

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

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	[]	
16	r_{yN}	r_y	y-coordinate	frame	m	[]	
17	r_{zN}	r_z	z-coordinate	frame	m	[]	

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	var	symbol	documentation	type	units	tokens	eqs
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}	mu	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	['energy', 'mass']	9
36	v_{xN}	v_x	velocity in x-direction	seconaryState	ms^{-1}	[]	20
37	v_{yN}	v_y	velocity in y-direction	seconaryState	ms^{-1}	[]	21
38	v_{zN}	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
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5 reactions

	var	symbol	documentation	type	units	tokens	eqs
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6 material

	var	symbol	documentation	type	units	tokens	eqs
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7 macroscopic

	var	symbol	documentation	type	units	tokens	eqs
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8 solid

	var	symbol	documentation	type	units	tokens	eqs
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9 fluid

	var	symbol	documentation	type	units	tokens	eqs
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10 liquid

	var	symbol	documentation	type	units	tokens	eqs
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11 gas

	var	symbol	documentation	type	units	tokens	eqs
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12 control-reactions

	var	symbol	documentation	type	units	tokens	eqs
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13 reactions-control

	var	symbol	documentation	type	units	tokens	eqs
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14 control-material

	var	symbol	documentation	type	units	tokens	eqs
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15 material-control

	var	symbol	documentation	type	units	tokens	eqs
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16 control-macroscopic

	var	symbol	documentation	type	units	tokens	eqs
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17 macroscopic-control

	var	symbol	documentation	type	units	tokens	eqs
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18 reactions–material

	var	symbol	documentation	type	units	tokens	eqs
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19 material–reactions

	var	symbol	documentation	type	units	tokens	eqs
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20 reactions–macroscopic

	var	symbol	documentation	type	units	tokens	eqs
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21 macroscopic–reactions

	var	symbol	documentation	type	units	tokens	eqs
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22 material–macroscopic

	var	symbol	documentation	type	units	tokens	eqs
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23 macroscopic–material

	var	symbol	documentation	type	units	tokens	eqs
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24 gas–liquid

	var	symbol	documentation	type	units	tokens	eqs
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25 gas–solid

	var	symbol	documentation	type	units	tokens	eqs
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26 liquid–solid

	var	symbol	documentation	type	units	tokens	eqs
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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	$R_N := B_N \cdot N^o$	gas constant	physical
13	$H_N := U_N + p_N \cdot V_N$	enthalpy	physical
14	$A_N := U_N - T_N \cdot S_N$	Helmholtz energy	physical
15	$G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$	Gibbs energy	physical
20	$v_{xN} := \frac{\partial r_{xN}}{\partial t}$	velocity in x-direction	physical
21	$v_{yN} := \frac{\partial r_{yN}}{\partial t}$	velocity in y-direction	physical

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no	equation	documentation	layer
22	$v_{zN} := \frac{\partial r_{zN}}{\partial t}$	velocity in z-direction	physical
23	$v_N := Stack(v_{xN}, v_{yN}, v_{zN})$	velocity vector	physical