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
120	one	one	one	constant		94
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	
104	r_N	r	radius	frame	m	

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	var	symbol	documentation	type	units	eqs
123	$gugus$	`gugus`	new	frame		
10	n_{NS}	`n`	species mass in moles	state	mol	65
11	U_N	`U`	internal energy	state	$kg\, m^2\, s^{-2}$	
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	kg	
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
111	A_N	`A`	definition of Helmholtz energy	secondaryState	$kg\, m^2\, s^{-2}$	90
112	G_N	`G`	definition of Gibbs free energy	secondaryState	$kg\, m^2\, s^{-2}$	91
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`	chemical potential from Gibbs free energy	effort	$kg\, m^2\, mol^{-1}\, s^{-2}$	18 92

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

Continued on next page

	var	symbol	documentation	type	units	eqs
81	$\hat{V}_{A,dt}$	`fV`	volumetric flow	transport	$m^3\, s^{-1}$	83
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	$mol\, s^{-1}$	82
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	$dndt_{NS,dt}$	`dndt`	zero accumulation	state	$mol\, s^{-1}$	62 97
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	$kg^{-1}\, m^{-2}\, mol\, s^2$	
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

Continued on next page

	var	symbol	documentation	type	units	eqs
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
94	λ_S	`mm`	molecular masses	constant	$kg\, mol^{-1}$	
106	$k_{granulate_{dt}}$	`k_granulate`	kinetic constant for granulation dynamics	constant	s^{-1}	
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
93	$k^{d_x}{}_{NS,AS,dt}$	`kd_x`	diffusional mass diffusivity per area.	property	$kg^{-1}\, m^{-4}\, mol^2\, s$	81
95	$k^{c_x}{}_{N,A,dt}$	`kc_x`	convective mass diffusivity per area	property	$m^{-1}\, s$	76
96	ρ_N	`rho`	mass density	property	$kg\, m^{-3}$	71
98	$k^{v_x}{}_{N,A,dt}$	`kv_x`	convective volume flow per area	property	$kg^{-1}\, m^2\, s$	78

7 mixing

	var	symbol	documentation	type	units	eqs
113	y_N	`y`	mixing index	state		
122	$dy_{N,dt}$	`dy`	mixing differential equation	state		96
114	β	`beta`	mixing beta parameter	constant		
115	γ	`gamma`	mixing gamma parameter	constant		
116	f	`f`	stirrer frequency	constant	s^{-1}	
117	$a_{N,dt}$	`a`	stirrer amplitude	constant		

Continued on next page

	var	symbol	documentation	type	units	eqs
121	1_N	`y_one`	a one of the same dimension as y	constant		95
118	$\alpha_{N,dt}$	`alpha`	stirrer function	parameter		93

8 fluid

	var	symbol	documentation	type	units	eqs

9 solid

	var	symbol	documentation	type	units	eqs
101	N_N	`N`	number of particles	state		
110	$N_{t\,N,dt}$	`dN`	population balance PDE	state	s^{-1}	89
108	$\tilde{N}_{N,dt}$	`pN`	granulation dynamics	conversion	ms^{-1}	87

10 liquid

	var	symbol	documentation	type	units	eqs

11 gas

	var	symbol	documentation	type	units	eqs

12 control–gas

	var	symbol	documentation	type	units	eqs

13 gas–control

	var	symbol	documentation	type	units	eqs

14 control–liquid

	var	symbol	documentation	type	units	eqs

15 liquid–control

	var	symbol	documentation	type	units	eqs

16 control–materialDB

	var	symbol	documentation	type	units	eqs

17 materialDB–control

	var	symbol	documentation	type	units	eqs

18 control–mixing

	var	symbol	documentation	type	units	eqs

19 mixing–control

	var	symbol	documentation	type	units	eqs

20 control–solid

	var	symbol	documentation	type	units	eqs

21 solid–control

	var	symbol	documentation	type	units	eqs

22 gas–materialDB

	var	symbol	documentation	type	units	eqs

23 materialDB–gas

	var	symbol	documentation	type	units	eqs

24 gas–mixing

	var	symbol	documentation	type	units	eqs

25 mixing–gas

	var	symbol	documentation	type	units	eqs

26 liquid–materialDB

	var	symbol	documentation	type	units	eqs

27 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
99	${k^{v_x}}_{N,A,dt}$	`kv_x`	link to get volumetric flow coefficient	transform	$kg^{-1}\,m^{2}\,s$	79
100	${k^{d_x}}_{NS,AS,dt}$	`kd_x`	link to get diffusional mass flow coefficient	transform	$kg^{-1}\,m^{-4}\,mol^{2}\,s$	80

28 liquid–mixing

	var	symbol	documentation	type	units	eqs

29 mixing–liquid

	var	symbol	documentation	type	units	eqs

30 materialDB–mixing

	var	symbol	documentation	type	units	eqs

31 mixing–materialDB

	var	symbol	documentation	type	units	eqs

32 materialDB–solid

	var	symbol	documentation	type	units	eqs
107	${k_{granulate}}_{dt}$	`k_granulate`	link to kinetic granulation constant	transform	s^{-1}	86

33 solid–materialDB

	var	symbol	documentation	type	units	eqs

34 mixing–solid

	var	symbol	documentation	type	units	eqs

35 solid–mixing

	var	symbol	documentation	type	units	eqs

36 gas–liquid

	var	symbol	documentation	type	units	eqs

37 gas–solid

	var	symbol	documentation	type	units	eqs

38 liquid–solid

	var	symbol	documentation	type	units	eqs

39 Equations

39.1 Model equations

no	equation	documentation	layer
1	$1\backslash 2 := Set(\#, -)$	one half	root
2	$0 := Set(\#, -)$	zero	root
3	$\partial t_{N,dt} := diffSpace(t_N)$	differential time	root
4	$T_N := \frac{\partial U_N}{\partial S_N}$	definition of temperature	physical
5	$p_N := \left(-\frac{\partial U_N}{\partial V_N}\right)$	definition of pressure	physical
7	$H_N := U_N + p_N \,.\, V_N$	definition of enthalpy	physical
8	$v_{x\,N} := \frac{\partial r_{x\,N}}{\partial t_N}$	definition of velocity in x direction	physical
10	$A_{x\,N} := r_{y\,N} \,.\, r_{z\,N}$	area at location x	physical
14	$c_{p\,N} := \frac{\partial H_N}{\partial T_N}$	heat capacity at constant pressure	materialDB
18	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	definition of chemical potential	physical
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	$k^{q_x}{}_{A,dt} := k^{q_x}{}_{A,dt}$	link to get heat transfer coefficient	materialDB »> liquid
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	$n^0{}_{NS} := Set(n_{NS}, -)$	initial condition	macroscopic
42	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar concentration	macroscopic

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no	equation	documentation	layer
43	$c_{KS} := P_{NS,KS} \overset{NS}{\star} c_{NS}$	molar concentrations assigned to reaction K	macroscopic
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	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature for reactions	macroscopic
46	$K_{NK,dt} := {K^o}_{K,dt} \odot exp({E^A}_K \odot (R \,.\, T_{NK})^{-1})$	reaction "constants"	macroscopic
47	${c^o}_{KS} := Set(c_{KS}, -)$	norming concentration – probability must have no units !	macroscopic
49	$x_{KS} := ({c^o}_{KS})^{-1} \,.\, c_{KS}$	normed concentration little like more fractions	macroscopic
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	$\xi_{NK,dt} := K_{NK,dt} \,.\, \phi_{NK}$	dyamic extend of reaction	macroscopic
54	$\tilde{n}_{NS,dt} := V_N \odot \left(N_{NS,NK} \overset{NK}{\star} \xi_{NK,dt}\right)$	production term	macroscopic
57	$d_A := \text{sign}\left(F_{N,A} \overset{N}{\star} p_N\right)$	direction of flow relative to reference coordinate	macroscopic
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	$c_{AS} := S_{NS,AS} \overset{NS}{\star} c_{NS}$	concentration in the convective flows	macroscopic
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
62	$dndt_{NS,dt} := \hat{n}^v_{NS,dt} + \hat{n}^d_{NS,dt} + \tilde{n}_{NS,dt}$	differential species balances	macroscopic
63	$to_N := Set(t_N, -)$	initial time	root
64	$te_N := Set(t_N, -)$	end time	root

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no	equation	documentation	layer
65	$n_{NS} := \int_{to_N}^{te_N} dndt_{NS,dt} \; d\,t_N + n^0{}_{NS}$	integration of differential species balances	macroscopic
71	$\rho_N := m_N \,.\, (V_N)^{-1}$	mass density	materialDB
76	$k^{c_x}{}_{N,A,dt} := (-P_{N,A,dt}) \overset{N}{\star} \left(\lambda_S \overset{S\in NS}{\star} (\mu_{NS})^{-1}\right) \,.\, (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial p_N} \,.\, v_{x\,N}$	convective mass diffusivity per area	materialDB
78	$k^{v_x}{}_{N,A,dt} := (\rho_N)^{-1} \,.\, k^{c_x}{}_{N,A,dt}$	convective volume flow per area	materialDB
79	$k^{v_x}{}_{N,A,dt} := k^{v_x}{}_{N,A,dt}$	link to get volumetric flow coefficient	materialDB »> liquid
80	$k^{d_x}{}_{NS,AS,dt} := k^{d_x}{}_{NS,AS,dt}$	link to get diffusional mass flow coefficient	materialDB »> liquid
81	$k^{d_x}{}_{NS,AS,dt} := (-P_{NS,AS,dt}) \overset{NS}{\star} \left(v_{x\,N} \,.\, (V_N)^{-1} \odot (\mu_{NS})^{-1}\right) \,.\, \frac{\partial U_N}{\partial \mu_{NS}}$	diffusional mass diffusivity per area.	materialDB
82	$\hat{n}^d_{NS,dt} := A_{x\,N} \odot F_{NS,AS} \overset{AS}{\star} \left(\left(-k^{d_x}{}_{NS,AS,dt}\right) \,.\, F_{NS,AS} \overset{NS}{\star} \mu_{NS}\right)$	diffusional species flows	macroscopic
83	$\hat{V}_{A,dt} := F_{N,A} \overset{A}{\star} (-k^{v_x}{}_{N,A,dt}) \,.\, A_{x\,N} \,.\, F_{N,A} \overset{N}{\star} p_N$	volumetric flow	macroscopic
86	$k_{granulate_{dt}} := k_{granulate_{dt}}$	link to kinetic granulation constant	materialDB »> solid
87	$\tilde{N}_{N,dt} := k_{granulate_{dt}} \,.\, r_N$	granulation dynamics	solid
89	$N_{t\,N,dt} := \frac{\partial \tilde{N}_{N,dt}}{\partial r_N}$	population balance PDE	solid
90	$A_N := U_N - T_N \,.\, S_N$	definition of Helmholtz energy	physical
91	$G_N := U_N + p_N \,.\, V_N - T_N \,.\, S_N$	definition of Gibbs free energy	physical
92	$\mu_{NS} := \frac{\partial G_N}{\partial n_{NS}}$	chemical potential from Gibbs free energy	physical
93	$\alpha_{N,dt} := a_{N,dt} \,.\, sin(t_N \,.\, f)$	stirrer function	mixing

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no	equation	documentation	layer
94	$one := Set(\#, -)$	one	root
95	$1_N := Set(y_N, -)$	one of the same dimension as y	mixing
96	$dy_{N,dt} := \alpha_{N,dt} \,.\, (\gamma \,.\, y_N - \beta \,.\, (y_N - 1_N))$	mixing differential equation	mixing
97	$dndt_{NS,dt} := Set(dndt_{NS,dt}, 0)$	zero accumulation	macroscopic

39.2 Instantiations

	no	equation	documentation	layer