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	$_{ m tokens}$	eqs
9	r_{xN}	r_x	x-coordinate	frame	m	[]	
10	r_{yN}	r_y	y-coordinate	frame	$\mid m \mid$		
23	r_{zN}	r_z	z-coordinate	frame	$\mid m \mid$		
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	н	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	Т	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	$\begin{array}{c} \text{identity to shift from differential space integral} \\ \text{space} \end{array}$	network			
130	$I_{A,D}$	I_A_D	identity to shift from differential space to arc	network			
137	x_N	х	controller state	state			112
138	$x^{o}{}_{N}$	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	$y^o{}_A$	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	е	control error	algebraic		[]	104

5 reactions

	var	symbol	documentation	type	units	$_{ m tokens}$	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	$K^o{}_K$	Ко	Arrhenius's frequency factor	constant	$m^{-3}mols^{-1}$		
89	K_{NK}	K_NK	Arrhenius reaction constant	$\operatorname{constant}$	$m^{-3}mols^{-1}$		65
114	c_{KS}	c_KS	molar concentrations in reactive system	$\operatorname{constant}$	$m^{-3} mol$		90
115	$c^{o}{}_{KS}$	co_KS	norming molar concentrations	$\operatorname{constant}$	$m^{-3} mol$	[]	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}	Ср	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	$k^q{}_N$	kq	Carthesian 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	$k^c{}_N$	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^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	$ ho_N$	density	mass density	property	$kg m^{-3}$		49
148	cp_N	ср	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	$\hat{n}^d{}_{AS}$	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	$\mod s^{-1}$		86
111	$\hat{n}^c{}_{NS}$	fnc	net convective molar mass flow	transport	$\mod s^{-1}$		87
120	$\hat{H}^c{}_A$	fHc_A	enthalpy flow due to convective mass flow	transport	$kg m^2 s^{-3}$		96
121	$\hat{H}^c{}_N$	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			

	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	$T_r e f_N$	T_ref	refernce temperature	$\operatorname{constant}$	K		117
69	m_N	m	mass	secondaryState	kg		47
108	c_{NS}	С	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	$ ilde{n}_{NS}$	pn	production term	conversion	$\mod s^{-1}$		94
119	\dot{n}_{NS}	dndt	differential molar mass balance	diffState	$\mod s^{-1}$		95
126	\dot{H}_N	dHdt	differential enthalpy balance	diffState	$kg m^2 s^{-3}$		102

8 solid

var symbol documentation type units tokens		var symbol	documentation	type			eqs
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9 fluid

var symbol documentation type units tokens		var symbol	documentation	type			eqs
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10 liquid

	var	symbol	documentation	type	units	tokens	eqs
--	-----	--------	---------------	------	-------	--------	-----

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

Vē	var	symbol	documentation	type	units	tokens	eqs
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17 solid-solid

var symbol documentation type units tokens		var symbol	documentation	type			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		var symbol	documentation	type			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 := Instantiate(#, #)	numerical value zero	root
2	1 := Instantiate(#, #)	numerical value one	root
3	0.5 := 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	$v_N := \operatorname{Stack}\left(v_{xN}, v_{yN}, v_{zN}\right)$	velocity vector	physical
16	$Bo_N := \operatorname{Instantiate}(S_N, \#)$	Boltzmann constant	physical
17	$R_N := A^v \cdot Bo_N$	Gas constant	physical

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	$k^q{}_N := \operatorname{Stack}\left(k^q_{xN}, k^q_{yN}, k^q_{zN}\right)$	Carthesian thermal conductivity vector	material
32	$\mu_{NS} := rac{\partial U_N}{\partial n_{NS}}$	chemical potential	physical
37	$k_{xN}^c := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass convectivity in x-direction	material
38	$k_{yN}^c := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$	convective mass convectivity in y-direction	material
39	$k_{zN}^c := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convective mass convectivity in z-direction	material
40	$k^c{}_N := \operatorname{Stack}\left(k^c_{xN}, k^c_{yN}, k^c_{zN}\right)$	Cartesian convective mass convectivity 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

no	equation	documentation	layer
44	$k^{d}_{NS} := \operatorname{Stack}\left(k^{d}_{xNS}, k^{d}_{yNS}, k^{d}_{zNS}\right)$	Cartesian dffusional mass conductivity vector	material
45	$h_{NS} := H_N \odot \left(n_{NS} \right)^{-1}$	partial molar enthalpies	material
46	$d_A := \operatorname{sign}\left(F_{N,A} \stackrel{N}{\star} p_N\right)$	direction of convective ow	macroscopic
47	$m_N := \lambda_S \overset{S \in NS}{\star} n_{NS}$	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	$E_{aNK} := \text{Instantiate}(P_{N,NK} \overset{N}{\star} R_N . T_{NK}, \#)$	Arrhenius's activation energy	reactions
65	$K_{NK} := K^o{}_K \odot exp((-E_{aNK}) \cdot \left(R_N * P_{N,NK} \cdot T_{NK}\right)^{-1})$	Arrhenius reaction constant	reactions
69	$N_{NS,NK} := P_{S,NS} \stackrel{S}{\star} \left(\left(P_{K,NK} \cdot T_{NK} \cdot \left(T_{NK} \right)^{-1} \right) \stackrel{K}{\star} N_{S,K} \right)$	extended stoichiometric matrix	macroscopic
71	$A_{yzN} := r_{yN} . r_{zN}$	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	$\hat{n}^d{}_{AS} := A_{yzN} \odot \left(-k^d_{xNS} \right) . D_{NS,AS} \overset{NS}{\star} \mu_{NS}$	diffusional mass transfer per arc	macroscopic
81	$\hat{n}^d{}_{NS} := F_{NS,AS} \stackrel{AS}{\star} \hat{n}^d{}_{AS}$	net diffusional mass transfer	macroscopic

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	$\hat{H}^d{}_N := F_{N,A} \stackrel{A}{\star} \hat{H}^d{}_A$	net enthalpy flow due to mass diffusion	macroscopic
84	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar concentration	macroscopic
85	$c_{AS} := (0.5 \cdot (F_{NS,AS} - d_A \odot F_{NS,AS})) \overset{NS}{\star} c_{NS}$	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	$\hat{n}^c{}_{NS} := F_{NS,AS} \stackrel{AS}{\star} \hat{n}^c{}_{AS}$	net convective molar mass flow	macroscopic
90	$c_{KS} := c_{NS} \overset{NS}{\star} P_{NS,KS}$	molar concentrations in reactive system	reactions
91	$c^o{}_{KS} := \operatorname{Instantiate}(c_{KS}, \#)$	norming molar concentrations	reactions
92	$\phi_{KS} := \prod \left(c_{KS} \cdot \left(c^o_{KS} \right)^{-1} right \right)$	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	$\hat{H}^c{}_N := F_{N,A} \stackrel{A}{\star} \hat{H}^c{}_A$	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	$\hat{w}_N := F_{N,A} \stackrel{A}{\star} \hat{w}_A$	net work flow	macroscopic

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

no	equation	documentation	layer
120	$cp_N := C_{pN} \cdot (m_N)^{-1}$	specific heat capacity at constant pressure	material
121	$cv_N := C_{vN} \cdot \left(m_N\right)^{-1}$	specific heat capacity at constant volume	material
122	$H_N := m_N \cdot \int_{T_r e f_N}^{T_N} c p_N \ dT_N$	enthalpy	macroscopic
123	$H_N := \int_{t_o}^{t_e} \dot{H}_N \ dt$	enthalpy	macroscopic