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
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

1

	var	symbol	documentation	type	units	tokens	eqs
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	$kg\,mol^{-1}$	[]	

Continued on next page

		var	symbol	documentation	type	units	tokens	eqs
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
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

Continued on next page

	var	symbol	documentation	type	units	tokens	eqs
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	$\hat{n}^c_{AS}$	fnc_AS	convective mass flow by stream	transport	$mol\,s^{-1}$	['mass']	68
86	$\hat{n}^c_{NS}$	fnc	net convective mass flow	transport	$mol\,s^{-1}$	['mass']	69
87	$\hat{n}^d_{AS}$	fnd_AS	diffusional mass flow by stream	transport	$mol\,s^{-1}$	['energy']	70
88	$\hat{n}^d_{NS}$	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 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		[]	
79	c_{NS}	c	molar concentration	seconaryState	$m^{-3}\,mol$	['mass']	62
81	m_N	m	mass in kg	seconaryState	kg	['mass']	64
82	ρ_N	density	density	seconaryState	$kg\,m^{-3}$	['mass']	65

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
89		T_N	T	link	transform	K	['energy']	72
90		c_{NS}	c	link	transform	$m^{-3}\,mol$	['mass']	73

22 material–macroscopic

		var	symbol	documentation	type	units	tokens	eqs
61		Mm_S	Mm	link to molar masses	transform	$kg\,mol^{-1}$	[]	44
62		kq_{x_N}	kq_x	link	transform	$kg\,K^{-1}\,s^{-3}$	['energy']	45
63		kq_{y_N}	kq_y	link	transform	$kg\,K^{-1}\,s^{-3}$	['energy']	46
64		kq_{z_N}	kq_z	link	transform	$kg\,K^{-1}\,s^{-3}$	['energy']	47
65		kq_N	kq	link	transform	$kg\,K^{-1}\,s^{-3}$	['energy']	48
66		kc_{x_N}	kc_x	link	transform	$m^{-1}\,s$	['energy', 'mass']	49
67		kc_{y_N}	kc_y	link	transform	$m^{-1}\,s$	['energy', 'mass']	50
68		kc_{z_N}	kc_z	link	transform	$m^{-1}\,s$	['energy', 'mass']	51
69		kc_N	kc	link	transform	$m^{-1}\,s$	['energy', 'mass']	52
70		$kd_{x_{NS}}$	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
71	kd_{NS}	kd	link	transform	$kg^{-1}\,m^{-4}\,mol^2\,s$	['energy', 'mass']	54
72	kd_{xNS}	kd_x	link	transform	$kg^{-1}\,m^{-4}\,mol^2\,s$	['energy', 'mass']	55
73	kd_{yNS}	kd_y	link	transform	$kg^{-1}\,m^{-4}\,mol^2\,s$	['energy', 'mass']	56
74	kd_{zNS}	kd_z	link	transform	$kg^{-1}\,m^{-4}\,mol^2\,s$	['energy', 'mass']	57
75	kd_{NS}	kd	link	transform	$kg^{-1}\,m^{-4}\,mol^2\,s$	['energy', 'mass']	58
76	cp_S	cp	link	transform	$m^2\,mol^2\,K^{-1}\,s^{-2}$	['energy', 'mass']	59
77	cv_S	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	$F_{NS,AS} := F_{N,A} \odot P_{NS,AS}$	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

no	equation	documentation	layer
22	$v_{zN} := \frac{\partial r_{zN}}{\partial t}$	velocity in z-direction	physical
23	$v_N := Stack\left(v_{xN}, v_{yN}, v_{zN}\right)$	velocity vector	physical
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	$c_{pS} := C_{pN} \cdot (\lambda_S)^{-1} \overset{N \in NS}{\star} n_{NS}$	specific heat capacity at constant pressure	material
27	$c_{vS} := C_{vN} \cdot (\lambda_S)^{-1} \overset{N \in NS}{\star} n_{NS}$	specific heat capacity at constant volume	material
28	$k^q_{xN} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}$	thermal conductivity in x-direction	material
29	$k^q_{yN} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{yN}$	thermal conductivity in y-direction	material
30	$k^q_{zN} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{zN}$	thermal conductivity in z-direction	material
31	$k^q_N := Stack\left(k^q_{xN}, k^q_{yN}, k^q_{zN}\right)$	Carthesian thermal conductivity vector	material
32	$k^c_{xN} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass convectivity in x-direction	material
33	$k^c_{yN} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$	convective mass convectivity in y-direction	material
34	$k^c_{zN} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convective mass convectivity in z-direction	material
35	$k^c_N := Stack\left(k^c_{xN}, k^c_{yN}, k^c_{zN}\right)$	Cartesian convective mass convectivity vector	material
36	$k^d_{xNS} := (\mu_{NS})^{-1} \cdot \left(v_{xN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in x-direction	material

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
43	$h_{NS} := H_N \odot (n_{NS})^{-1}$	partial molar enthalpies	material
44	$Mm_S := \lambda_S$	link to molar masses	material »> macroscopic
45	$kq_{x\,N} := k^q_{x\,N}$	link	material »> macroscopic
46	$kq_{y\,N} := k^q_{y\,N}$	link	material »> macroscopic
47	$kq_{z\,N} := k^q_{z\,N}$	link	material »> macroscopic
48	$kq_N := k^q{}_N$	link	material »> macroscopic
49	$kc_{x\,N} := k^c_{x\,N}$	link	material »> macroscopic

no	equation	documentation	layer
50	$kc_{y_N} := k^c_{y_N}$	link	material »> macro-scopic
51	$kc_{z_N} := k^c_{z_N}$	link	material »> macro-scopic
52	$kc_N := k^c_N$	link	material »> macro-scopic
53	$kd_{x_{NS}} := k^d_{x_{NS}}$	link	material »> macro-scopic
54	$kd_{NS} := k^d_{NS}$	link	material »> macro-scopic
55	$kd_{x_{NS}} := k^d_{x_{NS}}$	link	material »> macro-scopic
56	$kd_{y_{NS}} := k^d_{y_{NS}}$	link	material »> macro-scopic
57	$kd_{z_{NS}} := k^d_{z_{NS}}$	link	material »> macro-scopic
58	$kd_{NS} := k^d_{NS}$	link	material »> macro-scopic
59	$cp_S := c_{p_S}$	link	material »> macro-scopic
60	$cv_S := c_{v_S}$	link	material »> macro-scopic
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

no	equation	documentation	layer
63	$A_{y,z\,N} := r_{y\,N} \cdot r_{z\,N}$	cross sectional area in x-direction	macroscopic
64	$m_N := Mm_S \overset{S \in NS}{\star} n_{NS}$	mass in kg	macroscopic
65	$\rho_N := (V_N)^{-1} \cdot m_N$	density	macroscopic
66	$\hat{V}_A := (\rho_N)^{-1} \cdot kc_{x\,N} \cdot A_{y,z\,N} \cdot F_{N,A} \overset{N}{\star} p_N$	convective volumetric flow	macroscopic
67	$c_{AS} := (1/2 \cdot (F_{NS,AS} - d_A \odot \lvert F_{NS,AS} \rvert)) \overset{NS}{\star} c_{NS}$	molar species concentration in convective flow	macroscopic
68	$\hat{n}^c_{AS} := \hat{V}_A \odot c_{AS}$	convective mass flow by stream	macroscopic
69	$\hat{n}^c_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^c_{AS}$	net convective mass flow	macroscopic
70	$\hat{n}^d_{AS} := A_{y,z\,N} \odot (-kd_{x\,NS}) \cdot F_{NS,AS} \overset{NS}{\star} \mu_{NS}$	diffusional mass flow by stream	macroscopic
71	$\hat{n}^d_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^d_{AS}$	net diffusional mass flow	macroscopic
72	$T_N := T_N$	link	macroscopic »> reactions
73	$c_{NS} := c_{NS}$	link	macroscopic »> reactions