1 Variables

2 root

	var	symbol	documentation	type	units	eqs
2	$F_{N,A}$	F	incidence matrix of directed graph	network		
1	t_N	t	time	frame	s	
88	to_N	to	initial time	frame	s	63
89	te_N	te	end time	frame	s	64
5	$\#$	value	a value	constant		
6	$1\backslash 2$	half	one half	constant		1
7	0	zero	zero	constant		2
8	$\partial t_{N,dt}$	dt	differential time	*diffFrame	s	3

3 physical

	var	symbol	documentation	type	units	eqs
30	$F_{NS,AS}$	F_NS_AS	incidence matrix for species network	network		
41	$P_{N,A,dt}$	P_N_A_dt	projection of node to arc (used for mapping transport system material to application arc)	projection		
49	$P_{NS,AS,dt}$	P_NS_AS_dt	projection of node to arc (used for mapping transport system material to application arc)	projection		
9	$r_{x\,N}$	rx	spatial coordinate x	frame	m	
20	$r_{y\,N}$	ry	spatial coordinate y	frame	m	
21	$r_{z\,N}$	rz	spatial coordinate z	frame	m	
10	n_{NS}	n	species mass in moles	state	mol	65
11	U_N	U	internal energy	state	$kg\,m^2\,s^{-2}$	

Continued on next page

	var	symbol	documentation	type	units	eqs
12	S_N	S	entropy	state	$kg\,m^2\,K^{-1}\,s^{-2}$	
13	V_N	V	volume	state	m^3	
92	m_N	m	mass	state	mol	67
66	R	R	gas constant	constant	$kg^{-1}\,m^{-2}\,mol\,K^{-1}\,s^2$	
17	H_N	H	definition of enthalpy	secondaryState	$kg\,m^2\,s^{-2}$	7
18	$v_{x\,N}$	vx	definition of velocity in x direction	secondaryState	ms^{-1}	8
22	$A_{x\,N}$	Ax	area at location x	secondaryState	m^2	10
14	T_N	T	definition of temperature	effort	K	4
15	p_N	p	definition of pressure	effort	$kg\,m^{-1}\,s^{-2}$	5
31	μ_{NS}	mu	definition of chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	18

4 control

	var	symbol	documentation	type	units	eqs

5 macroscopic

	var	symbol	documentation	type	units	eqs
54	$\hat{q}_{N,dt}$	fq	heat flow	transport	$kg\,m^2\,s^{-3}$	39
81	$\hat{V}_{A,dt}$	fV	volumetric flow	transport	$m^3\,s^{-1}$	56
82	d_A	dir	direction of flow relative to reference coordinate	transport		57
83	$S_{NS,AS}$	S_NS_AS	selection of the flow sources	transport		58
84	c_{AS}	c_AS	concentration in the convective flows	transport	$m^{-3}\,mol$	59
85	$\hat{n}^v_{NS,dt}$	fnv	convective species flow	transport	$mol\,s^{-1}$	60
86	$\hat{n}^d_{NS,dt}$	fnd	diffusional species flows	transport	$mol\,s^{-1}$	61

Continued on next page

	var	symbol	documentation	type	units	eqs
57	$P_{NS,KS}$	P_NS_KS	projection of node species onto reaction species	projection		
58	$P_{K,NK}$	P_K_NK	projection reaction on node x reactions	projection		
59	$P_{N,NK}$	P_N_NK	projection node to node x reactions	projection		
74	$P_{NK,KS}$	P_NK_KS	projection node x conversion to conversion x species	projection		
56	${n^0}_{NS}$	n0	initial condition	state	mol	41
87	$\dot{n}_{NS,dt}$	dn	differential species balances	state	$mol\,s^{-1}$	62
62	$N_{K,KS}$	N_KS_K	stoichiometry for reaction k	constant		
64	${K^o}_{K,dt}$	Ko	Arrhenius prexponential factor (matrix)	constant	$m^{-3}\,mol\,s^{-1}$	
65	${E^A}_K$	ka	Arrhenius activation energy	constant	$kg^{-1}\,m^{-2}\,mol\,s^2$	
78	${k_x^{n_d}}_{AS,dt}$	knd_x	species diffusivity in x-direction	constant	$kg^{-1}\,m^{-4}\,mol^2\,s$	
79	${k_x^V}_{A,dt}$	kv_x	convective flow coefficient	constant	$kg^{-1}\,m^2\,s$	
61	c_{KS}	c_KS	molar concentrations assigned to reaction K	conversion	$m^{-3}\,mol$	43
63	$N_{NS,NK}$	N_NS_NK	global stoichiomety block matrix	conversion		44
67	T_{NK}	T_NK	temperature for reactions	conversion	K	45
68	$K_{NK,dt}$	K	reaction "constants"	conversion	$m^{-3}\,mol\,s^{-1}$	46
69	${c^o}_{KS}$	c_KS_o	norming concentration – probability must have no units !	conversion	$m^{-3}\,mol$	47
71	x_{KS}	x_KS	normed concentration little like more fractions	conversion		49
75	ϕ_{NK}	phi	probabiity for the reactions to occur	conversion		52
76	$\xi_{NK,dt}$	xi	dyamic extend of reaction	conversion	$m^{-3}\,mol\,s^{-1}$	53
77	$\tilde{n}_{NS,dt}$	pn	production term	conversion	$mol\,s^{-1}$	54
60	c_{NS}	c	molar concentration	secondaryState	$m^{-3}\,mol$	42

6 materialDB

	var	symbol	documentation	type	units	eqs
90	λ_S	`mm`	species molar mass	constant		
26	$c_{p\,N}$	`cp`	heat capacity at constant pressure	property	$kg\,m^2\,K^{-1}\,s^{-2}$	14
45	$k^{q_x}{}_{A,dt}$	`kq_x`	heat transfer coefficient for an event-dynamic transfer system	property	$kg\,K^{-1}\,s^{-3}$	31

7 fluid

	var	symbol	documentation	type	units	eqs

8 solid

	var	symbol	documentation	type	units	eqs

9 liquid

	var	symbol	documentation	type	units	eqs

10 gas

	var	symbol	documentation	type	units	eqs

11 control–gas

	var	symbol	documentation	type	units	eqs

12 gas–control

	var	symbol	documentation	type	units	eqs

13 control–liquid

	var	symbol	documentation	type	units	eqs

14 liquid–control

	var	symbol	documentation	type	units	eqs

15 control–materialDB

	var	symbol	documentation	type	units	eqs

16 materialDB–control

	var	symbol	documentation	type	units	eqs

17 control–solid

	var	symbol	documentation	type	units	eqs

18 solid–control

	var	symbol	documentation	type	units	eqs

19 gas–materialDB

	var	symbol	documentation	type	units	eqs

20 materialDB–gas

	var	symbol	documentation	type	units	eqs

21 liquid–materialDB

	var	symbol	documentation	type	units	eqs

22 materialDB–liquid

	var	symbol	documentation	type	units	eqs
46	${k^{q_x}}_{A,dt}$	`kq_x`	link to get heat transfer coefficient	transform	$kg\,K^{-1}\,s^{-3}$	32
91	S	`mm`	link to molar mass	transform		66

23 materialDB–solid

	var	symbol	documentation	type	units	eqs

24 solid–materialDB

	var	symbol	documentation	type	units	eqs

25 gas–liquid

	var	symbol	documentation	type	units	eqs

26 gas–solid

	var	symbol	documentation	type	units	eqs

27 liquid–solid

	var	symbol	documentation	type	units	eqs

28 Equations

28.1 Model equations

	no	equation	documentation	layer
1	1	$1\backslash 2 := Set(\#)$	one half	root
2	2	$0 := Set(\#)$	zero	root
3	3	$\partial t_{N,dt} := diffSpace(t_N)$	differential time	root
65	65	$n_{NS} := \int_{to_N}^{te_N} \dot{n}_{NS,dt} \; d\,t_N + n^0{}_{NS}$	integration of differential species balances	macroscopic
4	4	$T_N := \frac{\partial U_N}{\partial S_N}$	definition of temperature	physical
5	5	$p_N := \left(-\frac{\partial U_N}{\partial V_N}\right)$	definition of pressure	physical
7	7	$H_N := U_N + p_N \,.\, V_N$	definition of enthalpy	physical
8	8	$v_{x N} := \frac{\partial r_{x N}}{\partial t_N}$	definition of velocity in x direction	physical
10	10	$A_{x N} := r_{y N} \,.\, r_{z N}$	area at location x	physical
14	14	$c_{p N} := \frac{\partial H_N}{\partial T_N}$	heat capacity at constant pressure	materialDB
18	18	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	definition of chemical potential	physical
31	31	$k^{q_x}{}_{A,dt} := (-P_{N,A,dt}) \overset{N}{\star} \left((V_N)^{-1} \,.\, \frac{\partial U_N}{\partial T_N} \,.\, v_{x N}\right)$	heat transfer coefficient for an event-dynamic transfer system	materialDB
32	32	$k^{q_x}{}_{A,dt} := k^{q_x}{}_{A,dt}$	link to get heat transfer coefficient	materialDB »> liquid
39	39	$\hat{q}_{N,dt} := F_{N,A} \overset{A}{\star} \left((-k^{q_x}{}_{A,dt}) \,.\, A_{x N} \,.\, F_{N,A} \overset{N}{\star} T_N\right)$	heat flow	macroscopic
41	41	$n^0{}_{NS} := Set(n_{NS})$	initial condition	macroscopic

Continued on next page

	no	equation	documentation	layer
42	42	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar concentration	macroscopic
43	43	$c_{KS} := P_{NS,KS} \overset{NS}{\star} c_{NS}$	molar concentrations assigned to reaction K	macroscopic
44	44	$N_{NS,NK} := P_{NS,KS} \overset{KS}{\star} N_{K,KS} \overset{K}{\star} P_{K,NK}$	global stoichiomety block matrix	macroscopic
45	45	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature for reactions	macroscopic
46	46	$K_{NK,dt} := {K^o}_{K,dt} \odot exp({E^A}_K \odot (R \,.\, T_{NK})^{-1})$	reaction "constants"	macroscopic
47	47	${c^o}_{KS} := Set(c_{KS})$	norming concentration – probability must have no units !	macroscopic
49	49	$x_{KS} := ({c^o}_{KS})^{-1} \,.\, c_{KS}$	normed concentration little like more fractions	macroscopic
52	52	$\phi_{NK} := P_{NK,KS} \overset{KS}{\star} \left(\prod \left(x_{KS}^{N_{K,KS}}\right)\right)$	probabiity for the reactions to occur	macroscopic
53	53	$\xi_{NK,dt} := K_{NK,dt} \,.\, \phi_{NK}$	dyamic extend of reaction	macroscopic
54	54	$\tilde{n}_{NS,dt} := V_N \odot \left(N_{NS,NK} \overset{NK}{\star} \xi_{NK,dt}\right)$	production term	macroscopic
56	56	$\hat{V}_{A,dt} := F_{N,A} \overset{A}{\star} \left(-{k_x^V}_{A,dt}\right) \,.\, A_{xN} \,.\, F_{N,A} \overset{N}{\star} p_N$	volumetric flow	macroscopic
57	57	$d_A := \text{sign}\left(F_{N,A} \overset{N}{\star} p_N\right)$	direction of flow relative to reference coordinate	macroscopic
58	58	$S_{NS,AS} := 1\backslash 2 \,.\, (F_{NS,AS} - d_A \odot \lvert F_{NS,AS} \rvert)$	selection of the flow sources	macroscopic
59	59	$c_{AS} := S_{NS,AS} \overset{NS}{\star} c_{NS}$	concentration in the convective flows	macroscopic
60	60	$\hat{n}^v_{NS,dt} := F_{NS,AS} \overset{AS}{\star} \left(\hat{V}_{A,dt} \odot c_{AS}\right)$	convective species flow	macroscopic
61	61	$\hat{n}^d_{NS,dt} := A_{xN} \odot F_{NS,AS} \overset{AS}{\star} \left(\left(-{k_x^{n_d}}_{AS,dt}\right) \,.\, F_{NS,AS} \overset{NS}{\star} \mu_{NS}\right)$	diffusional species flows	macroscopic

Continued on next page

	no	equation	documentation	layer
62	62	$\dot{n}_{NS,dt} := \hat{n}^{v}_{NS,dt} + \hat{n}^{d}_{NS,dt} + \tilde{n}_{NS,dt}$	differential species balances	macroscopic
63	63	$to_N := Set(t_N)$	initial time	root
64	64	$te_N := Set(t_N)$	end time	root
66	66	$_S := \lambda_S$	link to molar mass	materialDB »> liquid
67	67	$m_N := (1\backslash 2 \, . \, _S) \overset{S \in NS}{\star} n_{NS}$	mass	physical

28.2 Instantiations

	no	equation	documentation	layer