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	to	`to`	starting time	constant	s	[]	41
59	te	`te`	end time	constant	s	[]	42

3 physical

	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	$P_{NS,KS}$	`P_NS_KS`	projection node x 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		[]	
15	r_{xN}	`r_x`	x-coordinate	frame	m	[]	

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	var	symbol	documentation	type	units	tokens	eqs
16	$r_{y\,N}$	`r_y`	y-coordinate	frame	m	[]	
17	$r_{z\,N}$	`r_z`	z-coordinate	frame	m	[]	
18	n_{NS}	`n`	foundation state – species mass	state	mol	['mass']	
19	U_N	`U`	foundation state – internal energy	state	$kg\,m^2\,s^{-2}$	['energy']	
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	$kg\,m^2\,s^{-2}$	['energy']	13
30	A_N	`A`	Helmholtz energy	state	$kg\,m^2\,s^{-2}$	['energy']	14
31	G_N	`G`	Gibbs energy	state	$kg\,m^2\,s^{-2}$	['energy']	15
26	N^o	`No`	Avogadro number	constant		[]	10
27	B_N	`B`	Boltzmann constant	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	[]	11
28	R_N	`R`	gas constant	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	[]	12
22	p_N	`p`	thermodynamic pressure	effort	$kg\,m^{-1}\,s^{-2}$	['energy']	7
23	T_N	`T`	temperature	effort	K	['energy']	8
24	μ_{NS}	`chem_potential`	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	['energy', 'mass']	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

5 reactions

	var	symbol	documentation	type	units	tokens	eqs

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	$kg\,m^2\,K^{-1}\,s^{-2}$	['energy']	24
42	$C_{v\,N}$	`Cv`	total heat capacity at constant volume	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	['energy']	25
43	$c_{p\,S}$	`cp`	specific heat capacity at constant pressure	constant	$m^2\,mol^2\,K^{-1}\,s^{-2}$	['energy', 'mass']	26
44	$c_{v\,S}$	`cv`	specific heat capacity at constant volume	constant	$m^2\,mol^2\,K^{-1}\,s^{-2}$	['energy', 'mass']	27
57	to	`to`	starting time	constant	s	[]	40
45	$k^q_{x\,N}$	`kq_x`	thermal conductivity in x-direction	seconaryState	$kg\,K^{-1}\,s^{-3}$	['energy']	28
46	$k^q_{y\,N}$	`kq_y`	thermal conductivity in y-direction	seconaryState	$kg\,K^{-1}\,s^{-3}$	['energy']	29
47	$k^q_{z\,N}$	`kq_z`	thermal conductivity in z-direction	seconaryState	$kg\,K^{-1}\,s^{-3}$	['energy']	30
48	$k^q{}_N$	`kq`	Carthesian thermal conductivity vector	seconaryState	$kg\,K^{-1}\,s^{-3}$	['energy']	31
49	$k^c_{x\,N}$	`kc_x`	convective mass convectivity in x-direction	seconaryState	$m^{-1}\,s$	['energy', 'mass']	32
50	$k^c_{y\,N}$	`kc_y`	convective mass convectivity in y-direction	seconaryState	$m^{-1}\,s$	['energy', 'mass']	33
51	$k^c_{z\,N}$	`kc_z`	convective mass convectivity in z-direction	seconaryState	$m^{-1}\,s$	['energy', 'mass']	34
52	$k^c{}_N$	`kc`	Cartesian convective mass convectivity vector	seconaryState	$m^{-1}\,s$	['energy', 'mass']	35

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	var	symbol	documentation	type	units	tokens	eqs
53	$k^d_{x\,NS}$	`kd_x`	diffusional mass conductivity in x-direction	seconaryState	$kg^{-1}\,m^{-4}\,mol^2\,s$	['energy', 'mass']	36
54	$k^d_{y\,NS}$	`kd_y`	diffusional mass conductivity in y-direction	seconaryState	$kg^{-1}\,m^{-4}\,mol^2\,s$	['energy', 'mass']	37
55	$k^d_{z\,NS}$	`kd_z`	diffusional mass conductivity in z-direction	seconaryState	$kg^{-1}\,m^{-4}\,mol^2\,s$	['energy', 'mass']	38
56	$k^d{}_{NS}$	`kd`	Cartesian diffusional mass conductivity vector	seconaryState	$kg^{-1}\,m^{-4}\,mol^2\,s$	['energy', 'mass']	39

7 macroscopic

	var	symbol	documentation	type	units	tokens	eqs

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

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

21 macroscopic–reactions

	var	symbol	documentation	type	units	tokens	eqs

22 material–macroscopic

	var	symbol	documentation	type	units	tokens	eqs

23 macroscopic–material

	var	symbol	documentation	type	units	tokens	eqs

24 gas–liquid

	var	symbol	documentation	type	units	tokens	eqs

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
10	$N^o := Set(\#, \#)$	Avogadro number	physical
11	$B_N := Set(S_N, \#)$	Boltzmann constant	physical
12	$R_N := B_N \,.\, N^o$	gas 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

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no	equation	documentation	layer
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
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

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no	equation	documentation	layer
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
38	$k^d_{z\,NS} := (\mu_{NS})^{-1} \,.\, \left(v_{z\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	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
40	$to := Set(t, t)$	starting time	material
41	$to := Set(t, t)$	starting time	root
42	$te := Set(t, t)$	end time	root