

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	<i>s</i>	
88	to_N	to	initial time	frame	<i>s</i>	63
89	te_N	te	end time	frame	<i>s</i>	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	<i>s</i>	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_{xN}	rx	spatial coordinate x	frame	<i>m</i>	
20	r_{yN}	ry	spatial coordinate y	frame	<i>m</i>	
21	r_{zN}	rz	spatial coordinate z	frame	<i>m</i>	
104	r_N	r	radius	frame	<i>m</i>	

Continued on next page

	var	symbol	documentation	type	units	eqs
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	$kg^{-1}\,m^{-2}\,mol\,K^{-1}\,s^2$	7 8 10 90 91 4 5 18 92
17	H_N	H	definition of enthalpy	secondaryState	$kg\,m^2\,s^{-2}$	
18	v_{xN}	vx	definition of velocity in x direction	secondaryState	ms^{-1}	
22	A_{xN}	Ax	area at location x	secondaryState	m^2	
111	A_N	A	definition of Helmholtz energy	secondaryState	$kg\,m^2\,s^{-2}$	
112	G_N	G	definition of Gibbs free energy	secondaryState	$kg\,m^2\,s^{-2}$	
14	T_N	T	definition of temperature	effort	K	
15	p_N	p	definition of pressure	effort	$kg\,m^{-1}\,s^{-2}$	
31	μ_{NS}	mu	chemical potential from Gibbs free energy	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	

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	$m^3\,s^{-1}$	83

Continued on next page

	var	symbol	documentation	type	units	eqs
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	$\hat{n}_{NS,dt}^v$	fnv	convective species flow	transport	$mol s^{-1}$	60
86	$\hat{n}_{NS,dt}^d$	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_{NS}^0	n0	initial condition	state	mol	41
87	$\dot{n}_{NS,dt}$	dn		state	$mol s^{-1}$	62
62	$N_{K,KS}$	N_KS_K	stoichiometry for reaction k	constant		
64	$K_{K,dt}^o$	Ko	Arrhenius prexponential factor (matrix)	constant	$m^{-3} mol s^{-1}$	
65	E_K^A	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 stoichiometry 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_{KS}^o	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

Continued on next page

	var	symbol	documentation	type	units	eqs
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	$kg mol^{-1}$	14 31 81 76 71 78
106	$k_{granulate\,dt}$	k_granulate	kinetic constant for granulation dynamics	constant	s^{-1}	
26	c_{pN}	cp	heat capacity at constant pressure	property	$kg m^2 K^{-1} s^{-2}$	
45	$k^{q_x}_{A,dt}$	kq_x	heat transfer coefficient for an event-dynamic transfer system	property	$kg K^{-1} s^{-3}$	
93	$k^{d_x}_{NS,AS,dt}$	kd_x	diffusional mass diffusivity per area.	property	$kg^{-1} m^{-4} mol^2 s$	
95	$k^{c_x}_{N,A,dt}$	kc_x	convective mass diffusivity per area	property	$m^{-1} s$	
96	ρ_N	rho	mass density	property	$kg m^{-3}$	
98	$k^{v_x}_{N,A,dt}$	kv_x	convective volume flow per area	property	$kg^{-1} m^2 s$	

7 mixing

	var	symbol	documentation	type	units	eqs
113	y_N	y	mixing index	state	s^{-1}	96
122	$dy_{N,dt}$	dy	mixing differential equation	state		
114	β	beta	mixing beta parameter	constant		
115	γ	gamma	mixing gamma parameter	constant		
116	f	f	stirrer frequency	constant		
117	$a_{N,dt}$	a	stirrer amplitude	constant		
121	1_N	y_one	a one of the same dimension as y	constant		95

Continued on next page

	var	symbol	documentation	type	units	eqs
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		89
110	$N_{tN,dt}$	dN	population balance PDE	state	s^{-1}	
108	$\tilde{N}_{N,dt}$	pN	granulation dynamics	conversion	ms^{-1}	

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	$1 \setminus 2 := Set(\#, -)$	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	$H_N := U_N + p_N \cdot V_N$	definition of enthalpy	physical
8	$v_{xN} := \frac{\partial r_{xN}}{\partial t_N}$	definition of velocity in x direction	physical
10	$A_{xN} := r_{yN} \cdot r_{zN}$	area at location x	physical
14	$c_{pN} := \frac{\partial H_N}{\partial T_N}$	heat capacity at constant pressure	materialDB
18	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	definition of chemical potential	physical
31	$k^{qx}_{A,dt} := (-P_{N,A,dt}) \stackrel{N}{\star} \left((V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}\right)$	heat transfer coefficient for an event-dynamic transfer system	materialDB
32	$k^{qx}_{A,dt} := k^{qx}_{A,dt}$	link to get heat transfer coefficient	materialDB » > liquid
39	$\hat{q}_{N,dt} := F_{N,A} \stackrel{A}{\star} \left((-k^{qx}_{A,dt}) \cdot A_{xN} \cdot F_{N,A} \stackrel{N}{\star} T_N\right)$	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

Continued on next page

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 stoichiometry block matrix	macroscopic
45	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature for reactions	macroscopic
46	$K_{NK,dt} := K^o_{K,dt} \odot \exp(E^A_K \odot (R \cdot T_{NK})^{-1})$	reaction "constants"	macroscopic
47	$c^o_{KS} := Set(c_{KS}, -)$	norming concentration – probability must have no units !	macroscopic
49	$x_{KS} := (c^o_{KS})^{-1} \cdot c_{KS}$	normed concentration little like more fractions	macroscopic
52	$\phi_{NK} := P_{NK,KS} \overset{KS}{\star} \left(\prod (x_{KS}^{N_{K,KS}}) \right)$	probability for the reactions to occur	macroscopic
53	$\xi_{NK,dt} := K_{NK,dt} \cdot \phi_{NK}$	dynamic 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	$S_{NS,AS} := 1 \setminus 2 \cdot (F_{NS,AS} - d_A \odot F_{NS,AS})$	selection of the flow sources	macroscopic
59	$c_{AS} := S_{NS,AS} \overset{NS}{\star} c_{NS}$	concentration in the convective flows	macroscopic
60	$\hat{n}_{NS,dt}^v := F_{NS,AS} \overset{AS}{\star} \left(\hat{V}_{A,dt} \odot c_{AS} \right)$	convective species flow	macroscopic
62	$\dot{n}_{NS,dt} := \hat{n}_{NS,dt}^v + \hat{n}_{NS,dt}^d + \tilde{n}_{NS,dt}$	differential species balances	macroscopic
63	$to_N := Set(t_N, -)$	initial time	root
64	$te_N := Set(t_N, -)$	end time	root

Continued on next page

no	equation	documentation	layer
65	$n_{NS} := \int_{t_0^N}^{t_N} \dot{n}_{NS,dt} dt + n_{NS}^0$	integration of differential species balances	macroscopic
71	$\rho_N := m_N \cdot (V_N)^{-1}$	mass density	materialDB
76	$k_{N,A,dt}^{c_x} := (-P_{N,A,dt}) \overset{N}{\star} \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass diffusivity per area	materialDB
78	$k_{N,A,dt}^{v_x} := (\rho_N)^{-1} \cdot k_{N,A,dt}^{c_x}$	convective volume flow per area	materialDB
79	$k_{N,A,dt}^{v_x} := k_{N,A,dt}^{v_x}$	link to get volumetric flow coefficient	materialDB »> liquid
80	$k_{NS,AS,dt}^{d_x} := k_{NS,AS,dt}^{d_x}$	link to get diffusional mass flow coefficient	materialDB »> liquid
81	$k_{NS,AS,dt}^{d_x} := (-P_{NS,AS,dt}) \overset{NS}{\star} \left(v_{xN} \cdot (V_N)^{-1} \odot (\mu_{NS})^{-1} \right) \cdot \frac{\partial U_N}{\partial \mu_{NS}}$	diffusional mass diffusivity per area.	materialDB
82	$\hat{n}_{NS,dt}^d := A_{xN} \odot F_{NS,AS} \overset{AS}{\star} \left((-k_{NS,AS,dt}^{d_x}) \cdot F_{NS,AS} \overset{NS}{\star} \mu_{NS} \right)$	diffusional species flows	macroscopic
83	$\hat{V}_{A,dt} := F_{N,A} \overset{A}{\star} (-k_{N,A,dt}^{v_x}) \cdot A_{xN} \cdot F_{N,A} \overset{N}{\star} p_N$	volumetric flow	macroscopic
86	$k_{granulate_{dt}} := k_{granulate_{dt}}$	link to kinetic granulation constant	materialDB »> solid
87	$\tilde{N}_{N,dt} := k_{granulate_{dt}} \cdot r_N$	granulation dynamics	solid
89	$N_{tN,dt} := \frac{\partial \tilde{N}_{N,dt}}{\partial r_N}$	population balance PDE	solid
90	$A_N := U_N - T_N \cdot S_N$	definition of Helmholtz energy	physical
91	$G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$	definition of Gibbs free energy	physical
92	$\mu_{NS} := \frac{\partial G_N}{\partial n_{NS}}$	chemical potential from Gibbs free energy	physical
93	$\alpha_{N,dt} := a_{N,dt} \cdot \sin(t_N \cdot f)$	stirrer function	mixing

Continued on next page

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

39.2 Instantiations

	no	equation	documentation	layer
--	----	----------	---------------	-------