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		
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	
20	H_N	`H`	enthalpy	state	$kg\,m^2\,s^{-2}$	9
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
18	T_N	`T`	temperature	effort	K	7

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	var	symbol	documentation	type	units	eqs
19	μ_{NS}	`chemPot`	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	8
27	$U^C{}_N$	`UC`	electrical potential – voltage	effort	$kg\,m^2\,A^{-1}s^{-3}$	14
28	v_{xN}	`v_x`	velocitiy 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

5 reactions

	var	symbol	documentation	type	units	eqs
31	$N_{S,K}$	N	soichiometric matrix	constant		
38	$K^o{}_K$	Ko	Arrhenius frequency factor	constant	$m^{-3}\,mol\,s^{-1}$	
39	$E^a{}_{N,NK}$	Ea	Arrhenius activation energy	constant	$kg\,m^2\,mol^{-1}\,s^{-2}$	18 19
60	$T_N K_{NK}$	T_NK	temperature of the reactive system	effort	K	39
61	$K_N K_{N,NK}$	K_NK	reaction 'constant'	effort	$m^{-3}\,mol\,s^{-1}$	40

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^q_{xN}	`kq_x`	thermal conductivity in x-direction	property	$kg\,K^{-1}\,s^{-3}$	23
45	k^q_{yN}	`kq_y`	thermal conductivity in y-direction	property	$kg\,K^{-1}\,s^{-3}$	24
46	k^q_{zN}	`kq_z`	thermal conductivity in z-direction'	property	$kg\,K^{-1}\,s^{-3}$	25
47	kq_N	`kq`	thermal conductivity	property	$kg\,K^{-1}\,s^{-3}$	26
48	k^c_{xN}	`kc_x`	convecitve mass conductivity in x-direction	property	$m^{-1}\,s$	27
49	k^c_{yN}	`kc_y`	convecitve mass conductivity in y-direction	property	$m^{-1}\,s$	28
50	k^c_{zN}	`kc_z`	convecitve mass conductivity in z-direction	property	$m^{-1}\,s$	29
51	$k^c{}_N$	`kc`	convective mass conductivity	property	$m^{-1}\,s$	30
52	k^d_{xNS}	`kd_x`	diffusional mass conductivity in x-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	31
53	k^d_{yNS}	`kd_y`	diffusional mass conductivity in y-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	32
54	k^d_{zNS}	`kd_z`	diffusional mass conductivity in z-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	33
55	$k^d{}_{NS}$	`kd`	diffusional mass condctivity	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	$density_N$	`density`	density	property	$kg\,m^{-3}$	38

7 macroscopic

	var	symbol	documentation	type	units	eqs
57	m_N	`m`	total mass	secondaryState	kg	36

8 solid

	var	symbol	documentation	type	units	eqs

9 fluid

	var	symbol	documentation	type	units	eqs

10 liquid

	var	symbol	documentation	type	units	eqs

11 gas

	var	symbol	documentation	type	units	eqs

12 control–control

	var	symbol	documentation	type	units	eqs

13 gas–liquid

	var	symbol	documentation	type	units	eqs

14 gas–gas

	var	symbol	documentation	type	units	eqs

15 liquid–liquid

	var	symbol	documentation	type	units	eqs

16 gas–solid

	var	symbol	documentation	type	units	eqs

17 solid–solid

	var	symbol	documentation	type	units	eqs

18 liquid–solid

	var	symbol	documentation	type	units	eqs

19 material–material

	var	symbol	documentation	type	units	eqs

20 reactions–reactions

	var	symbol	documentation	type	units	eqs

21 control–reactions

	var	symbol	documentation	type	units	eqs

22 reactions–control

	var	symbol	documentation	type	units	eqs

23 control–material

	var	symbol	documentation	type	units	eqs

24 material–control

	var	symbol	documentation	type	units	eqs

25 control–macroscopic

	var	symbol	documentation	type	units	eqs

26 macroscopic–control

	var	symbol	documentation	type	units	eqs

27 reactions–material

	var	symbol	documentation	type	units	eqs

28 material–reactions

	var	symbol	documentation	type	units	eqs

29 reactions–macroscopic

	var	symbol	documentation	type	units	eqs

30 macroscopic–reactions

	var	symbol	documentation	type	units	eqs

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

32 macroscopic–material

	var	symbol	documentation	type	units	eqs
58	m_N	`m`	link variable m to interface macroscopic »> material	get	kg	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	$H_N := U_N - p_N \,.\, V_N$	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 free energy	physical
12	${k^B}_N := \text{Instantiate}(S_N, \#)$	Boltzmann constant	physical
13	$R_N := A^v \,.\, {k^B}_N$	gas constant	physical
14	${U^C}_N := (C_N)^{-1} \,.\, U_N$	electrical potential – voltage	physical
15	$v_{xN} := \frac{\partial r_{xN}}{\partial t}$	velocitiy 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
18	$E^a{}_{N,NK} := P_{N,NK} \overset{N}{\star} R_N \,.\, T_N$	Arrhenius activation energy	reactions
19	$E^a{}_{N,NK} := \text{Instantiate}(E^a{}_{N,NK}, \#)$	Arrhenius activation energy	reactions
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	$k^q_{xN} := (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial T_N} \,.\, v_{xN}$	thermal conductivity in x-direction	material
24	$k^q_{yN} := (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial T_N} \,.\, v_{yN}$	thermal conductivity in y-direction	material
25	$k^q_{zN} := (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial T_N} \,.\, v_{zN}$	thermal conductivity in z-direction'	material
26	$kq_N := \text{Stack}\left(k^q_{xN}, k^q_{yN}, k^q_{zN}\right)$	thermal conductivity	material
27	$k^c_{xN} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \,.\, (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial p_N} \,.\, v_{xN}$	convecitve mass conductivity in x-direction	material
28	$k^c_{yN} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \,.\, (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial p_N} \,.\, v_{yN}$	convecitve mass conductivity in y-direction	material
29	$k^c_{zN} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \,.\, (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial p_N} \,.\, v_{zN}$	convecitve mass conductivity in z-direction	material
30	$k^c{}_N := \text{Stack}\left(k^c_{xN}, k^c_{yN}, k^c_{zN}\right)$	convective mass conductivity	material
31	$k^d_{xNS} := (\mu_{NS})^{-1} \,.\, \left(v_{xN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in x-direction	material
32	$k^d_{yNS} := (\mu_{NS})^{-1} \,.\, \left(v_{yN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in y-direction	material

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no	equation	documentation	layer
33	$k^d_{z\,NS} := (\mu_{NS})^{-1} \,.\, \left(v_{z\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in z-direction	material
34	$k^d{}_{NS} := \text{Stack}\left(k^d_{x\,NS}, k^d_{y\,NS}, k^d_{z\,NS}\right)$	diffusional mass condctivity	material
35	$h_{NS} := H_N \odot (n_{NS})^{-1}$	partial molar enthalpies	material
36	$m_N := Mm_S \overset{S \in NS}{\star} n_{NS}$	total mass	macroscopic
38	$density_N := m_N \,.\, (V_N)^{-1}$	density	material
39	$T_N K_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature of the reactive system	reactions
40	$K_N K_{N,NK} := K^o{}_K \odot exp((-E^a{}_{N,NK}) \,.\, \left(R_N \overset{N}{\star} P_{N,NK} \,.\, T_N K_{NK}\right)^{-1})$	reaction 'constant'	reactions

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