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	s	[]	
7	t_o	`to`	starting time	frame	s	[]	4
8	t_e	`te`	end time	frame	s	[]	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	seconaryState	ms^{-1}	[]	12
22	v_{yN}	`v_y`	velocity in y direction	seconaryState	ms^{-1}	[]	13
24	v_{zN}	`v_z`	velocity in z-direction	seconaryState	ms^{-1}	[]	14
25	v_N	`v`	velocity vector	seconaryState	ms^{-1}	[]	15

4 control

	var	symbol	documentation	type	units	tokens	eqs

5 reactions

	var	symbol	documentation	type	units	tokens	eqs
86	$N_{S,K}$	`N`	stoichiometric matrix	constant		[]	
87	E_{aNK}	`Ea`	Arrhenius's activation energy	constant	$kg\, m^2\, mol^{-1}\, s^{-2}$	[]	64
88	${K^o}_K$	`Ko`	Arrhenius's frequency factor	constant	$m^{-3}\, mol\, s^{-1}$	[]	
89	K_{NK}	`K_NK`	Arrhenius reaction constant	constant	$m^{-3}\, mol\, s^{-1}$	[]	65
114	c_{KS}	`c_KS`	molar concentrations in reactive system	constant	$m^{-3}\, mol$	[]	90
115	${c^o}_{KS}$	`co_KS`	norming molar concentrations	constant	$m^{-3}\, mol$	[]	91
116	ϕ_{KS}	`phi_KS`	probability of species to meet	constant		[]	92

6 material

	var	symbol	documentation	type	units	tokens	eqs
29	$_{S}$	`Mm`	species molecular masses	constant	$kg\,mol^{-1}$	[]	
46	$C_{p\,N}$	`C_p`	total heat capacity at constant pressure	seconaryState	$kg\,m^{2}\,K^{-1}\,s^{-2}$	[]	33
47	$C_{v\,N}$	`C_v`	specific heat capacity at constant volume	seconaryState	$kg\,m^{2}\,K^{-1}\,s^{-2}$	[]	34
48	$c_{p\,S}$	`cp`	specific heat capacity at constant pressure	seconaryState	$m^{2}\,mol^{2}\,K^{-1}\,s^{-2}$	[]	35
49	$c_{v\,S}$	`cv`	specific heat capacity at constant volume	seconaryState	$m^{2}\,mol^{2}\,K^{-1}\,s^{-2}$	[]	36
30	$C_{p\,N}$	`Cp`	total heat capacity at constant pressure	property	$kg\,m^{2}\,K^{-1}\,s^{-2}$	[]	18
31	$C_{v\,N}$	`Cv`	total heat capacity at constant volume	property	$kg\,m^{2}\,K^{-1}\,s^{-2}$	[]	19
34	$k^{q}_{x\,N}$	`kq_x`	thermal conductivity in x-direction	property	$kg\,K^{-1}\,s^{-3}$	[]	22
35	$k^{q}_{y\,N}$	`kq_y`	thermal conductivity in y-direction	property	$kg\,K^{-1}\,s^{-3}$	[]	23
36	$k^{q}_{z\,N}$	`kq_z`	thermal conductivity in z-direction	property	$kg\,K^{-1}\,s^{-3}$	[]	24
37	$k^{q}{}_{N}$	`kq`	Carthesian thermal conductivity vector	property	$kg\,K^{-1}\,s^{-3}$	[]	25
50	$k^{c}_{x\,N}$	`kc_x`	convective mass convectivity in x-direction	property	$m^{-1}\,s$	[]	37
51	$k^{c}_{y\,N}$	`kc_y`	convective mass convectivity in y-direction	property	$m^{-1}\,s$	[]	38
52	$k^{c}_{z\,N}$	`kc_z`	convective mass convectivity in z-direction	property	$m^{-1}\,s$	[]	39
53	$k^{c}{}_{N}$	`kc`	Cartesian convective mass convectivity vector	property	$m^{-1}\,s$	[]	40
54	$k^{d}_{x\,NS}$	`kd_x`	diffusional mass conductivity in x-direction	property	$kg^{-1}\,m^{-4}\,mol^{2}\,s$	[]	41
55	$k^{d}_{y\,NS}$	`kd_y`	diffusional mass conductivity in y-direction	property	$kg^{-1}\,m^{-4}\,mol^{2}\,s$	[]	42
56	$k^{d}_{z\,NS}$	`kd_z`	diffusional mass conductivity in z-direction	property	$kg^{-1}\,m^{-4}\,mol^{2}\,s$	[]	43
57	$k^{d}{}_{NS}$	`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
98	$\hat{V}_A$	`fV`	volumetric flow in x-direction	transport	$m^3\,s^{-1}$	[]	74
104	$\hat{n}^d{}_{AS}$	`fnd_AS`	diffusional mass transfer per arc	transport	$mol\,s^{-1}$	[]	80
105	$\hat{n}^d{}_{NS}$	`fnd`	net diffusional mass transfer	transport	$mol\,s^{-1}$	[]	81
106	$\hat{H}^d{}_A$	`fHd_A`	enthalpy flow due to mass diffusion per arc	transport	$kg\,m^2\,s^{-3}$	[]	82
107	$\hat{H}^d{}_N$	`fHd`	net enthalpy flow due to mass diffusion	transport	$kg\,m^2\,s^{-3}$	[]	83
109	c_{AS}	`c_AS`	moler concentration in convective arc	transport	$m^{-3}\,mol$	[]	85
110	$\hat{n}^c{}_{AS}$	`fnc_AS`	convective molar mass flow per arc	transport	$mol\,s^{-1}$	[]	86
111	$\hat{n}^c{}_{NS}$	`fnc`	net convective molar mass flow	transport	$mol\,s^{-1}$	[]	87
95	$A_{yz\,N}$	`Ayz`	cross sectional area in x-direction	geometry	m^2	[]	71
96	$A_{xz\,N}$	`Axz`	cross sectional area in y direction	geometry	m^2	[]	72
97	$A_{xy\,N}$	`Axy`	cross sectional area in z-direction	geometry	m^2	[]	73
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
108	c_{NS}	`c`	molar concentration	seconaryState	$m^{-3}\,mol$	[]	84

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	var	symbol	documentation	type	units	tokens	eqs
77	T_{NK}	T_NK	temperature in reactive systems	conversion	K	[]	55
93	$N_{NS,NK}$	N_NS_NK	extended stoichiometric matrix	conversion		[]	69
117	ξ_{NK}	xi	extend of reaction per volume	conversion	$m^{-3}\,mol\,s^{-1}$	[]	93
118	$\tilde{n}_{NS}$	pn	production term	conversion	$mol\,s^{-1}$	[]	94
119	$\dot{n}_{NS}$	dndt	differential molar mass balance	diffState	$mol\,s^{-1}$	[]	95

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–control

	var	symbol	documentation	type	units	tokens	eqs

13 gas–liquid

	var	symbol	documentation	type	units	tokens	eqs

14 gas–gas

	var	symbol	documentation	type	units	tokens	eqs

15 liquid–liquid

	var	symbol	documentation	type	units	tokens	eqs

16 gas–solid

	var	symbol	documentation	type	units	tokens	eqs

17 solid–solid

	var	symbol	documentation	type	units	tokens	eqs

18 liquid–solid

	var	symbol	documentation	type	units	tokens	eqs

19 material–material

	var	symbol	documentation	type	units	tokens	eqs

20 reactions–reactions

	var	symbol	documentation	type	units	tokens	eqs

21 Equations

22 Generic

no	equation	documentation	layer
1	$0 := \mathrm{Instantiate}(\#, \#)$	numerical value zero	root
2	$1 := \mathrm{Instantiate}(\#, \#)$	numerical value one	root
3	$0.5 := \mathrm{Instantiate}(\#, \#)$	numerical value one half	root
4	$t_o := \mathrm{Instantiate}(t, \#)$	starting time	root
5	$t_e := \mathrm{Instantiate}(t, \#)$	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	$H_N := U_N - p_N \, . \, V_N$	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 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	$v_N := \mathrm{Stack}\left(v_{xN}, v_{yN}, v_{zN}\right)$	velocity vector	physical
16	$Bo_N := \mathrm{Instantiate}(S_N, \#)$	Boltzmann constant	physical
17	$R_N := A^v \, . \, Bo_N$	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	$k^q_{xN} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}$	thermal conductivity in x-direction	material
23	$k^q_{yN} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{yN}$	thermal conductivity in y-direction	material
24	$k^q_{zN} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{zN}$	thermal conductivity in z-direction	material
25	$k^q{}_N := \mathrm{Stack}\left(k^q_{xN}, k^q_{yN}, k^q_{zN}\right)$	Carthesian 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	$c_{pS} := C_{pN} \cdot (_S)^{-1} \overset{N \in NS}{\star} n_{NS}$	specific heat capacity at constant pressure	material
36	$c_{vS} := C_{vN} \cdot (_S)^{-1} \overset{N \in NS}{\star} n_{NS}$	specific heat capacity at constant volume	material
37	$k^c_{xN} := \left(_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass convectivity in x-direction	material
38	$k^c_{yN} := \left(_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$	convective mass convectivity in y-direction	material
39	$k^c_{zN} := \left(_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convective mass convectivity in z-direction	material
40	$k^c{}_N := \mathrm{Stack}\left(k^c_{xN}, k^c_{yN}, k^c_{zN}\right)$	Cartesian convective mass convectivity vector	material

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no	equation	documentation	layer
41	$k^d_{x\,NS} := (\mu_{NS})^{-1} \,.\, \left(v_{x\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in x-direction	material
42	$k^d_{y\,NS} := (\mu_{NS})^{-1} \,.\, \left(v_{y\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in y-direction	material
43	$k^d_{z\,NS} := (\mu_{NS})^{-1} \,.\, \left(v_{z\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in z-direction	material
44	$k^d{}_{NS} := \mathrm{Stack}\left(k^d_{x\,NS}, k^d_{y\,NS}, k^d_{z\,NS}\right)$	Cartesian dffusional mass conductivity vector	material
45	$h_{NS} := H_N \odot (n_{NS})^{-1}$	partial molar enthalpies	material
46	$d_A := \mathrm{sign}\left(F_{N,A} \overset{N}{\star} p_N\right)$	direction of convective ow	macroscopic
47	$m_N := {}_S \overset{S \in NS}{\star} n_{NS}$	mass	macroscopic
49	$\rho_N := m_N \,.\, (V_N)^{-1}$	mass density	material
51	$F_{NS,AS} := F_{N,A} \odot P_{NS,AS}$	incidence matrix of directed graphs for for species NS x AS	macroscopic
55	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature in reactive systems	macroscopic
64	$E_{a\,NK} := \mathrm{Instantiate}(P_{N,NK} \overset{N}{\star} R_N \,.\, T_{NK}, \#)$	Arrhenius's activation energy	reactions
65	$K_{NK} := K^o{}_K \odot exp((-E_{a\,NK}) \,.\, \left(R_N \overset{N}{\star} P_{N,NK} \,.\, T_{NK}\right)^{-1})$	Arrhenius reaction constant	reactions
69	$N_{NS,NK} := P_{S,NS} \overset{S}{\star} \left(\left(P_{K,NK} \,.\, T_{NK} \,.\, (T_{NK})^{-1}\right) \overset{K}{\star} N_{S,K}\right)$	extended stoichiometric matrix	macroscopic
71	$A_{yz\,N} := r_{y\,N} \,.\, r_{z\,N}$	cross sectional area in x-direction	macroscopic
72	$A_{xz\,N} := r_{x\,N} \,.\, r_{z\,N}$	cross sectional area in y direction	macroscopic

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no	equation	documentation	layer
73	$A_{xyN} := r_{xN} \,.\, r_{yN}$	cross sectional area in z-direction	macroscopic
74	$\hat{V}_A := (\rho_N)^{-1} \,.\, k^c_{xN} \,.\, A_{yzN} \,.\, F_{N,A} \overset{N}{\star} p_N$	volumetric flow in x-direction	macroscopic
80	$\hat{n}^d{}_{AS} := A_{yzN} \odot \left(-k^d_{xNS}\right) \,.\, F_{NS,AS} \overset{NS}{\star} \mu_{NS}$	diffusional mass transfer per arc	macroscopic
81	$\hat{n}^d{}_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^d{}_{AS}$	net diffusional mass transfer	macroscopic
82	$\hat{H}^d{}_A := \left(F_{NS,AS} \overset{NS}{\star} h_{NS}\right) \overset{S \in AS}{\star} \hat{n}^d{}_{AS}$	enthalpy flow due to mass diffusion per arc	macroscopic
83	$\hat{H}^d{}_N := F_{N,A} \overset{A}{\star} \hat{H}^d{}_A$	net enthalpy flow due to mass diffusion	macroscopic
84	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar concentration	macroscopic
85	$c_{AS} := (0.5 \,.\, (F_{NS,AS} - d_A \odot \lvert F_{NS,AS} \rvert)) \overset{NS}{\star} c_{NS}$	moler concentration in convective arc	macroscopic
86	$\hat{n}^c{}_{AS} := \hat{V}_A \odot c_{AS}$	convective molar mass flow per arc	macroscopic
87	$\hat{n}^c{}_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^c{}_{AS}$	net convective molar mass flow	macroscopic
90	$c_{KS} := c_{NS} \overset{NS}{\star} P_{NS,KS}$	molar concentrations in reactive system	reactions
91	$c^o{}_{KS} := \text{Instantiate}(c_{KS}, \#)$	norming molar concentrations	reactions
92	$\phi_{KS} := \prod \left(c_{KS} \,.\, (c^o{}_{KS})^{-1} right\right)$	probability of species to meet	reactions
93	$\xi_{NK} := K_{NK} \,.\, P_{NK,KS} \overset{KS}{\star} \phi_{KS}$	extend of reaction per volume	macroscopic
94	$\tilde{n}_{NS} := V_N \odot \left(N_{NS,NK} \overset{NK}{\star} \xi_{NK}\right)$	production term	macroscopic
95	$\dot{n}_{NS} := \hat{n}^c{}_{NS} + \hat{n}^d{}_{NS} + \tilde{n}_{NS}$	differential molar mass balance	macroscopic