1 Variables

2 root

	var	symbol	documentation	type	units	tokens	eqs
5	$F_{N,A}$	`F`	incidence matrix of a directed graph	network		[]	
6	t	`t`	time	frame	s	[]	
7	t_o	`to`	starting time	frame	s	[]	4
8	t_e	`te`	end time	frame	s	[]	5
1	#	`value`	numerical value	constant		[]	
2	0	`zero`	numerical value zero	constant		[]	1
3	1	`one`	numerical value one	constant		[]	2
4	0.5	`onehalf`	numerical value one half	constant		[]	3

3 physical

	var	symbol	documentation	type	units	tokens	eqs
9	$r_{x\,N}$	`r_x`	x-coordinate	frame	m	[]	
10	$r_{y\,N}$	`r_y`	y-coordinate	frame	m	[]	
23	$r_{z\,N}$	`r_z`	z-coordinate	frame	m	[]	
11	U_N	`U`	foundation state – internal energy	state	$kg\,m^2\,s^{-2}$	[]	
12	S_N	`S`	foundation state – entropy	state	$kg\,m^2\,K^{-1}\,s^{-2}$	[]	
13	V_N	`V`	foundation state – volume	state	m^3	[]	
18	H_N	`H`	enthalpy	state	$kg\,m^2\,s^{-2}$	[]	9 122
19	A_N	`A`	Helmholtz energy	state	$kg\,m^2\,s^{-2}$	[]	10
20	G_N	`G`	Gibbs energy	state	$kg\,m^2\,s^{-2}$	[]	11
42	n_{NS}	`n`	species molar mass	state	mol	[]	116
26	A^v	`Avogadro`	Avogadro number	constant	mol^{-1}	[]	
27	Bo_N	`Boltzmann`	Boltzmann constant	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	[]	16
28	R_N	`GasConstant`	Gas constant	constant	$kg\,m^2\,mol^{-1}\,K^{-1}\,s^{-2}$	[]	17
15	p_N	`p`	thermodynamic pressure	effort	$kg\,m^{-1}\,s^{-2}$	[]	6 115
16	T_N	`T`	temperature	effort	K	[]	7 113
45	μ_{NS}	`chem_pot`	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	[]	32 114
21	$v_{x\,N}$	`v_x`	velocity in x-direction	secondaryState	ms^{-1}	[]	12
22	$v_{y\,N}$	`v_y`	velocity in y direction	secondaryState	ms^{-1}	[]	13
24	$v_{z\,N}$	`v_z`	velocity in z-direction	secondaryState	ms^{-1}	[]	14
25	v_N	`v`	velocity vector	secondaryState	ms^{-1}	[]	15

4 control

	var	symbol	documentation	type	units	tokens	eqs
139	m_A	mc	measurements	input		[]	
129	$I_{N,D}$	I_N_D	identity to shift from differential space integral space	network		[]	
130	$I_{A,D}$	I_A_D	identity to shift from differential space to arc	network		[]	
137	x_N	x	controller state	state		[]	112
138	$x^o{}_N$	xo	controller initial condition	state		[]	103
133	$C_{N,A}$	Cx	measurement matrix	constant		[]	
134	$D_{N,D}$	Dx	event matrix (dimension issue)	constant		[]	
135	$y^o{}_A$	setpoint	set point	constant		[]	
136	D_A	D_A	event diagonal matrix (no dimension problem)	constant		[]	
142	$A_{N,D}$	Ax	dynamic control matrix	constant	s^{-1}	[]	
143	$B_{A,D}$	Bx	input matrix	constant	s^{-1}	[]	
144	$\dot{x}_D$	dxdt	differential controller state	diffState	s^{-1}	[]	106
140	e_A	e	control error	algebraic		[]	104

5 reactions

	var	symbol	documentation	type	units	tokens	eqs
86	$N_{S,K}$	`N`	stoichiometric matrix	constant		[]	
87	$E_{a\,N\,K}$	`Ea`	Arrhenius's activation energy	constant	$kg\,m^2\,mol^{-1}\,s^{-2}$	[]	64
88	${K^o}_K$	`Ko`	Arrhenius's frequency factor	constant	$m^{-3}\,mol\,s^{-1}$	[]	
89	$K_{N\,K}$	`K_NK`	Arrhenius reaction constant	constant	$m^{-3}\,mol\,s^{-1}$	[]	65
114	$c_{K\,S}$	`c_KS`	molar concentrations in reactive system	constant	$m^{-3}\,mol$	[]	90
115	${c^o}_{K\,S}$	`co_KS`	norming molar concentrations	constant	$m^{-3}\,mol$	[]	91
116	$\phi_{K\,S}$	`phi_KS`	probability of species to meet	constant		[]	92

6 material

	var	symbol	documentation	type	units	tokens	eqs
29	λ_S	`Mm`	species molecular masses	constant	$kg\, mol^{-1}$	[]	
30	C_{pN}	`Cp`	total heat capacity at constant pressure	property	$kg\, m^2\, K^{-1}\, s^{-2}$	[]	18
31	C_{vN}	`Cv`	total heat capacity at constant volume	property	$kg\, m^2\, K^{-1}\, s^{-2}$	[]	19
34	$k^q_{x}{}_N$	`kq_x`	thermal conductivity in x-direction	property	$kg\, K^{-1}\, s^{-3}$	[]	22
35	$k^q_{y}{}_N$	`kq_y`	thermal conductivity in y-direction	property	$kg\, K^{-1}\, s^{-3}$	[]	23
36	$k^q_{z}{}_N$	`kq_z`	thermal conductivity in z-direction	property	$kg\, K^{-1}\, s^{-3}$	[]	24
37	$k^q{}_N$	`kq`	Carthesian thermal conductivity vector	property	$kg\, K^{-1}\, s^{-3}$	[]	25
50	$k^c_{x}{}_N$	`kc_x`	convective mass convectivity in x-direction	property	$m^{-1}\, s$	[]	37
51	$k^c_{y}{}_N$	`kc_y`	convective mass convectivity in y-direction	property	$m^{-1}\, s$	[]	38
52	$k^c_{z}{}_N$	`kc_z`	convective mass convectivity in z-direction	property	$m^{-1}\, s$	[]	39
53	$k^c{}_N$	`kc`	Cartesian convective mass convectivity vector	property	$m^{-1}\, s$	[]	40
54	$k^d_{x}{}_{NS}$	`kd_x`	diffusional mass conductivity in x-direction	property	$kg^{-1}\, m^{-4}\, mol^2\, s$	[]	41
55	$k^d_{y}{}_{NS}$	`kd_y`	diffusional mass conductivity in y-direction	property	$kg^{-1}\, m^{-4}\, mol^2\, s$	[]	42
56	$k^d_{z}{}_{NS}$	`kd_z`	diffusional mass conductivity in z-direction	property	$kg^{-1}\, m^{-4}\, mol^2\, s$	[]	43
57	$k^d{}_{NS}$	`kd`	Cartesian dffusional mass conductivity vector	property	$kg^{-1}\, m^{-4}\, mol^2\, s$	[]	44
58	h_{NS}	`h`	partial molar enthalpies	property	$kg\, m^2\, mol^{-1}\, s^{-2}$	[]	45
71	ρ_N	`density`	mass density	property	$kg\, m^{-3}$	[]	49
148	cp_N	`cp`	specific heat capacity at constant pressure	property	$m^2\, K^{-1}\, s^{-2}$	[]	120
149	cv_N	`cv`	specific heat capacity at constant volume	property	$m^2\, K^{-1}\, s^{-2}$	[]	121

7 macroscopic

	var	symbol	documentation	type	units	tokens	eqs
65	d_A	d	direction of convective flow	transport		[]	46
98	$\hat{V}_A$	fV	volumetric flow in x-direction	transport	$m^3\, s^{-1}$	[]	74
104	$\hat{n}^d{}_{AS}$	fnd_AS	diffusional mass transfer per arc	transport	$mol\, s^{-1}$	[]	80
105	$\hat{n}^d{}_{NS}$	fnd	net diffusional mass transfer	transport	$mol\, s^{-1}$	[]	81
106	$\hat{H}^d{}_A$	fHd_A	enthalpy flow due to mass diffusion per arc	transport	$kg\, m^2\, s^{-3}$	[]	82
107	$\hat{H}^d{}_N$	fHd	net enthalpy flow due to mass diffusion	transport	$kg\, m^2\, s^{-3}$	[]	83
109	c_{AS}	c_AS	moler concentration in convective arc	transport	$m^{-3}\, mol$	[]	85
110	$\hat{n}^c{}_{AS}$	fnc_AS	convective molar mass flow per arc	transport	$mol\, s^{-1}$	[]	86
111	$\hat{n}^c{}_{NS}$	fnc	net convective molar mass flow	transport	$mol\, s^{-1}$	[]	87
120	$\hat{H}^c{}_A$	fHc_A	enthalpy flow due to convective mass flow	transport	$kg\, m^2\, s^{-3}$	[]	96
121	$\hat{H}^c{}_N$	fHc	net enthalpy flow due to convective mass flow	transport	$kg\, m^2\, s^{-3}$	[]	97
122	$\hat{w}_A$	fw_A	example of work flow	transport	$kg\, m^2\, s^{-3}$	[]	98
123	$\hat{w}_N$	fw	net work flow	transport	$kg\, m^2\, s^{-3}$	[]	99
124	$\hat{q}_A$	fq_A_x	heat flow in x-direction	transport	$kg\, m^2\, s^{-3}$	[]	100
125	$\hat{q}_N$	fq	net heat flow	transport	$kg\, m^2\, s^{-3}$	[]	101
95	$A_{yz\,N}$	Ayz	cross sectional area in x-direction	geometry	m^2	[]	71
96	$A_{xz\,N}$	Axz	cross sectional area in y direction	geometry	m^2	[]	72
97	$A_{xy\,N}$	Axy	cross sectional area in z-direction	geometry	m^2	[]	73
73	$F_{NS,AS}$	F_NS_AS	incidence matrix of directed graphs for for species NS x AS	network		[]	51
59	$P_{NS,AS}$	P_NS_AS	node species to arc species projection	projection		[]	
60	$P_{K,NK}$	P_K_NK	projection of conversion to node x conversion	projection		[]	
61	$P_{S,NS}$	P_S_NS	projection species to conversion x species	projection		[]	

Continued on next page

	var	symbol	documentation	type	units	tokens	eqs
62	$P_{N,NK}$	P_N_NK	projection node to node x conversion	projection		[]	
63	$P_{NK,KS}$	P_NK_KS	projection node x conversion to conversion x species	projection		[]	
64	$P_{NS,KS}$	P_NS_KS	projection node x species to conversion x species	projection		[]	
127	$D_{N,A}$	D	difference operator	differenceOperator		[]	
128	$D_{NS,AS}$	D_NS_AS	block difference operator	differenceOperator		[]	
145	T_ref_N	T_ref	refernce temperature	constant	K	[]	117
69	m_N	m	mass	secondaryState	kg	[]	47
108	c_{NS}	c	molar concentration	secondaryState	$m^{-3}\,mol$	[]	84
77	T_{NK}	T_NK	temperature in reactive systems	conversion	K	[]	55
93	$N_{NS,NK}$	N_NS_NK	extended stoichiometric matrix	conversion		[]	69
117	ξ_{NK}	xi	extend of reaction per volume	conversion	$m^{-3}\,mol\,s^{-1}$	[]	93
118	$\tilde{n}_{NS}$	pn	production term	conversion	$mol\,s^{-1}$	[]	94
119	$\dot{n}_{NS}$	dndt	differential molar mass balance	diffState	$mol\,s^{-1}$	[]	95
126	$\dot{H}_N$	dHdt	differential enthalpy balance	diffState	$kg\,m^2\,s^{-3}$	[]	102

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–control

	var	symbol	documentation	type	units	tokens	eqs

13 gas–liquid

	var	symbol	documentation	type	units	tokens	eqs

14 gas–gas

	var	symbol	documentation	type	units	tokens	eqs

15 liquid–liquid

	var	symbol	documentation	type	units	tokens	eqs

16 gas–solid

	var	symbol	documentation	type	units	tokens	eqs

17 solid–solid

	var	symbol	documentation	type	units	tokens	eqs

18 liquid–solid

	var	symbol	documentation	type	units	tokens	eqs

19 material–material

	var	symbol	documentation	type	units	tokens	eqs

20 reactions–reactions

	var	symbol	documentation	type	units	tokens	eqs

21 Equations

22 Generic

no	equation	documentation	layer
1	$0 := \text{Instantiate}(\#, \#)$	numerical value zero	root
2	$1 := \text{Instantiate}(\#, \#)$	numerical value one	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
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
9	$H_N := U_N - p_N \,.\, V_N$	enthalpy	physical
10	$A_N := U_N - T_N \,.\, S_N$	Helmholtz energy	physical
11	$G_N := U_N + p_N \,.\, V_N - T_N \,.\, S_N$	Gibbs energy	physical
12	$v_{x\,N} := \frac{\partial r_{x\,N}}{\partial t}$	velocity in x-direction	physical
13	$v_{y\,N} := \frac{\partial r_{y\,N}}{\partial t}$	velocity in y direction	physical
14	$v_{z\,N} := \frac{\partial r_{z\,N}}{\partial t}$	velocity in z-direction	physical
15	$v_N := \text{Stack}\left(v_{x\,N}, v_{y\,N}, v_{z\,N}\right)$	velocity vector	physical
16	$Bo_N := \text{Instantiate}(S_N, \#)$	Boltzmann constant	physical
17	$R_N := A^v \,.\, Bo_N$	Gas constant	physical

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no	equation	documentation	layer
18	$C_{p\,N} := \frac{\partial H_N}{\partial T_N}$	total heat capacity	material
19	$C_{v\,N} := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	material
22	$k^q_{x\,N} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{x\,N}$	thermal conductivity in x-direction	material
23	$k^q_{y\,N} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{y\,N}$	thermal conductivity in y-direction	material
24	$k^q_{z\,N} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{z\,N}$	thermal conductivity in z-direction	material
25	$k^q{}_N := \text{Stack}\left(k^q_{x\,N}, k^q_{y\,N}, k^q_{z\,N}\right)$	Carthesian thermal conductivity vector	material
32	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	chemical potential	physical
37	$k^c_{x\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{x\,N}$	convective mass convectivity in x-direction	material
38	$k^c_{y\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{y\,N}$	convective mass convectivity in y-direction	material
39	$k^c_{z\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{z\,N}$	convective mass convectivity in z-direction	material
40	$k^c{}_N := \text{Stack}\left(k^c_{x\,N}, k^c_{y\,N}, k^c_{z\,N}\right)$	Cartesian convective mass convectivity vector	material
41	$k^d_{x\,NS} := (\mu_{NS})^{-1} \cdot \left(v_{x\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in x-direction	material
42	$k^d_{y\,NS} := (\mu_{NS})^{-1} \cdot \left(v_{y\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in y-direction	material
43	$k^d_{z\,NS} := (\mu_{NS})^{-1} \cdot \left(v_{z\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in z-direction	material

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no	equation	documentation	layer
44	${k^d}_{NS} := \text{Stack}\left(k^d_{x}{}_{NS}, k^d_{y}{}_{NS}, k^d_{z}{}_{NS}\right)$	Cartesian dffusional mass conductivity vector	material
45	$h_{NS} := H_N \odot (n_{NS})^{-1}$	partial molar enthalpies	material
46	$d_A := \text{sign}\left(F_{N,A} \overset{N}{\star} p_N\right)$	direction of convective ow	macroscopic
47	$m_N := \lambda_S \overset{S \in NS}{\star} n_{NS}$	mass	macroscopic
49	$\rho_N := m_N \, . \, (V_N)^{-1}$	mass density	material
51	$F_{NS,AS} := F_{N,A} \odot P_{NS,AS}$	incidence matrix of directed graphs for for species NS x AS	macroscopic
55	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature in reactive systems	macroscopic
64	$E_{aNK} := \text{Instantiate}(P_{N,NK} \overset{N}{\star} R_N \, . \, T_{NK}, \#)$	Arrhenius's activation energy	reactions
65	$K_{NK} := {K^o}_K \odot exp((-E_{aNK}) \, . \, \left(R_N \overset{N}{\star} P_{N,NK} \, . \, T_{NK}\right)^{-1})$	Arrhenius reaction constant	reactions
69	$N_{NS,NK} := P_{S,NS} \overset{S}{\star} \left(\left(P_{K,NK} \, . \, T_{NK} \, . \, (T_{NK})^{-1}\right) \overset{K}{\star} N_{S,K}\right)$	extended stoichiometric matrix	macroscopic
71	$A_{yzN} := r_{yN} \, . \, r_{zN}$	cross sectional area in x-direction	macroscopic
72	$A_{xzN} := r_{xN} \, . \, r_{zN}$	cross sectional area in y direction	macroscopic
73	$A_{xyN} := r_{xN} \, . \, r_{yN}$	cross sectional area in z-direction	macroscopic
74	$\hat{V}_A := (\rho_N)^{-1} \, . \, k^c_{x}{}_N \, . \, A_{yzN} \, . \, D_{N,A} \overset{N}{\star} p_N$	volumetric flow in x-direction	macroscopic
80	${\hat{n}^d}_{AS} := A_{yzN} \odot \left(-k^d_{x}{}_{NS}\right) \, . \, D_{NS,AS} \overset{NS}{\star} \mu_{NS}$	diffusional mass transfer per arc	macroscopic
81	${\hat{n}^d}_{NS} := F_{NS,AS} \overset{AS}{\star} {\hat{n}^d}_{AS}$	net diffusional mass transfer	macroscopic

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no	equation	documentation	layer
82	$\hat{H}^{d}{}_{A} := \left(F_{NS,AS} \overset{NS}{\star} h_{NS}\right) \overset{S \in AS}{\star} \hat{n}^{d}{}_{AS}$	enthalpy flow due to mass diffusion per arc	macroscopic
83	$\hat{H}^{d}{}_{N} := F_{N,A} \overset{A}{\star} \hat{H}^{d}{}_{A}$	net enthalpy flow due to mass diffusion	macroscopic
84	$c_{NS} := (V_{N})^{-1} \odot n_{NS}$	molar concentration	macroscopic
85	$c_{AS} := (0.5 \,.\, (F_{NS,AS} - d_{A} \odot \lvert F_{NS,AS} \rvert)) \overset{NS}{\star} c_{NS}$	moler concentration in convective arc	macroscopic
86	$\hat{n}^{c}{}_{AS} := \hat{V}_{A} \odot c_{AS}$	convective molar mass flow per arc	macroscopic
87	$\hat{n}^{c}{}_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^{c}{}_{AS}$	net convective molar mass flow	macroscopic
90	$c_{KS} := c_{NS} \overset{NS}{\star} P_{NS,KS}$	molar concentrations in reactive system	reactions
91	$c^{o}{}_{KS} := \text{Instantiate}(c_{KS}, \#)$	norming molar concentrations	reactions
92	$\phi_{KS} := \prod \left(c_{KS} \,.\, (c^{o}{}_{KS})^{-1} right\right)$	probability of species to meet	reactions
93	$\xi_{NK} := K_{NK} \,.\, P_{NK,KS} \overset{KS}{\star} \phi_{KS}$	extend of reaction per volume	macroscopic
94	$\tilde{n}_{NS} := V_{N} \odot \left(N_{NS,NK} \overset{NK}{\star} \xi_{NK}\right)$	production term	macroscopic
95	$\dot{n}_{NS} := \hat{n}^{c}{}_{NS} + \hat{n}^{d}{}_{NS} + \tilde{n}_{NS}$	differential molar mass balance	macroscopic
96	$\hat{H}^{c}{}_{A} := \left(F_{NS,AS} \overset{NS}{\star} h_{NS}\right) \overset{S \in AS}{\star} \hat{n}^{c}{}_{AS}$	enthalpy flow due to convective mass flow	macroscopic
97	$\hat{H}^{c}{}_{N} := F_{N,A} \overset{A}{\star} \hat{H}^{c}{}_{A}$	net enthalpy flow due to convective mass flow	macroscopic
98	$\hat{w}_{A} := \text{Instantiate}(\hat{H}^{c}{}_{A}, \#)$	example of work flow	macroscopic
99	$\hat{w}_{N} := F_{N,A} \overset{A}{\star} \hat{w}_{A}$	net work flow	macroscopic

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no	equation	documentation	layer
100	$\hat{q}_A := A_{yz\,N} \,.\, k^q_{x\,N} \,.\, D_{N,A} \overset{N}{\star} T_N$	heat flow in x-direction	macroscopic
101	$\hat{q}_N := F_{N,A} \overset{A}{\star} \hat{q}_A$	net heat flow	macroscopic
102	$\dot{H}_N := \hat{H}^c{}_N + \hat{H}^d{}_N + \hat{q}_N + \hat{w}_N$	differential enthalpy balance	macroscopic
103	$x^o{}_N := \mathrm{Instantiate}(x_N, \#)$	controller initial condition	control
104	$e_A := m_A - y^o{}_A$	control error	control
106	$\dot{x}_D := A_{N,D} \overset{N}{\star} x_N + B_{A,D} \overset{A}{\star} e_A$	differential controller state	control
112	$x_N := \int_{t_o}^{t_e} \; I_{N,D} \overset{D}{\star} \dot{x}_D \;\; d\,t$	controller state	control
113	$T_N := \mathrm{Instantiate}(T_N, \#)$	temperature	physical
114	$\mu_{NS} := \mathrm{Instantiate}(\mu_{NS}, \#)$	chemical potential	physical
115	$p_N := \mathrm{Instantiate}(p_N, \#)$	thermodynamic pressure	physical
116	$n_{NS} := \int_{t_o}^{t_e} \; \dot{n}_{NS} \;\; d\,t$	species molar mass	macroscopic
117	$T_ref_N := \mathrm{Instantiate}(T_N, \#)$	refernce temperature	macroscopic

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no	equation	documentation	layer
120	$cp_N := C_{pN} \cdot (m_N)^{-1}$	specific heat capacity at constant pressure	material
121	$cv_N := C_{vN} \cdot (m_N)^{-1}$	specific heat capacity at constant volume	material
122	$H_N := m_N \cdot \int_{Tref_N}^{T_N} cp_N \; dT_N$	enthalpy	macroscopic