

# 1 Variables

## 2 root

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

## 3 physical

	var	symbol	documentation	type	units	eqs
30	$F_{NS,AS}$	<b>F_NS_AS</b>	incidence matrix for species network	network		
41	$P_{N,A,dt}$	<b>P_N_A_dt</b>	projection of node to arc (used for mapping transport system material to application arc)	projection		
49	$P_{NS,AS,dt}$	<b>P_NS_AS_dt</b>	projection of node to arc (used for mapping transport system material to application arc)	projection		
9	$r_{xN}$	<b>rx</b>	spatial coordinate x	frame	<i>m</i>	
20	$r_{yN}$	<b>ry</b>	spatial coordinate y	frame	<i>m</i>	
21	$r_{zN}$	<b>rz</b>	spatial coordinate z	frame	<i>m</i>	
104	$r_N$	<b>r</b>	radius	frame	<i>m</i>	
10	$n_{NS}$	<b>n</b>	species mass in moles	state	<i>mol</i>	65

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	var	symbol	documentation	type	units	eqs
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	$v_{xN}$	vx	definition of velocity in x direction	secondaryState	$ms^{-1}$	8
22	$A_{xN}$	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	$\mu_{NS}$	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
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## 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
82	$d_A$	dir	direction of flow relative to reference coordinate	transport		57

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	var	symbol	documentation	type	units	eqs
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	$\hat{n}_{NS,dt}^v$	f <sub>nv</sub>	convective species flow	transport	$mol s^{-1}$	60
86	$\hat{n}_{NS,dt}^d$	f <sub>nd</sub>	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	$\phi_{NK}$	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
94	$\lambda_S$	mm	molecular masses	constant	$kg\ mol^{-1}$	
106	$k_{granulate\ dt}$	k_granulate	kinetic constant for granulation dynamics	constant	$s^{-1}$	
26	$c_{pN}$	cp	heat capacity at constant pressure	property	$kg\ m^2\ K^{-1}\ s^{-2}$	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	$\rho_N$	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		
114	$\beta$	beta	mixing beta parameter	constant		
115	$\gamma$	gamma	mixing gamma parameter	constant		
116	$f$	f	stirrer frequency	constant	$s^{-1}$	
117	$a_{N,dt}$	a	stirrer amplitude	constant		
118	$\alpha$	alpha	stirrer function	parameter		93

## 8 fluid

	var	symbol	documentation	type	units	eqs
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## 9 solid

	var	symbol	documentation	type	units	eqs
101	$N_N$	N	number of particles	state		
110	$N_{tN,dt}$	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
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## 11 gas

	var	symbol	documentation	type	units	eqs
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## 12 control–gas

	var	symbol	documentation	type	units	eqs
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## 13 gas–control

	var	symbol	documentation	type	units	eqs
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## 14 control-liquid

	var	symbol	documentation	type	units	eqs
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## 15 liquid-control

	var	symbol	documentation	type	units	eqs
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## 16 control-materialDB

	var	symbol	documentation	type	units	eqs
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## 17 materialDB-control

	var	symbol	documentation	type	units	eqs
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## 18 control-mixing

	var	symbol	documentation	type	units	eqs
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## 19 mixing-control

	var	symbol	documentation	type	units	eqs
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## 20 control-solid

	var	symbol	documentation	type	units	eqs
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## 21 solid-control

	var	symbol	documentation	type	units	eqs
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## 22 gas-materialDB

	var	symbol	documentation	type	units	eqs
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## 23 materialDB-gas

	var	symbol	documentation	type	units	eqs
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## 24 liquid-materialDB

	var	symbol	documentation	type	units	eqs
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## 25 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

## 26 materialDB–mixing

	var	symbol	documentation	type	units	eqs
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## 27 mixing–materialDB

	var	symbol	documentation	type	units	eqs
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## 28 materialDB–solid

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

## 29 solid–materialDB

	var	symbol	documentation	type	units	eqs
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## 30 gas–liquid

	var	symbol	documentation	type	units	eqs
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## 31 gas–mixing

	var	symbol	documentation	type	units	eqs
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## 32 gas–solid

	var	symbol	documentation	type	units	eqs
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## 33 liquid–mixing

	var	symbol	documentation	type	units	eqs
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## 34 liquid–solid

	var	symbol	documentation	type	units	eqs
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## 35 mixing–solid

	var	symbol	documentation	type	units	eqs
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## 36 Equations

### 36.1 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

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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 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

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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	$\alpha := a_{N,dt} \cdot \sin(t_N \cdot f)$	stirrer function	mixing

## 36.2 Instantiations

	no	equation	documentation	layer
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