

## 1 Variables

### 2 root

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

### 3 physical

	var	symbol	documentation	type	units	tokens	eqs
9	$r_{xN}$	<b>r_x</b>	x-coordinate	frame	$m$	[]	
10	$r_{yN}$	<b>r_y</b>	y-coordinate	frame	$m$	[]	
23	$r_{zN}$	<b>r_z</b>	z-coordinate	frame	$m$	[]	
11	$U_N$	<b>U</b>	foundation state – internal energy	state	$kg\ m^2\ s^{-2}$	[]	
12	$S_N$	<b>S</b>	foundation state – entropy	state	$kg\ m^2\ K^{-1}\ s^{-2}$	[]	
13	$V_N$	<b>V</b>	foundation state – volume	state	$m^3$	[]	
18	$H_N$	<b>H</b>	enthalpy	state	$kg\ m^2\ s^{-2}$	[]	9
19	$A_N$	<b>A</b>	Helmholtz energy	state	$kg\ m^2\ s^{-2}$	[]	10
20	$G_N$	<b>G</b>	Gibbs energy	state	$kg\ m^2\ s^{-2}$	[]	11
42	$n_{NS}$	<b>n</b>	species molar mass	state	$mol$	[]	
26	$A^v$	<b>Avogadro</b>	Avogadro number	constant	$mol^{-1}$	[]	
27	$Bo_N$	<b>Boltzmann</b>	Boltzmann constant	constant	$kg\ m^2\ K^{-1}\ s^{-2}$	[]	16
28	$R_N$	<b>GasConstant</b>	Gas constant	constant	$kg\ m^2\ mol^{-1}\ K^{-1}\ s^{-2}$	[]	17
15	$p_N$	<b>p</b>	thermodynamic pressure	effort	$kg\ m^{-1}\ s^{-2}$	[]	6
16	$T_N$	<b>T</b>	temperature	effort	$K$	[]	7
45	$\mu_{NS}$	<b>chem_pot</b>	chemical potential	effort	$kg\ m^2\ mol^{-1}\ s^{-2}$	[]	32
21	$v_{xN}$	<b>v_x</b>	velocity in x-direction	secondaryState	$ms^{-1}$	[]	12
22	$v_{yN}$	<b>v_y</b>	velocity in y direction	secondaryState	$ms^{-1}$	[]	13
24	$v_{zN}$	<b>v_z</b>	velocity in z-direction	secondaryState	$ms^{-1}$	[]	14
25	$v_N$	<b>v</b>	velocity vector	secondaryState	$ms^{-1}$	[]	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	$E_{a,NK}$	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	$\phi_{KS}$	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	$C_{pN}$	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	$\rho_N$	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	$\hat{n}_{AS}^d$	fnd_AS	diffusional mass transfer per arc	transport	$mol s^{-1}$	[]	80
105	$\hat{n}_{NS}^d$	fnd	net diffusional mass transfer	transport	$mol s^{-1}$	[]	81
106	$\hat{H}_A^d$	fHd_A	enthalpy flow due to mass diffusion per arc	transport	$kg m^2 s^{-3}$	[]	82
107	$\hat{H}_N^d$	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	$\hat{n}_{AS}^c$	fnc_AS	convective molar mass flow per arc	transport	$mol s^{-1}$	[]	86
111	$\hat{n}_{NS}^c$	fnc	net convective molar mass flow	transport	$mol s^{-1}$	[]	87
120	$\hat{H}_A^c$	fHc_A	enthalpy flow due to convective mass flow	transport	$kg m^2 s^{-3}$	[]	96
121	$\hat{H}_N^c$	fHc	net enthalpy flow due to convective mass flow	transport	$kg m^2 s^{-3}$	[]	97
122	$\hat{w}_A$	fw_A	example of work flow	transport	$kg m^2 s^{-3}$	[]	98
123	$\hat{w}_N$	fw	net work flow	transport	$kg m^2 s^{-3}$	[]	99
124	$\hat{q}_A$	fq_A_x	heat flow in x-direction	transport	$kg m^2 s^{-3}$	[]	100
125	$\hat{q}_N$	fq	net heat flow	transport	$kg m^2 s^{-3}$	[]	101
95	$A_{yzN}$	Ayz	cross sectional area in x-direction	geometry	$m^2$	[]	71
96	$A_{xzN}$	Axz	cross sectional area in y direction	geometry	$m^2$	[]	72
97	$A_{xyN}$	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		[]	

*Continued on next page*

	var	symbol	documentation	type	units	tokens	eqs
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
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	$\xi_{NK}$	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
126	$\dot{H}_N$	dHdt	differential enthalpy balance	diffState	$kg m^2 s^{-3}$	[]	102

## 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	$0 := \text{Instantiate}(\#, \#)$	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

*Continued on next page*

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

*Continued on next page*

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	$m_N := \overset{S \in NS}{S} \overset{\star}{\star} n_{NS}$	mass	macroscopic
49	$\rho_N := m_N \cdot (V_N)^{-1}$	mass density	material
51	$F_{NS,AS} := F_{N,A} \odot P_{NS,AS}$	incidence matrix of directed graphs for species NS x AS	macroscopic
55	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature in reactive systems	macroscopic
64	$E_{aNK} := \text{Instantiate}(P_{N,NK} \overset{N}{\star} R_N \cdot T_{NK}, \#)$	Arrhenius's activation energy	reactions
65	$K_{NK} := K^o_K \odot \exp((-E_{aNK}) \cdot \left( R_N \overset{N}{\star} P_{N,NK} \cdot T_{NK} \right)^{-1})$	Arrhenius reaction constant	reactions
69	$N_{NS,NK} := P_{S,NS} \overset{S}{\star} \left( \left( P_{K,NK} \cdot T_{NK} \cdot (T_{NK})^{-1} \right) \overset{K}{\star} N_{S,K} \right)$	extended stoichiometric matrix	macroscopic
71	$A_{yzN} := r_{yN} \cdot r_{zN}$	cross sectional area in x-direction	macroscopic
72	$A_{xzN} := r_{xN} \cdot r_{zN}$	cross sectional area in y direction	macroscopic

*Continued on next page*

no	equation	documentation	layer
73	$A_{xyN} := r_{xN} \cdot r_{yN}$	cross sectional area in z-direction	macroscopic
74	$\hat{V}_A := (\rho_N)^{-1} \cdot k_{xN}^c \cdot A_{yzN} \cdot F_{N,A} \stackrel{N}{\star} p_N$	volumetric flow in x-direction	macroscopic
80	$\hat{n}_{AS}^d := A_{yzN} \odot (-k_{xNS}^d) \cdot F_{NS,AS} \stackrel{NS}{\star} \mu_{NS}$	diffusional mass transfer per arc	macroscopic
81	$\hat{n}_{NS}^d := F_{NS,AS} \stackrel{AS}{\star} \hat{n}_{AS}^d$	net diffusional mass transfer	macroscopic
82	$\hat{H}_A^d := \left( F_{NS,AS} \stackrel{NS}{\star} h_{NS} \right) \stackrel{S \in AS}{\star} \hat{n}_{AS}^d$	enthalpy flow due to mass diffusion per arc	macroscopic
83	$\hat{H}_N^d := F_{N,A} \stackrel{A}{\star} \hat{H}_A^d$	net enthalpy flow due to mass diffusion	macroscopic
84	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar concentration	macroscopic
85	$c_{AS} := (0.5 \cdot (F_{NS,AS} - d_A \odot  F_{NS,AS} )) \stackrel{NS}{\star} c_{NS}$	molar concentration in convective arc	macroscopic
86	$\hat{n}_{AS}^c := \hat{V}_A \odot c_{AS}$	convective molar mass flow per arc	macroscopic
87	$\hat{n}_{NS}^c := F_{NS,AS} \stackrel{AS}{\star} \hat{n}_{AS}^c$	net convective molar mass flow	macroscopic
90	$c_{KS} := c_{NS} \stackrel{NS}{\star} P_{NS,KS}$	molar concentrations in reactive system	reactions
91	$c_{KS}^o := \text{Instantiate}(c_{KS}, \#)$	norming molar concentrations	reactions
92	$\phi_{KS} := \prod \left( c_{KS} \cdot (c_{KS}^o)^{-1} \text{right} \right)$	probability of species to meet	reactions
93	$\xi_{NK} := K_{NK} \cdot P_{NK,KS} \stackrel{KS}{\star} \phi_{KS}$	extend of reaction per volume	macroscopic
94	$\tilde{n}_{NS} := V_N \odot \left( N_{NS,NK} \stackrel{NK}{\star} \xi_{NK} \right)$	production term	macroscopic
95	$\dot{n}_{NS} := \hat{n}_{NS}^c + \hat{n}_{NS}^d + \tilde{n}_{NS}$	differential molar mass balance	macroscopic
96	$\hat{H}_A^c := \left( F_{NS,AS} \stackrel{NS}{\star} h_{NS} \right) \stackrel{S \in AS}{\star} \hat{n}_{AS}^c$	enthalpy flow due to convective mass flow	macroscopic

Continued on next page



no	equation	documentation	layer
97	$\hat{H}^c_N := F_{N,A} \overset{A}{\star} \hat{H}^c_A$	net enthalpy flow due to convective mass flow	macroscopic
98	$\hat{w}_A := \text{Instantiate}(\hat{H}^c_A, \#)$	example of work flow	macroscopic
99	$\hat{w}_N := F_{N,A} \overset{A}{\star} \hat{w}_A$	net work flow	macroscopic
100	$\hat{q}_A := A_{yzN} \cdot k_{xN}^q \cdot F_{N,A} \overset{N}{\star} T_N$	heat flow in x-direction	macroscopic
101	$\hat{q}_N := F_{N,A} \overset{A}{\star} \hat{q}_A$	net heat flow	macroscopic
102	$\dot{H}_N := \hat{H}^c_N + \hat{H}^d_N + \hat{q}_N + \hat{w}_N$	differential enthalpy balance	macroscopic