

1 Variables

2 root

	var	symbol	documentation	type	units	tokens	eqs
5	$F_{N,A}$	F	incidence matrix of a directed graph	network		[]	
6	t	t	time	frame	<i>s</i>	[]	
7	t_o	to	starting time	frame	<i>s</i>	[]	4
8	t_e	te	end time	frame	<i>s</i>	[]	5
1	#	value	numerical value	constant		[]	
2	0	zero	numerical value zero	constant		[]	1
3	1	one	numerical value one	constant		[]	2
4	0.5	onehalf	numerical value one half	constant		[]	3

3 physical

	var	symbol	documentation	type	units	tokens	eqs
9	r_{xN}	r_x	x-coordinate	frame	m	[]	
10	r_{yN}	r_y	y-coordinate	frame	m	[]	
23	r_{zN}	r_z	z-coordinate	frame	m	[]	
11	U_N	U	foundation state – internal energy	state	$kg\ m^2\ s^{-2}$	[]	
12	S_N	S	foundation state – entropy	state	$kg\ m^2\ K^{-1}\ s^{-2}$	[]	
13	V_N	V	foundation state – volume	state	m^3	[]	
18	H_N	H	enthalpy	state	$kg\ m^2\ s^{-2}$	[]	9
19	A_N	A	Helmholtz energy	state	$kg\ m^2\ s^{-2}$	[]	10
20	G_N	G	Gibbs energy	state	$kg\ m^2\ s^{-2}$	[]	11
42	n_{NS}	n	species molar mass	state	mol	[]	
26	A^v	Avogadro	Avogadro number	constant	mol^{-1}	[]	
27	Bo_N	Boltzmann	Boltzmann constant	constant	$kg\ m^2\ K^{-1}\ s^{-2}$	[]	16
28	R_N	GasConstant	Gas constant	constant	$kg\ m^2\ mol^{-1}\ K^{-1}\ s^{-2}$	[]	17
15	p_N	p	thermodynamic pressure	effort	$kg\ m^{-1}\ s^{-2}$	[]	6
16	T_N	T	temperature	effort	K	[]	7
45	μ_{NS}	chem_pot	chemical potential	effort	$kg\ m^2\ mol^{-1}\ s^{-2}$	[]	32
21	v_{xN}	v_x	velocity in x-direction	secondaryState	ms^{-1}	[]	12
22	v_{yN}	v_y	velocity in y direction	secondaryState	ms^{-1}	[]	13
24	v_{zN}	v_z	velocity in z-direction	secondaryState	ms^{-1}	[]	14
25	v_N	v	velocity vector	secondaryState	ms^{-1}	[]	15

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
29	S	Mm	species molecular masses	constant	$kg\ mol^{-1}$	[]	
46	C_{pN}	C_p	total heat capacity at constant pressure	seconaryState	$kg\ m^2\ K^{-1}\ s^{-2}$	[]	33
47	C_{vN}	C_v	specific heat capacity at constant volume	seconaryState	$kg\ m^2\ K^{-1}\ s^{-2}$	[]	34
48	c_{pS}	cp	specific heat capacity at constant pressure	seconaryState	$m^2\ mol^2\ K^{-1}\ s^{-2}$	[]	35
49	c_{vS}	cv	specific heat capacity at constant volume	seconaryState	$m^2\ mol^2\ K^{-1}\ s^{-2}$	[]	36
30	C_{pN}	Cp	total heat capacity at constant pressure	property	$kg\ m^2\ K^{-1}\ s^{-2}$	[]	18
31	C_{vN}	Cv	total heat capacity at constant volume	property	$kg\ m^2\ K^{-1}\ s^{-2}$	[]	19
34	k_{xN}^q	kq_x	thermal conductivity in x-direction	property	$kg\ K^{-1}\ s^{-3}$	[]	22
35	k_{yN}^q	kq_y	thermal conductivity in y-direction	property	$kg\ K^{-1}\ s^{-3}$	[]	23
36	k_{zN}^q	kq_z	thermal conductivity in z-direction	property	$kg\ K^{-1}\ s^{-3}$	[]	24
37	k_N^q	kq	Cartesian thermal conductivity vector	property	$kg\ K^{-1}\ s^{-3}$	[]	25
50	k_{xN}^c	kc_x	convective mass convectivity in x-direction	property	$m^{-1}\ s$	[]	37
51	k_{yN}^c	kc_y	convective mass convectivity in y-direction	property	$m^{-1}\ s$	[]	38
52	k_{zN}^c	kc_z	convective mass convectivity in z-direction	property	$m^{-1}\ s$	[]	39
53	k_N^c	kc	Cartesian convective mass convectivity vector	property	$m^{-1}\ s$	[]	40
54	k_{xNS}^d	kd_x	diffusional mass conductivity in x-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	[]	41
55	k_{yNS}^d	kd_y	diffusional mass conductivity in y-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	[]	42
56	k_{zNS}^d	kd_z	diffusional mass conductivity in z-direction	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	[]	43
57	k_{NS}^d	kd	Cartesian dffusional mass conductivity vector	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	[]	44
58	h_{NS}	h	partial molar enthalpies	property	$kg\ m^2\ mol^{-1}\ s^{-2}$	[]	45
71	ρ_N	density	mass density	property	$kg\ m^{-3}$	[]	49

7 macroscopic

	var	symbol	documentation	type	units	tokens	eqs
65	d_A	d	direction of convective flow	transport		[]	46
72	\hat{V}_A	fV	volumetric flow in x-direction	transport	ms^{-1}	[]	50
74	$c_{N,AS}$	c_AS	concentration in convective flow	transport	$m^{-3} mol$	[]	52
75	$\hat{n}_{N,AS}^c$	fnc_AS	convective mass flow by stream	transport	$m^{-2} mol s^{-1}$	[]	53
76	$\hat{n}_{N,NS}^c$	fnc	net convective mass flow	transport	$m^{-2} mol s^{-1}$	[]	54
79	$\hat{m}_{N,A}$	fm_A	mass flow in arc	transport	$kg m^{-2} s^{-1}$	[]	57
80	$\hat{H}_{N,A}^c$	fHc_A	enthalpy flow due to convection	transport	$kg s^{-3}$	[]	58
81	\hat{H}_N^c	fHc	net enthalpy flow due to convection	transport	$kg s^{-3}$	[]	59
66	A_{yz}	A_yz	cross sectional area in x-direction	geometry		[]	
67	A_{xz}	A_xz	cross sectional area in y-direction	geometry		[]	
68	A_{xy}	A_xy	cross sectional area in z-direction	geometry		[]	
73	$F_{NS,AS}$	F_NS_AS	incidence matrix of directed graphs for for species NS x AS	network		[]	51
59	$P_{NS,AS}$	P_NS_AS	node species to arc species projection	projection		[]	
60	$P_{K,NK}$	P_K_NK	projection of conversion to node x conversion	projection		[]	
61	$P_{S,NS}$	P_S_NS	projection species to conversion x species	projection		[]	
62	$P_{N,NK}$	P_N_NK	projection node to node x conversion	projection		[]	
63	$P_{NK,KS}$	P_NK_KS	projection node x conversion to conversion x species	projection		[]	
64	$P_{NS,KS}$	P_NS_KS	projection node x species to conversion x species	projection		[]	
69	m_N	m	mass	seconaryState	kg	[]	47
70	$c_{N,NS}$	c	molar concentration	seconaryState	$m^{-3} mol$	[]	48
77	T_{NK}	T_NK	temperature in reactive systems	conversion	K	[]	55

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	var	symbol	documentation	type	units	tokens	eqs
78	$c_{N,KS}$	c_KS	concentration in the reactive systems	conversion	$m^{-3} mol$	[]	56

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-control

	var	symbol	documentation	type	units	tokens	eqs
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13 gas–liquid

	var	symbol	documentation	type	units	tokens	eqs
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14 gas–gas

	var	symbol	documentation	type	units	tokens	eqs
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15 liquid–liquid

	var	symbol	documentation	type	units	tokens	eqs
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16 gas–solid

	var	symbol	documentation	type	units	tokens	eqs
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17 solid–solid

	var	symbol	documentation	type	units	tokens	eqs
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18 liquid–solid

	var	symbol	documentation	type	units	tokens	eqs
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19 material–material

	var	symbol	documentation	type	units	tokens	eqs
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20 reactions-reactions

	var	symbol	documentation	type	units	tokens	eqs
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21 Equations

22 Generic

no	equation	documentation	layer
1	$0 := \text{Instantiate}(\#, \#)$	numerical value zero	root
2	$1 := \text{Instantiate}(\#, \#)$	numerical value one	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
9	$H_N := U_N - p_N \cdot V_N$	enthalpy	physical
10	$A_N := U_N - T_N \cdot S_N$	Helmholtz energy	physical
11	$G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$	Gibbs energy	physical
12	$v_{xN} := \frac{\partial r_{xN}}{\partial t}$	velocity in x-direction	physical
13	$v_{yN} := \frac{\partial r_{yN}}{\partial t}$	velocity in y direction	physical
14	$v_{zN} := \frac{\partial r_{zN}}{\partial t}$	velocity in z-direction	physical
15	$v_N := \text{Stack}(v_{xN}, v_{yN}, v_{zN})$	velocity vector	physical
16	$Bo_N := \text{Instantiate}(S_N, \#)$	Boltzmann constant	physical
17	$R_N := A^v \cdot Bo_N$	Gas constant	physical

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no	equation	documentation	layer
18	$C_{pN} := \frac{\partial H_N}{\partial T_N}$	total heat capacity	material
19	$C_{vN} := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	material
22	$k_{xN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}$	thermal conductivity in x-direction	material
23	$k_{yN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{yN}$	thermal conductivity in y-direction	material
24	$k_{zN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{zN}$	thermal conductivity in z-direction	material
25	$k_N^q := \text{Stack}(k_{xN}^q, k_{yN}^q, k_{zN}^q)$	Cartesian thermal conductivity vector	material
32	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	chemical potential	physical
33	$C_{pN} := \frac{\partial H_N}{\partial T_N}$	total heat capacity at constant pressure	material
34	$C_{vN} := \frac{\partial U_N}{\partial T_N}$	specic heat capacity at constant volume	material
35	$c_{pS} := C_{pN} \cdot (S)^{-1} \stackrel{N \in NS}{\star} n_{NS}$	specific heat capacity at constant pressure	material
36	$c_{vS} := C_{vN} \cdot (S)^{-1} \stackrel{N \in NS}{\star} n_{NS}$	specific heat capacity at constant volume	material
37	$k_{xN}^c := \left(S \stackrel{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass convectivity in x-direction	material
38	$k_{yN}^c := \left(S \stackrel{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$	convective mass convectivity in y-direction	material
39	$k_{zN}^c := \left(S \stackrel{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convective mass convectivity in z-direction	material
40	$k_N^c := \text{Stack}(k_{xN}^c, k_{yN}^c, k_{zN}^c)$	Cartesian convective mass convectivity vector	material

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no	equation	documentation	layer
41	$k_{xNS}^d := (\mu_{NS})^{-1} \cdot \left(v_{xN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in x-direction	material
42	$k_{yNS}^d := (\mu_{NS})^{-1} \cdot \left(v_{yN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in y-direction	material
43	$k_{zNS}^d := (\mu_{NS})^{-1} \cdot \left(v_{zN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in z-direction	material
44	$k_{NS}^d := \text{Stack}(k_{xNS}^d, k_{yNS}^d, k_{zNS}^d)$	Cartesian diffusional mass conductivity vector	material
45	$h_{NS} := H_N \odot (n_{NS})^{-1}$	partial molar enthalpies	material
46	$d_A := \text{sign} \left(F_{N,A} \overset{N}{\star} p_N \right)$	direction of convective ow	macroscopic
47	$m_N := \overset{S \in NS}{\star} n_{NS}$	mass	macroscopic
48	$c_{N,NS} := (V_N)^{-1} \cdot n_{NS}$	molar concentration	macroscopic
49	$\rho_N := m_N \cdot (V_N)^{-1}$	mass density	material
50	$\hat{V}_A := (\rho_N)^{-1} \cdot k_{xN}^c \cdot A_{yz} \cdot F_{N,A} \overset{N}{\star} p_N$	volumetric flow in x-direction	macroscopic
51	$F_{NS,AS} := F_{N,A} \odot P_{NS,AS}$	incidence matrix of directed graphs for species NS x AS	macroscopic
52	$c_{N,AS} := (0.5 \cdot (F_{NS,AS} - d_A \odot F_{NS,AS})) \overset{NS}{\star} c_{N,NS}$	concentration in convective flow	macroscopic
53	$\hat{n}_{N,AS}^c := \hat{V}_A \odot c_{N,AS}$	convective mass ow by stream	macroscopic
54	$\hat{n}_{N,NS}^c := F_{NS,AS} \overset{AS}{\star} \hat{n}_{N,AS}^c$	net convective mass flow	macroscopic
55	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature in reactive systems	macroscopic
56	$c_{N,KS} := c_{N,NS} \overset{NS}{\star} P_{NS,KS}$	concentration in the reactive systems	macroscopic

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no	equation	documentation	layer
57	$\hat{m}_{N,A} := {}_S \overset{S \in AS}{\star} \hat{n}_{N,AS}^c$	mass ow in arc	macroscopic
58	$\hat{H}_{N,A}^c := \left(F_{NS,AS} \overset{NS}{\star} h_{NS} \right) {}_S \overset{S \in AS}{\star} \hat{n}_{N,AS}^c$	enthalpy ow due to convection	macroscopic
59	$\hat{H}_N^c := F_{N,A} \overset{A}{\star} \hat{H}_{N,A}^c$	net enthalpy ow due to convection	macroscopic