

1 Variables

2 root

	var	symbol	documentation	type	units	eqs
8	$F_{N,A}$	F_N_A	fudamental incidence matrix	network		
5	t	t	time	frame	s	
6	t^o	to	starting time	frame	s	4
7	t^e	te	end time	frame	s	5
1	#	value	numerical value	constant		
2	1	one	numerical value one	constant		1
3	0	zero	numerical value zero	constant		2
4	0.5	onehalf	numerical value one half	constant		3

3 physical

	var	symbol	documentation	type	units	eqs
9	$P_{N,A}$	P_N_A	projection from node to arc for arc properties	projection		
32	$P_{NS,AS}$	P_NS_AS	projection node species to arc species	projection		
33	$P_{K,NK}$	P_K_NK	projection of conversion to node conversion	projection		
34	$P_{S,NS}$	P_S_NS	projection species to node species	projection		
35	$P_{N,NK}$	P_N_NK	projection node to node conversion	projection		
36	$P_{NS,KS}$	P_NS_KS	projection node species to conversion species	projection		
37	$P_{A,NS}$	P_A_NS	projection arc to node species for conductivity	projection		
65	$P_{NK,KS}$	P_NK_KS	projection node conversion to conversion species	projection		
10	r_{xN}	r_x	x-coordinate	frame	m	
11	r_{yN}	r_y	y-coordinate	frame	m	
12	r_{zN}	r_z	z coordinate	frame	m	
13	U_N	U	fundamental state – internal energy	state	$kg\,m^2\,s^{-2}$	
14	S_N	S	fundamental state – entropy	state	$kg\,m^2\,K^{-1}\,s^{-2}$	
15	V_N	V	fundamental state – volume	state	m^3	
16	n_{NS}	n	fundamental state – molar mass	state	mol	86
20	H_N	H	enthalpy	state	$kg\,m^2\,s^{-2}$	9 87
21	A_N	A	Helmholtz energy	state	$kg\,m^2\,s^{-2}$	10
22	G_N	G	Gibbs free energy	state	$kg\,m^2\,s^{-2}$	11
23	C_N	charge	fundamental state – charge	state	$A\,s$	
24	A^v	Avogadro	Avogadro number	constant	mol^{-1}	
25	k^B_N	Boltzmann	Boltzmann constant	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	12
26	R_N	GasConstant	gas constant	constant	$kg\,m^2\,mol^{-1}\,K^{-1}\,s^{-2}$	13
17	p_N	p	thermodynamic pressure	effort	$kg\,m^{-1}\,s^{-2}$	6

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	var	symbol	documentation	type	units	eqs
18	T_N	T	temperature	effort	K	7
19	μ_{NS}	chemPot	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	8
27	U_N^C	UC	electrical potential – voltage	effort	$kg\,m^2\,A^{-1}\,s^{-3}$	14
28	v_{xN}	v_x	velocity in x-direction	secondaryState	ms^{-1}	15
29	v_{yN}	v_y	velocity in y-direction	secondaryState	ms^{-1}	16
30	v_{zN}	v_z	velocity in z-direction	secondaryState	ms^{-1}	17

4 control

	var	symbol	documentation	type	units	eqs
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5 reactions

	var	symbol	documentation	type	units	eqs
31	$N_{S,K}$	N	stoichiometric matrix	constant		
38	K^o_K	Ko	Arrhenius frequency factor	constant	$m^{-3} mol s^{-1}$	
62	E^a_{NK}	Ea	Arrhenius activation energy	constant	$kg m^2 mol^{-1} s^{-2}$	41
63	K_{NK}	K_NK	Arrhenius reaction 'constant'	constant	$m^{-3} mol s^{-1}$	42
64	$N_{NS,NK}$	N_NS_NK	stoichiometric block matrix node species and node reaction	constant		43
60	T_{NK}	T_NK	temperature of the reactive system	effort	K	39
68	$c_K S_{KS}$	c_KS	concentrations associated with reactions	secondaryState	$m^{-3} mol$	46
69	$co_K S_{KS}$	co_KS	normalizing concentrations	secondaryState	$m^{-3} mol$	47

6 material

	var	symbol	documentation	type	units	eqs
40	λ_S	Mm	species molecular mass	constant	$kg\ mol^{-1}$	
42	C_{pN}	Cp	total heat capacity at constant pressure	property	$kg\ m^2\ K^{-1}\ s^{-2}$	21
43	C_{VN}	Cv	total heat capacity at constant volume	property	$kg\ m^2\ K^{-1}\ s^{-2}$	22
44	k_{xN}^q	kq_x	thermal conductivity in x-direction	property	$kg\ K^{-1}\ s^{-3}$	23
45	k_{yN}^q	kq_y	thermal conductivity in y-direction	property	$kg\ K^{-1}\ s^{-3}$	24
46	k_{zN}^q	kq_z	thermal conductivity in z-direction'	property	$kg\ K^{-1}\ s^{-3}$	25
47	k_{qN}	kq	thermal conductivity	property	$kg\ K^{-1}\ s^{-3}$	26
48	k_{xN}^c	kc_x	convective mass conductivity in x-direction	property	$m^{-1}\ s$	27
49	k_{yN}^c	kc_y	convective mass conductivity in y-direction	property	$m^{-1}\ s$	28
50	k_{zN}^c	kc_z	convective mass conductivity in z-direction	property	$m^{-1}\ s$	29
51	k_{cN}^c	kc	convective mass conductivity	property	$m^{-1}\ s$	30
52	k_{xNS}^d	kd_x	diffusional mass conductivity in x-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	31
53	k_{yNS}^d	kd_y	diffusional mass conductivity in y-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	32
54	k_{zNS}^d	kd_z	diffusional mass conductivity in z-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	33
55	k_{dNS}^d	kd	diffusional mass conductivity	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	34
56	h_{NS}	h	partial molar enthalpies	property	$kg\ m^2\ mol^{-1}\ s^{-2}$	35
59	ρ_N	density	density	property	$kg\ m^{-3}$	38

7 macroscopic

	var	symbol	documentation	type	units	eqs
92	\hat{V}_A	fV	volumetric flow	transport	$m^3 s^{-1}$	67
93	\hat{n}_{AS}^d	fnd_AS	diffusional mass flow in a given stream	transport	$mol s^{-1}$	68
94	\hat{n}_{NS}^d	fnd	net diffusional mass flow	transport	$mol s^{-1}$	69
95	\hat{H}_{AS}^d	fHd_A	enthalpy flow per diffusional mass stream	transport	$kg m^2 s^{-3}$	70
96	\hat{H}_N^d	fHd	net enthaply stream due to diffusion	transport	$kg m^2 s^{-3}$	71
97	d_A	d	flow direction of convectional flow	transport		72
102	\hat{H}_{AS}^c	fHc_A	convective enthalpy flow for given stream	transport	$kg m^2 s^{-3}$	77
103	\hat{H}_N^c	fHc	net convectional enthalpy stream	transport	$kg m^2 s^{-3}$	78
104	\hat{w}_A	fw_A	sample work stream	transport	$kg m^2 s^{-3}$	79
105	fw_N	fw	net work stream	transport	$kg m^2 s^{-3}$	80
106	\hat{q}_{xA}	fq_A_x	heat flow in x-direction for given stream	transport	$kg m^2 s^{-3}$	81
107	\hat{q}_N	fq	net heat flow	transport	$kg m^2 s^{-3}$	82
71	A_{yzN}	Ayz	cross sectional area yz	geometry	m^2	48
72	A_{xzN}	Axz	cross sectional area xz	geometry	m^2	49
73	A_{xyN}	Axy	cross sectional area xy	geometry	m^2	50
70	$F_{NS,AS}$	F_NS_AS	species related incidence matrix	network		
90	$D_{N,A}$	D	difference operator	differenceOperator		
91	$D_{NS,AS}$	D_NS_AS	difference operator for species topology	differenceOperator		
109	H_N^o	Ho	initial enthalpy	state	$kg m^2 s^{-2}$	84
110	n_{NS}^o	no	initial species	state	mol	85
57	m_N	m	total mass	secondaryState	kg	36
66	c_{NS}	c	molar composition	secondaryState	$m^{-3} mol$	44
98	c_{AS}	c_AS	concentration in convectional flow	secondaryState	$m^{-3} mol$	73

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	var	symbol	documentation	type	units	eqs
99	\hat{n}_{AS}^c	fnc_AS	molar convetional mass flow in the given stream	secondaryState	$mol\ s^{-1}$	74
100	\hat{n}_{NS}^c	fnc	net molar convectional mass flow	secondaryState	$mol\ s^{-1}$	75
101	\dot{n}_{NS}	dndt	differential species balance	diffState	$mol\ s^{-1}$	76
108	\dot{H}_N	dHdt	differential enthalpy balance	diffState	$kg\ m^2\ s^{-3}$	83

8 solid

	var	symbol	documentation	type	units	eqs
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9 fluid

	var	symbol	documentation	type	units	eqs
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10 liquid

	var	symbol	documentation	type	units	eqs
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11 gas

	var	symbol	documentation	type	units	eqs
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12 control-control

	var	symbol	documentation	type	units	eqs
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13 gas–liquid

	var	symbol	documentation	type	units	eqs
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14 gas–gas

	var	symbol	documentation	type	units	eqs
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15 liquid–liquid

	var	symbol	documentation	type	units	eqs
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16 gas–solid

	var	symbol	documentation	type	units	eqs
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17 solid–solid

	var	symbol	documentation	type	units	eqs
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18 liquid–solid

	var	symbol	documentation	type	units	eqs
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19 material–material

	var	symbol	documentation	type	units	eqs
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20 reactions-reactions

	var	symbol	documentation	type	units	eqs
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21 control-reactions

	var	symbol	documentation	type	units	eqs
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22 reactions-control

	var	symbol	documentation	type	units	eqs
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23 control-material

	var	symbol	documentation	type	units	eqs
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24 material-control

	var	symbol	documentation	type	units	eqs
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25 control-macroscopic

	var	symbol	documentation	type	units	eqs
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26 macroscopic-control

	var	symbol	documentation	type	units	eqs
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27 reactions-material

	var	symbol	documentation	type	units	eqs
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28 material-reactions

	var	symbol	documentation	type	units	eqs
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29 reactions–macroscopic

	var	symbol	documentation	type	units	eqs
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30 macroscopic-reactions

	var	symbol	documentation	type	units	eqs
67	c_{NS}	c	link variable c to interface macroscopic »> reactions	get	$m^{-3} mol$	45

31 material–macroscopic

	var	symbol	documentation	type	units	eqs
41	Mm_S	Mm	link variable Mm to interface material »> macroscopic	get	$kg\,mol^{-1}$	20
74	$density_N$	density	link variable density to interface material »> macroscopic	get	$kg\,m^{-3}$	51
75	h_{NS}	h	link variable h to interface material »> macroscopic	get	$kg\,m^2\,mol^{-1}\,s^{-2}$	52
76	kq_{xN}	kq_x	link variable kq x to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	53
77	Cv_N	Cv	link variable Cv to interface material »> macroscopic	get	$kg\,m^2\,K^{-1}\,s^{-2}$	54
78	kq_{yN}	kq_y	link variable kq y to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	55
79	kq_{zN}	kq_z	link variable kq z to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	56
80	kq_N	kq	link variable kq to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	57
81	kc_{xN}	kc_x	link variable kc x to interface material »> macroscopic	get	$m^{-1}\,s$	58
82	Cp_N	Cp	link variable Cp to interface material »> macroscopic	get	$kg\,m^2\,K^{-1}\,s^{-2}$	59
83	kc_{yN}	kc_y	link variable kc y to interface material »> macroscopic	get	$m^{-1}\,s$	60
84	kc_{zN}	kc_z	link variable kc z to interface material »> macroscopic	get	$m^{-1}\,s$	61
85	kc_N	kc	link variable kc to interface material »> macroscopic	get	$m^{-1}\,s$	62
86	kd_{xNS}	kd_x	link variable kd x to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	63
87	kd_{yNS}	kd_y	link variable kd y to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	64
88	kd_{zNS}	kd_z	link variable kd z to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	65

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	var	symbol	documentation	type	units	eqs
89	kd_{NS}	kd	link variable kd to interface material » > macroscopic	get	$kg^{-1} m^{-4} mol^2 s$	66

32 macroscopic-material

	var	symbol	documentation	type	units	eqs
58	m_N	m	link variable m to interface macroscopic » > material	get	<i>kg</i>	37

33 Equations

34 Generic

no	equation	documentation	layer
1	$1 := \text{Instantiate}(\#, \#)$	numerical value 1	root
2	$0 := \text{Instantiate}(\#, \#)$	numerical value zero	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
8	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	chemical potential	physical
9	$H_N := U_N - p_N \cdot V_N$	enthalpy	physical
10	$A_N := U_N - T_N \cdot S_N$	Helmholtz energy	physical
11	$G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$	Gibbs free energy	physical
12	$k^B_N := \text{Instantiate}(S_N, \#)$	Boltzmann constant	physical
13	$R_N := A^v \cdot k^B_N$	gas constant	physical
14	$U^C_N := (C_N)^{-1} \cdot U_N$	electrical potential – voltage	physical
15	$v_{xN} := \frac{\partial r_{xN}}{\partial t}$	velocity in x-direction	physical
16	$v_{yN} := \frac{\partial r_{yN}}{\partial t}$	velocity in y direction	physical

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no	equation	documentation	layer
17	$v_{zN} := \frac{\partial r_{zN}}{\partial t}$	velocity in z-direction	physical
21	$C_{pN} := \frac{\partial H_N}{\partial T_N}$	total heat capacity at constant pressure	material
22	$C_{VN} := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	material
23	$k_{xN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}$	thermal conductivity in x-direction	material
24	$k_{yN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{yN}$	thermal conductivity in y-direction	material
25	$k_{zN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{zN}$	thermal conductivity in z-direction'	material
26	$kq_N := \text{Stack}(k_{xN}^q, k_{yN}^q, k_{zN}^q)$	thermal conductivity	material
27	$k_{xN}^c := \left(\lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass conductivity in x-direction	material
28	$k_{yN}^c := \left(\lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$	convective mass conductivity in y-direction	material
29	$k_{zN}^c := \left(\lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convective mass conductivity in z-direction	material
30	$k^c_N := \text{Stack}(k_{xN}^c, k_{yN}^c, k_{zN}^c)$	convective mass conductivity	material
31	$k_{xNS}^d := (\mu_{NS})^{-1} \cdot \left(v_{xN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in x-direction	material
32	$k_{yNS}^d := (\mu_{NS})^{-1} \cdot \left(v_{yN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in y-direction	material
33	$k_{zNS}^d := (\mu_{NS})^{-1} \cdot \left(v_{zN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in z-direction	material
34	$k^d_{NS} := \text{Stack}(k_{xNS}^d, k_{yNS}^d, k_{zNS}^d)$	diffusional mass conductivity	material

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no	equation	documentation	layer
35	$h_{NS} := H_N \odot (n_{NS})^{-1}$	partial molar enthalpies	material
36	$m_N := M m_S \overset{S \in NS}{\star} n_{NS}$	total mass	macroscopic
38	$\rho_N := m_N \cdot (V_N)^{-1}$	density	material
39	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature of the reactive system	reactions
41	$E^a_{NK} := \text{Instantiate}(P_{N,NK} \overset{N}{\star} R_N \cdot T_{NK}, \#)$	Arrhenius activation energy	reactions
42	$K_{NK} := K^o_K \odot \exp((-E^a_{NK}) \cdot (R_N \overset{N}{\star} P_{N,NK} \cdot T_{NK})^{-1})$	Arrhenius reaction 'constant'	reactions
43	$N_{NS,NK} := P_{S,NS} \overset{S}{\star} (P_{K,NK} \overset{K}{\star} N_{S,K})$	soichiometric block matrix node species and node reaction	reactions
44	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar composition	macroscopic
46	$c_K S_{KS} := c_{NS} \overset{NS}{\star} P_{NS,KS}$	concentrations associated with reactions	reactions
47	$co_K S_{KS} := \text{Instantiate}(c_K S_{KS}, \#)$	norming concentrations	reactions
48	$A_{yzN} := r_{yN} \cdot r_{zN}$	cross sectional area yz	macroscopic
49	$A_{xzN} := r_{xN} \cdot r_{zN}$	cross sectional area xz	macroscopic
50	$A_{xyN} := r_{xN} \cdot r_{yN}$	cross sectional area xy	macroscopic
67	$\hat{V}_A := (density_N)^{-1} \cdot k c_{xN} \cdot A_{yzN} \cdot D_{N,A} \overset{N}{\star} p_N$	volumetric flow	macroscopic
68	$\hat{n}^d_{AS} := A_{yzN} \odot (-k d_{xNS}) \cdot D_{NS,AS} \overset{NS}{\star} \mu_{NS}$	diffusional mass flow in a given stream	macroscopic
69	$\hat{n}^d_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^d_{AS}$	net diffusional mass flow	macroscopic

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no	equation	documentation	layer
70	$\hat{H}^d_A := \left(F_{NS,AS} \overset{NS}{\star} h_{NS} \right) \overset{S \in AS}{\star} \hat{n}^d_{AS}$	enthalpy flow per diffusional mass stream	macroscopic
71	$\hat{H}^d_N := F_{N,A} \overset{A}{\star} \hat{H}^d_A$	net enthaply stream due to diffusion	macroscopic
72	$d_A := \text{sign} \left(F_{N,A} \overset{N}{\star} p_N \right)$	flow direction of convectional flow	macroscopic
73	$c_{AS} := (0.5 \cdot (F_{NS,AS} - d_A \odot F_{NS,AS})) \overset{NS}{\star} c_{NS}$	concentration in convectional flow	macroscopic
74	$\hat{n}^c_{AS} := \hat{V}_A \odot c_{AS}$	molar convetional mass flow in the given stream	macroscopic
75	$\hat{n}^c_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^c_{AS}$	net molar convectional mass flow	macroscopic
76	$\dot{n}_{NS} := \hat{n}^c_{NS} + \hat{n}^d_{NS}$	differential species balance	macroscopic
77	$\hat{H}^c_A := \left(F_{NS,AS} \overset{NS}{\star} h_{NS} \right) \overset{S \in AS}{\star} \hat{n}^c_{AS}$	convective enthalpy flow for given stream	macroscopic
78	$\hat{H}^c_N := F_{N,A} \overset{A}{\star} \hat{H}^c_A$	net convectional enthalpy stream	macroscopic
79	$\hat{w}_A := \text{Instantiate}(\hat{H}^c_A, \#)$	sample work stream	macroscopic
80	$fw_N := F_{N,A} \overset{A}{\star} \hat{w}_A$	net work stream	macroscopic
81	$\hat{q}_{xA} := A_{yzN} \cdot kq_{xN} \cdot D_{N,A} \overset{N}{\star} T_N$	heat flow in x-direction for given stream	macroscopic
82	$\hat{q}_N := F_{N,A} \overset{A}{\star} \hat{q}_{xA}$	net heat flow	macroscopic
83	$\dot{H}_N := \hat{H}^c_N + \hat{H}^d_N + \hat{q}_N + fw_N$	differential enthalpy balance	macroscopic
84	$H^o_N := \text{Instantiate}(H_N, \#)$	initial enthalpy	macroscopic
85	$n^o_{NS} := \text{Instantiate}(n_{NS}, \#)$	initial species	macroscopic
86	$n_{NS} := \int_{t^o}^{t^e} \dot{n}_{NS} dt$	fundamental state – molar mass	macroscopic

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no	equation	documentation	layer
87	$H_N := \int_{t^o}^{t^e} \dot{H}_N \, dt$	enthalpy	macroscopic

35 Interface Link Equation

no	equation	documentation	layer
20	$Mm_S := Mm_S$	interface equation	material → macroscopic
37	$m_N := m_N$	interface equation	macroscopic → material
45	$c_{NS} := c_{NS}$	interface equation	macroscopic → reactions
51	$density_N := density_N$	interface equation	material → macroscopic
52	$h_{NS} := h_{NS}$	interface equation	material → macroscopic
53	$kq_{xN} := kq_{xN}$	interface equation	material → macroscopic
54	$Cv_N := Cv_N$	interface equation	material → macroscopic
55	$kq_{yN} := kq_{yN}$	interface equation	material → macroscopic
56	$kq_{zN} := kq_{zN}$	interface equation	material → macroscopic
57	$kq_N := kq_N$	interface equation	material → macroscopic
58	$kc_{xN} := kc_{xN}$	interface equation	material → macroscopic

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no	equation	documentation	layer
59	$Cp_N := Cp_N$	interface equation	material → macroscopic
60	$kc_{yN} := kc_{yN}$	interface equation	material → macroscopic
61	$kc_{zN} := kc_{zN}$	interface equation	material → macroscopic
62	$kc_N := kc_N$	interface equation	material → macroscopic
63	$kd_{xNS} := kd_{xNS}$	interface equation	material → macroscopic
64	$kd_{yNS} := kd_{yNS}$	interface equation	material → macroscopic
65	$kd_{zNS} := kd_{zNS}$	interface equation	material → macroscopic
66	$kd_{NS} := kd_{NS}$	interface equation	material → macroscopic