

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	t^o	to	starting time	constant	s	[]	41
59	t^e	te	end time	constant	s	[]	42

3 physical

	var	symbol	documentation	type	units	tokens	eqs
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	[]	
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

Continued on next page

	var	symbol	documentation	type	units	tokens	eqs
31	G_N	G	Gibbs energy	state	$kg\,m^2\,s^{-2}$	['energy']	15
27	B_N	B	Boltzmann constant	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	[]	11
99	Av	Av	Avogadro number	constant	mol^{-1}	[]	
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_{xN}	v_x	velocity in x-direction	secondaryState	ms^{-1}	[]	20
37	v_{yN}	v_y	velocity in y-direction	secondaryState	ms^{-1}	[]	21
38	v_{zN}	v_z	velocity in z-direction	secondaryState	ms^{-1}	[]	22
39	v_N	v	velocity vector	secondaryState	ms^{-1}	[]	23

4 control

	var	symbol	documentation	type	units	tokens	eqs
--	-----	--------	---------------	------	-------	--------	-----

5 reactions

	var	symbol	documentation	type	units	tokens	eqs
98	$N_{S,K}$	N	stoichiometric matrix	constant		[]	

6 material

	var	symbol	documentation	type	units	tokens	eqs
40	λ_S	Mm	species molecular masses	constant	$kg\,mol^{-1}$	[]	

Continued on next page

	var	symbol	documentation	type	units	tokens	eqs
41	C_{pN}	Cp	total heat capacity at constant pressure	constant	$kg\ m^2\ K^{-1}\ s^{-2}$	['energy']	24
42	C_{vN}	Cv	total heat capacity at constant volume	constant	$kg\ m^2\ K^{-1}\ s^{-2}$	['energy']	25
43	c_{pS}	cp	specific heat capacity at constant pressure	constant	$m^2\ mol^2\ K^{-1}\ s^{-2}$	['energy', 'mass']	26
44	c_{vS}	cv	specific heat capacity at constant volume	constant	$m^2\ mol^2\ K^{-1}\ s^{-2}$	['energy', 'mass']	27
45	k_{xN}^q	kq_x	thermal conductivity in x-direction	seconaryState	$kg\ K^{-1}\ s^{-3}$	['energy']	28
46	k_{yN}^q	kq_y	thermal conductivity in y-direction	seconaryState	$kg\ K^{-1}\ s^{-3}$	['energy']	29
47	k_{zN}^q	kq_z	thermal conductivity in z-direction	seconaryState	$kg\ K^{-1}\ s^{-3}$	['energy']	30
48	k_N^q	kq	Cartesian thermal conductivity vector	seconaryState	$kg\ K^{-1}\ s^{-3}$	['energy']	31
49	k_{xN}^c	kc_x	convective mass convectivity in x-direction	seconaryState	$m^{-1}\ s$	['energy', 'mass']	32
50	k_{yN}^c	kc_y	convective mass convectivity in y-direction	seconaryState	$m^{-1}\ s$	['energy', 'mass']	33
51	k_{zN}^c	kc_z	convective mass convectivity in z-direction	seconaryState	$m^{-1}\ s$	['energy', 'mass']	34
52	k_N^c	kc	Cartesian convective mass convectivity vector	seconaryState	$m^{-1}\ s$	['energy', 'mass']	35
53	k_{xNS}^d	kd_x	diffusional mass conductivity in x-direction	seconaryState	$kg^{-1}\ m^{-4}\ mol^2\ s$	['energy', 'mass']	36
54	k_{yNS}^d	kd_y	diffusional mass conductivity in y-direction	seconaryState	$kg^{-1}\ m^{-4}\ mol^2\ s$	['energy', 'mass']	37
55	k_{zNS}^d	kd_z	diffusional mass conductivity in z-direction	seconaryState	$kg^{-1}\ m^{-4}\ mol^2\ s$	['energy', 'mass']	38
56	k_{NS}^d	kd	Cartesian diffusional mass conductivity vector	seconaryState	$kg^{-1}\ m^{-4}\ mol^2\ s$	['energy', 'mass']	39
60	h_{NS}	h	partial molar enthalpies	seconaryState	$kg\ m^2\ mol^{-1}\ s^{-2}$	['energy', 'mass']	43

7 macroscopic

	var	symbol	documentation	type	units	tokens	eqs
78	d_A	d	direction of convective flow	transport		[]	61
80	A_{y,z_N}	Ayz	cross sectional area in x-direction	transport	m^2	[]	63
83	\hat{V}_A	fV	convective volumetric flow	transport	$m^3 s^{-1}$	['mass']	66
84	c_{AS}	c_AS	molar species concentration in convective flow	transport	$m^{-3} mol$	['mass']	67
85	\hat{n}_{AS}^c	fnc_AS	convective mass flow by stream	transport	$mol s^{-1}$	['mass']	68
86	\hat{n}_{NS}^c	fnc	net convective mass flow	transport	$mol s^{-1}$	['mass']	69
87	\hat{n}_{AS}^d	fnd_AS	diffusional mass flow by stream	transport	$mol s^{-1}$	['energy']	70
88	\hat{n}_{NS}^d	fnd	net diffusional mass flow	transport	$mol s^{-1}$	['energy']	71
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	$P_{S,NS}$	P_S_NS	projection 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		[]	
95	$P_N S_K S_{NS,KS}$	P_NS_KS	projection node x species to conversion x species	projection		[]	
92	$one_N K_{NK}$	one_NK	one with energy	effort		['energy']	75
79	c_{NS}	c	molar concentration	secondaryState	$m^{-3} mol$	['mass']	62
81	m_N	m	mass in kg	secondaryState	kg	['mass']	64
82	ρ_N	density	density	secondaryState	$kg m^{-3}$	['mass']	65
91	$T_N K_{NK}$	T_NK	temperature in reactive systems	conversion	K	['energy']	74
96	$c_K S_{KS}$	c_KS	concentration in the reactive systems	conversion	$m^{-3} mol$	['mass']	78

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
94	$T_N K_{NK}$	T_NK	temperature of reactive systems	transform	K	['energy']	77
97	$c_K S_{KS}$	c_KS	link	transform	$m^{-3} mol$	['mass']	79

22 material-macroscopic

	var	symbol	documentation	type	units	tokens	eqs
61	λ_S	Mm	link to molar masses	transform	$kg mol^{-1}$	[]	44
62	k_{xN}^a	kq_x	link	transform	$kg K^{-1} s^{-3}$	['energy']	45
63	k_{yN}^a	kq_y	link	transform	$kg K^{-1} s^{-3}$	['energy']	46
64	k_{zN}^a	kq_z	link	transform	$kg K^{-1} s^{-3}$	['energy']	47
65	k_N^a	kq	link	transform	$kg K^{-1} s^{-3}$	['energy']	48
66	k_{xN}^c	kc_x	link	transform	$m^{-1} s$	['energy', 'mass']	49
67	k_{yN}^c	kc_y	link	transform	$m^{-1} s$	['energy', 'mass']	50
68	k_{zN}^c	kc_z	link	transform	$m^{-1} s$	['energy', 'mass']	51
69	k_N^c	kc	link	transform	$m^{-1} s$	['energy', 'mass']	52
70	k_{xNS}^d	kd_x	link	transform	$kg^{-1} m^{-4} mol^2 s$	['energy', 'mass']	53

Continued on next page

	var	symbol	documentation	type	units	tokens	eqs
73	k_{yNS}^d	kd_y	link	transform	$kg^{-1} m^{-4} mol^2 s$	['energy', 'mass']	56
74	k_{zNS}^d	kd_z	link	transform	$kg^{-1} m^{-4} mol^2 s$	['energy', 'mass']	57
75	k_{NS}^d	kd	link	transform	$kg^{-1} m^{-4} mol^2 s$	['energy', 'mass']	58
76	c_{pS}	cp	link	transform	$m^2 mol^2 K^{-1} s^{-2}$	['energy', 'mass']	59
77	c_{vS}	cv	link	transform	$m^2 mol^2 K^{-1} s^{-2}$	['energy', 'mass']	60

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	$F_{NS,AS} := F_{N,A} \odot P_{NS,AS}$	block 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
11	$B_N := Set(S_N, \#)$	Boltzmann 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
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

Continued on next page

no	equation	documentation	layer
24	$C_{pN} := \frac{\partial H_N}{\partial T_N}$	total heat capacity at constant pressure	material
25	$C_{vN} := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	material
26	$c_{pS} := C_{pN} \cdot (\lambda_S)^{-1} \stackrel{N \in NS}{\star} n_{NS}$	specific heat capacity at constant pressure	material
27	$c_{vS} := C_{vN} \cdot (\lambda_S)^{-1} \stackrel{N \in NS}{\star} n_{NS}$	specific heat capacity at constant volume	material
28	$k_{xN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}$	thermal conductivity in x-direction	material
29	$k_{yN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{yN}$	thermal conductivity in y-direction	material
30	$k_{zN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{zN}$	thermal conductivity in z-direction	material
31	$k_N^q := \text{Stack} \left(k_{xN}^q, k_{yN}^q, k_{zN}^q \right)$	Cartesian thermal conductivity vector	material
32	$k_{xN}^c := \left(\lambda_S \stackrel{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass conductivity in x-direction	material
33	$k_{yN}^c := \left(\lambda_S \stackrel{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$	convective mass conductivity in y-direction	material
34	$k_{zN}^c := \left(\lambda_S \stackrel{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convective mass conductivity in z-direction	material
35	$k_N^c := \text{Stack} \left(k_{xN}^c, k_{yN}^c, k_{zN}^c \right)$	Cartesian convective mass conductivity vector	material
36	$k_{xNS}^d := (\mu_{NS})^{-1} \cdot \left(v_{xN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in x-direction	material
37	$k_{yNS}^d := (\mu_{NS})^{-1} \cdot \left(v_{yN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in y-direction	material

Continued on next page

no	equation	documentation	layer
38	$k_{zNS}^d := (\mu_{NS})^{-1} \cdot \left(v_{zN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in z-direction	material
39	$k_{NS}^d := Stack \left(k_{xNS}^d, k_{yNS}^d, k_{zNS}^d \right)$	Cartesian diffusional mass conductivity vector	material
41	$t^o := Set(t, t)$	starting time	root
42	$t^e := Set(t, t)$	end time	root
43	$h_{NS} := H_N \odot (n_{NS})^{-1}$	partial molar enthalpies	material
44	$\lambda_S := \lambda_S$	link to molar masses	material » macroscopic
45	$k_{xN}^q := k_{xN}^q$	link	material » macroscopic
46	$k_{yN}^q := k_{yN}^q$	link	material » macroscopic
47	$k_{zN}^q := k_{zN}^q$	link	material » macroscopic
48	$k_N^q := k_N^q$	link	material » macroscopic
49	$k_{xN}^c := k_{xN}^c$	link	material » macroscopic
50	$k_{yN}^c := k_{yN}^c$	link	material » macroscopic
51	$k_{zN}^c := k_{zN}^c$	link	material » macroscopic

Continued on next page

no	equation	documentation	layer
52	$k_N^c := k_N^c$	link	material » macroscopic
53	$k_{NS}^d := k_{NS}^d$	link	material » macroscopic
56	$k_{yNS}^d := k_{yNS}^d$	link	material » macroscopic
57	$k_{zNS}^d := k_{zNS}^d$	link	material » macroscopic
58	$k_{NS}^d := k_{NS}^d$	link	material » macroscopic
59	$c_{pS} := c_{pS}$	link	material » macroscopic
60	$c_{vS} := c_{vS}$	link	material » macroscopic
61	$d_A := \text{sign} \left(F_{N,A} \overset{N}{\star} p_N \right)$	direction of convective flow	macroscopic
62	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar concentration	macroscopic
63	$A_{y,zN} := r_{yN} \cdot r_{zN}$	cross sectional area in x-direction	macroscopic
64	$m_N := \lambda_S \overset{S \in NS}{\star} n_{NS}$	mass in kg	macroscopic
65	$\rho_N := (V_N)^{-1} \cdot m_N$	density	macroscopic
66	$\hat{V}_A := (\rho_N)^{-1} \cdot k_{xN}^c \cdot A_{y,zN} \cdot F_{N,A} \overset{N}{\star} p_N$	convective volumetric flow	macroscopic
67	$c_{AS} := (1/2 \cdot (F_{NS,AS} - d_A \odot F_{NS,AS})) \overset{NS}{\star} c_{NS}$	molar species concentration in convective flow	macroscopic

Continued on next page

no	equation	documentation	layer
68	$\hat{n}_{AS}^c := \hat{V}_A \odot c_{AS}$	convective mass flow by stream	macroscopic
69	$\hat{n}_{NS}^c := F_{NS,AS} \overset{AS}{\star} \hat{n}_{AS}^c$	net convective mass flow	macroscopic
70	$\hat{n}_{AS}^d := A_{y,z_N} \odot (-k_{x_{NS}}^d) \cdot F_{NS,AS} \overset{NS}{\star} \mu_{NS}$	diffusional mass flow by stream	macroscopic
71	$\hat{n}_{NS}^d := F_{NS,AS} \overset{AS}{\star} \hat{n}_{AS}^d$	net diffusional mass flow	macroscopic
74	$T_N K_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature in reactive systems	macroscopic
75	$one_N K_{NK} := (T_N K_{NK})^{-1} \cdot T_N K_{NK}$	one with energy	macroscopic
77	$T_N K_{NK} := T_N K_{NK}$	temperature of reactive systems	macroscopic »> re- actions
78	$c_K S_{KS} := c_{NS} \overset{NS}{\star} P_N S_K S_{NS,KS}$	concentration in the reactive systems	macroscopic
79	$c_K S_{KS} := c_K S_{KS}$	link	macroscopic »> re- actions