset{NS}{\star} \mu_{NS}$	diffusional mass transfer in arc	macroscopic
108	$\hat{n}^d_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^d_{AS}$	net diffusional mass transfer	macroscopic
109	$\hat{H}^d_A := \left(F_{NS,AS} \overset{NS}{\star} h_{NS}\right) \overset{S \in AS}{\star} \hat{n}^d_{AS}$	enthalpy flow due to mass diffusion	macroscopic
110	$\hat{H}^d_N := F_{N,A} \overset{A}{\star} \hat{H}^d_A$	net enthalpy flow due to diffusion	macroscopic
111	$\dot{n}_{NS} := \hat{n}^c_{NS} + \hat{n}^d_{NS} + \tilde{n}_{NS}$	species mass accumulation	macroscopic

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no	equation	documentation	layer
114	$\hat{w}_A := Set(\hat{H}^c_A, \#)$	example of work flow	macroscopic
115	$\hat{w}_N := F_{N,A} \overset{A}{\star} \hat{w}_A$	net work flow	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
123	$xo_N := Set(x_N, \#)$	initial state	control
125	$s_{T\,A} := F_{N,A} \overset{N}{\star} \left(T_N \,.\, (T^n{}_N)^{-1}\right)$	normed temperature signal	macroscopic »> control
126	$s_{p\,A} := F_{N,A} \overset{N}{\star} \left(p_N \,.\, (p^n{}_N)^{-1}\right)$	normed pressure signal	macroscopic »> control
127	$s_{c\,A} := F_{A,NS} \overset{NS}{\star} \left(c_{NS} \,.\, (c^n{}_{NS})^{-1}\right)$	noremed concentration signal vector	macroscopic »> control
128	$u_A := Stack\left(s_{T\,A}, s_{p\,A}, s_{c\,A}\right)$	controller input	control
130	$\dot{x}_D := A_{N,D} \overset{N}{\star} x_N + B_{A,D} \overset{A}{\star} u_A$	controller dynamics	control

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no	equation	documentation	layer
131	$x_N := \int_{t^o}^{t^e} I_{N,D} \overset{D}{\star} \dot{x}_D \; dt$	state	control
132	$X := MixedStack\left(n_{NS}, H_N\right)$	state for nodes with mass and energy	macroscopic
133	$c_{p\,S} := Set(c_{p\,S}, \#)$	specific heat capacity at constant pressure	material
134	$c_{v\,S} := Set(c_{v\,S}, \#)$	specific heat capacity at constant volume	material
135	${\mu^{\alpha}}_{NS} := \mu^{-\epsilon}_{NS}$	left chemical potential	gas »> liquid
136	${\mu^{\beta}}_{NS} := \mu^{+\epsilon}_{NS}$	right chemical potential	gas »> liquid
137	${\mu^{\alpha}}_{NS} := Root\left({\mu^{\alpha}}_{NS} - {\mu^{\beta}}_{NS}, {\mu^{\alpha}}_{NS}\right)$	left chemical potential	gas »> liquid
138	${\mu^{\beta}}_{NS} := Root\left({\mu^{\beta}}_{NS} - {\mu^{\alpha}}_{NS}, {\mu^{\beta}}_{NS}\right)$	right chemical potential	gas »> liquid
139	$\hat{q}^{-\epsilon}_{AS} := {\hat{n}^{d}_{AS}}^{-\epsilon}$	left diffusional mass flow	gas »> liquid
140	$\hat{q}^{+\epsilon}_{AS} := {\hat{n}^{d}_{AS}}^{+\epsilon}$	right diffusional mass flow	gas »> liquid
141	$\hat{q}^{-\epsilon}_{AS} := Root\left(\hat{q}^{-\epsilon}_{AS} - \hat{q}^{+\epsilon}_{AS}, \hat{q}^{-\epsilon}_{AS}\right)$	left diffusional mass flow	gas »> liquid
142	$\hat{q}^{+\epsilon}_{AS} := Root\left(\hat{q}^{-\epsilon}_{AS} - \hat{q}^{+\epsilon}_{AS}, \hat{q}^{+\epsilon}_{AS}\right)$	right diffusional mass flow	gas »> liquid

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no	equation	documentation	layer
143	$T^{-\epsilon}{}_{N} := T_{N}^{-\epsilon}$	temparture left	gas »> liquid
144	$T^{+\epsilon}{}_{N} := T_{N}^{+\epsilon}$	right temperature	gas »> liquid
145	$T^{-\epsilon}{}_{N} := Root\left(T^{-\epsilon}{}_{N} - T^{+\epsilon}{}_{N}, T^{-\epsilon}{}_{N}\right)$	temparture left	gas »> liquid
146	$T^{+\epsilon}{}_{N} := Root\left(T^{-\epsilon}{}_{N} - T^{+\epsilon}{}_{N}, T^{+\epsilon}{}_{N}\right)$	right temperature	gas »> liquid
147	$p^{-\epsilon}{}_{N} := p_{N}^{-\epsilon}$	left pressure	gas »> liquid
148	$p^{+\epsilon}{}_{N} := p_{N}^{+\epsilon}$	right pressure	gas »> liquid
150	$p^{+\epsilon}{}_{N} := Root\left(p^{-\epsilon}{}_{N} - p^{+\epsilon}{}_{N}, p^{+\epsilon}{}_{N}\right)$	right pressure	gas »> liquid
151	$p^{-\epsilon}{}_{N} := Root\left(p^{-\epsilon}{}_{N} - p^{+\epsilon}{}_{N}, p^{-\epsilon}{}_{N}\right)$	left pressure	gas »> liquid
152	$\hat{n}^{c-\epsilon}{}_{AS} := \hat{n}^{c}_{AS}{}^{-\epsilon}$	left convective mass flow	gas »> liquid
153	$\hat{n}^{c+\epsilon}{}_{AS} := \hat{n}^{c}_{AS}{}^{+\epsilon}$	right convective mass flow	gas »> liquid
154	$\hat{n}^{c-\epsilon}{}_{AS} := Root\left(\hat{n}^{c-\epsilon}{}_{AS} - \hat{n}^{c+\epsilon}{}_{AS}, \hat{n}^{c-\epsilon}{}_{AS}\right)$	left convective mass flow	gas »> liquid
155	$\hat{n}^{c+\epsilon}{}_{AS} := Root\left(\hat{n}^{c-\epsilon}{}_{AS} - \hat{n}^{c+\epsilon}{}_{AS}, \hat{n}^{c+\epsilon}{}_{AS}\right)$	right convective mass flow	gas »> liquid

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no	equation	documentation	layer
162	$fq_{Ax\,A} := A_{y,z\,N} \cdot k^{q}_{x\,N} \cdot F_{N,A} \overset{N}{\star} T_N$	conductive heat transfer in x-direction	macroscopic
163	$fq_{x\,N} := F_{N,A} \overset{A}{\star} fq_{Ax\,A}$	net convective heat transfer in x-direction	macroscopic
164	$\dot{H}_N := \hat{H}^c_N + \hat{H}^d_N + fq_{x\,N} + \hat{w}_N$	differential enthalpy balance	macroscopic