

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	$kg\ m^2\ s^{-2}$	[]	9 122 123
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	[]	116
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	$kg\ m^{-1}\ s^{-2}$	[]	6 115
16	T_N	T	temperature	effort	K	[]	7 113
45	μ_{NS}	chem_pot	chemical potential	effort	$kg\ m^2\ mol^{-1}\ s^{-2}$	[]	32 114
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
139	m_A	mc	measurements	input		[]	
129	$I_{N,D}$	I_N_D	identity to shift from differential space integral space	network		[]	
130	$I_{A,D}$	I_A_D	identity to shift from differential space to arc	network		[]	
137	x_N	x	controller state	state		[]	112
138	x_N^o	xo	controller initial condition	state		[]	103
133	$C_{N,A}$	Cx	measurement matrix	constant		[]	
134	$D_{N,D}$	Dx	event matrix (dimension issue)	constant		[]	
135	y_A^o	setpoint	set point	constant		[]	
136	D_A	D_A	event diagonal matrix (no dimension problem)	constant		[]	
142	$A_{N,D}$	Ax	dynamic control matrix	constant	s^{-1}	[]	
143	$B_{A,D}$	Bx	input matrix	constant	s^{-1}	[]	
144	\dot{x}_D	dxdt	differential controller state	diffState	s^{-1}	[]	106
140	e_A	e	control error	algebraic		[]	104

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	ϕ_{KS}	phi_KS	probability of species to meet	constant		[]	92

6 material

	var	symbol	documentation	type	units	tokens	eqs
29	λ_S	Mm	species molecular masses	constant	$kg\ mol^{-1}$	[]	
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 conductivity in x-direction	property	$m^{-1}\ s$	[]	37
51	k_{yN}^c	kc_y	convective mass conductivity in y-direction	property	$m^{-1}\ s$	[]	38
52	k_{zN}^c	kc_z	convective mass conductivity in z-direction	property	$m^{-1}\ s$	[]	39
53	k_N^c	kc	Cartesian convective mass conductivity 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 diffusional 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
148	cp_N	cp	specific heat capacity at constant pressure	property	$m^2\ K^{-1}\ s^{-2}$	[]	120
149	cv_N	cv	specific heat capacity at constant volume	property	$m^2\ K^{-1}\ s^{-2}$	[]	121

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		[]	
127	$D_{N,A}$	D	difference operator	differenceOperator		[]	
128	$D_{NS,AS}$	D_NS_AS	block difference operator	differenceOperator		[]	
145	T_{ref_N}	T_ref	refernce temperature	constant	K	[]	117
150	n^o_{NS}	no	initial condition for species mass in nodes	constant	mol	[]	124
151	H^o_N	Ho	initial condition for enthalpy in nodes	constant	$kg\ m^2\ s^{-2}$	[]	125
69	m_N	m	mass	secondaryState	kg	[]	47
108	c_{NS}	c	molar concentration	secondaryState	$m^{-3}\ mol$	[]	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	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
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
37	$k_{xN}^c := \left(\lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass conductivity in x-direction	material
38	$k_{yN}^c := \left(\lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$	convective mass conductivity in y-direction	material
39	$k_{zN}^c := \left(\lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convective mass conductivity in z-direction	material
40	$k_N^c := \text{Stack}(k_{xN}^c, k_{yN}^c, k_{zN}^c)$	Cartesian convective mass conductivity vector	material
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

Continued on next page

no	equation	documentation	layer
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	$d_A := \text{sign}\left(F_{N,A} \stackrel{N}{\star} p_N\right)$	direction of convective ow	macroscopic
47	$m_N := \lambda_S \stackrel{S \in NS}{\star} n_{NS}$	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 for species NS x AS	macroscopic
55	$T_{NK} := P_{N,NK} \stackrel{N}{\star} T_N$	temperature in reactive systems	macroscopic
64	$E_{aNK} := \text{Instantiate}(P_{N,NK} \stackrel{N}{\star} R_N \cdot T_{NK}, \#)$	Arrhenius's activation energy	reactions
65	$K_{NK} := K^o_K \odot \exp((-E_{aNK}) \cdot (R_N \stackrel{N}{\star} P_{N,NK} \cdot T_{NK})^{-1})$	Arrhenius reaction constant	reactions
69	$N_{NS,NK} := P_{S,NS} \stackrel{S}{\star} \left((P_{K,NK} \cdot T_{NK} \cdot (T_{NK})^{-1}) \stackrel{K}{\star} N_{S,K} \right)$	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
73	$A_{xyN} := r_{xN} \cdot r_{yN}$	cross sectional area in z-direction	macroscopic
74	$\hat{V}_A := (\rho_N)^{-1} \cdot k_{xN}^c \cdot A_{yzN} \cdot D_{N,A} \stackrel{N}{\star} p_N$	volumetric flow in x-direction	macroscopic
80	$\hat{n}_{AS}^d := A_{yzN} \odot (-k_{xNS}^d) \cdot D_{NS,AS} \stackrel{NS}{\star} \mu_{NS}$	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

Continued on next page

no	equation	documentation	layer
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	$c_{AS} := (0.5 \cdot (F_{NS,AS} - d_A \odot F_{NS,AS})) \overset{NS}{\star} c_{NS}$	molar 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	$\phi_{KS} := \prod \left(c_{KS} \cdot (c^o_{KS})^{-1} \text{right} \right)$	probability of species to meet	reactions
93	$\xi_{NK} := K_{NK} \cdot P_{NK,KS} \overset{KS}{\star} \phi_{KS}$	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
96	$\hat{H}^c_A := \left(F_{NS,AS} \overset{NS}{\star} h_{NS} \right) \overset{S \in AS}{\star} \hat{n}^c_{AS}$	enthalpy flow due to convective mass flow	macroscopic
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

Continued on next page

no	equation	documentation	layer
100	$\hat{q}_A := A_{yzN} \cdot k_{xN}^q \cdot D_{N,A} \overset{N}{\star} T_N$	heat flow in x-direction	macroscopic
101	$\hat{q}_N := F_{N,A} \overset{A}{\star} \hat{q}_A$	net heat flow	macroscopic
102	$\dot{H}_N := \hat{H}_N^c + \hat{H}_N^d + \hat{q}_N + \hat{w}_N$	differential enthalpy balance	macroscopic
103	$x_N^o := \text{Instantiate}(x_N, \#)$	controller initial condition	control
104	$e_A := m_A - y_A^o$	control error	control
106	$\dot{x}_D := A_{N,D} \overset{N}{\star} x_N + B_{A,D} \overset{A}{\star} e_A$	differential controller state	control
112	$x_N := \int_{t_o}^{t_e} I_{N,D} \overset{D}{\star} \dot{x}_D \, dt$	controller state	control
113	$T_N := \text{Instantiate}(T_N, \#)$	temperature	physical
114	$\mu_{NS} := \text{Instantiate}(\mu_{NS}, \#)$	chemical potential	physical
115	$p_N := \text{Instantiate}(p_N, \#)$	thermodynamic pressure	physical
116	$n_{NS} := \int_{t_o}^{t_e} \dot{n}_{NS} \, dt$	species molar mass	macroscopic
117	$T_{refN} := \text{Instantiate}(T_N, \#)$	reference temperature	macroscopic

Continued on next page

no	equation	documentation	layer
120	$cp_N := C_{pN} \cdot (m_N)^{-1}$	specific heat capacity at constant pressure	material
121	$cv_N := C_{vN} \cdot (m_N)^{-1}$	specific heat capacity at constant volume	material
122	$H_N := m_N \cdot \int_{T_{ref_N}}^{T_N} cp_N \, dT_N$	enthalpy	macroscopic
123	$H_N := \int_{t_o}^{t_e} \dot{H}_N \, dt$	enthalpy	macroscopic
124	$n^o_{NS} := \text{Instantiate}(n_{NS}, \#)$	initial condition for species mass in nodes	macroscopic
125	$H^o_N := \text{Instantiate}(H_N, \#)$	initial condition for enthalpy in nodes	macroscopic