

# 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\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	$r_{xN}$	rx	spatial coordinate x	frame	m	
20	$r_{yN}$	ry	spatial coordinate y	frame	m	
21	$r_{zN}$	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 <sup>2</sup> s <sup>-2</sup>	

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	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	$kg$	
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
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	definition of chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	18

## 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	$m^3\,s^{-1}$	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	$\hat{n}_{NS,dt}^v$	fnv	convective species flow	transport	$mol\,s^{-1}$	60
86	$\hat{n}_{NS,dt}^d$	fnd	diffusional species flows	transport	$mol\,s^{-1}$	61

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	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	$n_{NS}^0$	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 preexponential factor (matrix)	constant	$m^{-3}\ mol\ s^{-1}$	
65	$E_K^A$	ka	Arrhenius activation energy	constant	$kg^{-1}\ m^{-2}\ mol\ s^2$	
78	$k_{x\ AS,dt}^{n_d}$	knd_x	species diffusivity in x-direction	constant	$kg^{-1}\ m^{-4}\ mol^2\ s$	
79	$k_{x\ A,dt}^V$	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 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	probability for the reactions to occur	conversion		52
76	$\xi_{NK,dt}$	xi	dynamic 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	$mm_S$	mm	molecular masses	constant	$kg\ mol^{-1}$	
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	$kd_x$	kd_x	diffusional mass diffusivity per area	property	$kg^{-1}\ m^{-4}\ mol^2\ s$	69
95	$kc_x$	kc_x	convective mass diffusivity per area	property	$m^{-1}\ s$	70

## 7 fluid

	var	symbol	documentation	type	units	eqs
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## 8 solid

	var	symbol	documentation	type	units	eqs
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## 9 liquid

	var	symbol	documentation	type	units	eqs
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## 10 gas

	var	symbol	documentation	type	units	eqs
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## 11 control-gas

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

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

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

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

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

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

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

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

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

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

	var	symbol	documentation	type	units	eqs
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## 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

## 23 materialDB-solid

	var	symbol	documentation	type	units	eqs
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24 solid–materialDB

	var	symbol	documentation	type	units	eqs
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25 gas–liquid

	var	symbol	documentation	type	units	eqs
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26 gas–solid

	var	symbol	documentation	type	units	eqs
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27 liquid–solid

	var	symbol	documentation	type	units	eqs
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## 28 Equations

### 28.1 Model equations

	no	equation	documentation	layer
1	1	$1 \setminus 2 := Set(\#, -)$	one half	root
2	2	$0 := Set(\#, -)$	zero	root
3	3	$\partial t_{N,dt} := diffSpace(t_N)$	differential time	root
65	65	$n_{NS} := \int_{t_{oN}}^{t_{eN}} \dot{n}_{NS,dt} dt_N + n_{NS}^0$	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	$H_N := U_N + p_N \cdot V_N$	definition of enthalpy	physical
8	8	$v_{xN} := \frac{\partial r_{xN}}{\partial t_N}$	definition of velocity in x direction	physical
10	10	$A_{xN} := r_{yN} \cdot r_{zN}$	area at location x	physical
14	14	$c_{PN} := \frac{\partial H_N}{\partial T_N}$	heat capacity at constant pressure	materialDB
18	18	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	definition of chemical potential	physical
31	31	$k^{qx}_{A,dt} := (-P_{N,A,dt}) \stackrel{N}{\star} \left( (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN} \right)$	heat transfer coefficient for an event-dynamic transfer system	materialDB
32	32	$k^{qx}_{A,dt} := k^{qx}_{A,dt}$	link to get heat transfer coefficient	materialDB »> liquid
39	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	41	$n_{NS}^0 := Set(n_{NS}, -)$	initial condition	macroscopic

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	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 stoichiometry block matrix	macroscopic
45	45	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature for reactions	macroscopic
46	46	$K_{NK,dt} := K^o_{K,dt} \odot \exp(E^A_K \odot (R \cdot T_{NK})^{-1})$	reaction "constants"	macroscopic
47	47	$c^o_{KS} := Set(c_{KS}, -)$	norming concentration – probability must have no units !	macroscopic
49	49	$x_{KS} := (c^o_{KS})^{-1} \cdot c_{KS}$	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	$\xi_{NK,dt} := K_{NK,dt} \cdot \phi_{NK}$	dynamic 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	$\hat{V}_{A,dt} := F_{N,A} \overset{A}{\star} \left( -k_{x_{A,dt}}^V \right) \cdot A_{xN} \cdot F_{N,A} \overset{N}{\star} p_N$	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	$S_{NS,AS} := 1 \setminus 2 \cdot (F_{NS,AS} - d_A \odot  F_{NS,AS} )$	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	$\hat{n}_{NS,dt}^v := F_{NS,AS} \overset{AS}{\star} \left( \hat{V}_{A,dt} \odot c_{AS} \right)$	convective species flow	macroscopic
61	61	$\hat{n}_{NS,dt}^d := A_{xN} \odot F_{NS,AS} \overset{AS}{\star} \left( \left( -k_{x_{AS,dt}}^{n_d} \right) \cdot F_{NS,AS} \overset{NS}{\star} \mu_{NS} \right)$	diffusional species flows	macroscopic

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	no	equation	documentation	layer
<b>62</b>	62	$\dot{n}_{NS,dt} := \hat{n}_{NS,dt}^v + \hat{n}_{NS,dt}^d + \tilde{n}_{NS,dt}$	differential species balances	macroscopic
<b>63</b>	63	$to_N := Set(t_N, -)$	initial time	root
<b>64</b>	64	$te_N := Set(t_N, -)$	end time	root
<b>69</b>	69	$kd_x := (\mu_{NS})^{-1} \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{NS}} \cdot v_{xN}$	diffusional mass diffusivity per area	materialDB
<b>70</b>	70	$kc_x := \left( mm_S \odot (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass diffusivity per area	materialDB

## 28.2 Instantiations

	no	equation	documentation	layer
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