

# 1 Variables

## 2 root

	var	symbol	documentation	type	units	tokens	eqs
1	$F_{N,A}$	<b>F</b>	incidence matrix of directed graph	network		[]	
2	$t$	<b>t</b>	time	frame	$s$	[]	98
3	$\#$	<b>value</b>	numerical value	constant		[]	
4	1	<b>one</b>	numerical value 1	constant		[]	1
5	0	<b>zero</b>	numerical value 0	constant		[]	2
6	1/2	<b>onehalf</b>	numerical value 1/2	constant		[]	3
58	$t^o$	<b>to</b>	starting time	constant	$s$	[]	41
59	$t^e$	<b>te</b>	end time	constant	$s$	[]	42

## 3 physical

	var	symbol	documentation	type	units	tokens	eqs
15	$r_{xN}$	<b>r_x</b>	x-coordinate	frame	$m$	[]	101
16	$r_{yN}$	<b>r_y</b>	y-coordinate	frame	$m$	[]	99
17	$r_{zN}$	<b>r_z</b>	z-coordinate	frame	$m$	[]	100
18	$n_{NS}$	<b>n</b>	foundation state – species mass	state	$mol$	['mass']	94
19	$U_N$	<b>U</b>	foundation state – internal energy	state	$kg\,m^2\,s^{-2}$	['energy']	95
20	$S_N$	<b>S</b>	foundation state – entropy	state	$kg\,m^2\,K^{-1}\,s^{-2}$	[]	96
21	$V_N$	<b>V</b>	foundation state – volume	state	$m^3$	[]	97
29	$H_N$	<b>H</b>	enthalpy	state	$kg\,m^2\,s^{-2}$	['energy']	13
30	$A_N$	<b>A</b>	Helmholtz energy	state	$kg\,m^2\,s^{-2}$	['energy']	14

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	var	symbol	documentation	type	units	tokens	eqs
31	$G_N$	G	Gibbs energy	state	$kg\,m^2\,s^{-2}$	['energy']	15
27	$B_N$	B	Boltzmann constant	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	[]	11
101	$Av_N$	Av	Avogadro number	constant	$mol^{-1}$	[]	
102	$R_N$	R	Gas constant	constant	$kg\,m^2\,mol^{-1}\,K^{-1}\,s^{-2}$	[]	82
22	$p_N$	p	thermodynamic pressure	effort	$kg\,m^{-1}\,s^{-2}$	['energy']	7
23	$T_N$	T	temperature	effort	$K$	['energy']	8
24	$\mu_{NS}$	chem_potential	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	['energy', 'mass']	9
36	$v_{xN}$	v_x	velocity in x-direction	secondaryState	$ms^{-1}$	[]	20
37	$v_{yN}$	v_y	velocity in y-direction	secondaryState	$ms^{-1}$	[]	21
38	$v_{zN}$	v_z	velocity in z-direction	secondaryState	$ms^{-1}$	[]	22
39	$v_N$	v	velocity vector	secondaryState	$ms^{-1}$	[]	23

## 4 control

	var	symbol	documentation	type	units	tokens	eqs
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## 5 reactions

	var	symbol	documentation	type	units	tokens	eqs
98	$N_{S,K}$	N	stoichiometric matrix	constant		[]	
104	$E_{aNK}$	Ea	Arrhenius's activation energy	constant	$kg\,m^2\,mol^{-1}\,s^{-2}$	['energy']	84
105	$K^o_K$	Ko	Arrhenius's frequency factor	constant	$m^{-3}\,mol\,s^{-1}$	[]	
108	$c^o_{KS}$	co_KS	standardisation of concentration	constant	$m^{-3}\,mol$	['mass']	87
106	$K_{NK}$	K_NK	Arrhenius reaction constants	secondaryState	$m^{-3}\,mol\,s^{-1}$	['energy']	85

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	var	symbol	documentation	type	units	tokens	eqs
109	$\phi_{KS}$	phi_KS	propabilities to meet	seconaryState		['mass']	88

## 6 material

	var	symbol	documentation	type	units	tokens	eqs
40	$\lambda_S$	Mm	species molecular masses	constant	$kg\ mol^{-1}$	[]	
41	$C_{pN}$	Cp	total heat capacity at constant pressure	constant	$kg\ m^2\ K^{-1}\ s^{-2}$	['energy']	24
42	$C_{vN}$	Cv	total heat capacity at constant volume	constant	$kg\ m^2\ K^{-1}\ s^{-2}$	['energy']	25
43	$c_{pS}$	cp	specific heat capacity at constant pressure	constant	$m^2\ mol^2\ K^{-1}\ s^{-2}$	['energy', 'mass']	26
44	$c_{vS}$	cv	specific heat capacity at constant volume	constant	$m^2\ mol^2\ K^{-1}\ s^{-2}$	['energy', 'mass']	27
45	$k_{xN}^q$	kq_x	thermal conductivity in x-direction	seconaryState	$kg\ K^{-1}\ s^{-3}$	['energy']	28
46	$k_{yN}^q$	kq_y	thermal conductivity in y-direction	seconaryState	$kg\ K^{-1}\ s^{-3}$	['energy']	29
47	$k_{zN}^q$	kq_z	thermal conductivity in z-direction	seconaryState	$kg\ K^{-1}\ s^{-3}$	['energy']	30
48	$k_N^q$	kq	Cartesian thermal conductivity vector	seconaryState	$kg\ K^{-1}\ s^{-3}$	['energy']	31
49	$k_{xN}^c$	kc_x	convective mass convectivity in x-direction	seconaryState	$m^{-1}\ s$	['energy', 'mass']	32
50	$k_{yN}^c$	kc_y	convective mass convectivity in y-direction	seconaryState	$m^{-1}\ s$	['energy', 'mass']	33
51	$k_{zN}^c$	kc_z	convective mass convectivity in z-direction	seconaryState	$m^{-1}\ s$	['energy', 'mass']	34
52	$k_N^c$	kc	Cartesian convective mass convectivity vector	seconaryState	$m^{-1}\ s$	['energy', 'mass']	35
53	$k_{xNS}^d$	kd_x	diffusional mass conductivity in x-direction	seconaryState	$kg^{-1}\ m^{-4}\ mol^2\ s$	['energy', 'mass']	36
54	$k_{yNS}^d$	kd_y	diffusional mass conductivity in y-direction	seconaryState	$kg^{-1}\ m^{-4}\ mol^2\ s$	['energy', 'mass']	37

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	var	symbol	documentation	type	units	tokens	eqs
55	$k_{zNS}^d$	kd_z	diffusional mass conductivity in z-direction	seconaryState	$kg^{-1} m^{-4} mol^2 s$	['energy', 'mass']	<b>38</b>
56	$k_{NS}^d$	kd	Cartesian diffusional mass conductivity vector	seconaryState	$kg^{-1} m^{-4} mol^2 s$	['energy', 'mass']	<b>39</b>
60	$h_{NS}$	h	partial molar enthalpies	seconaryState	$kg m^2 mol^{-1} s^{-2}$	['energy', 'mass']	<b>43</b>

## 7 macroscopic

	var	symbol	documentation	type	units	tokens	eqs
78	$d_A$	d	direction of convective flow	transport		[]	<b>61</b>
80	$A_{y,zN}$	Ayz	cross sectional area in x-direction	transport	$m^2$	[]	<b>63</b>
83	$\hat{V}_A$	fV	convective volumetric flow	transport	$m^3 s^{-1}$	['mass']	<b>66</b>
84	$c_{AS}$	c_AS	molar species concentration in convective flow	transport	$m^{-3} mol$	['mass']	<b>67</b>
85	$\hat{n}_{AS}^c$	fnc_AS	convective mass flow by stream	transport	$mol s^{-1}$	['mass']	<b>68</b>
86	$\hat{n}_{NS}^c$	fnc	net convective mass flow	transport	$mol s^{-1}$	['mass']	<b>69</b>
87	$\hat{n}_{AS}^d$	fnd_AS	diffusional mass flow by stream	transport	$mol s^{-1}$	['energy']	<b>70</b>
88	$\hat{n}_{NS}^d$	fnd	net diffusional mass flow	transport	$mol s^{-1}$	['energy']	<b>71</b>
10	$F_{NS,AS}$	F_NS_AS	click incidence matrix of directed species graph	network		[]	<b>6</b>
9	$P_{NS,AS}$	P_NS_AS	node species to arc species projection	projection		[]	
11	$P_{K,NK}$	P_K_NK	projection of conversion to node x conversion	projection		[]	
12	$P_{S,NS}$	P_S_NS	projection species to conversion x species	projection		[]	
13	$P_{N,NK}$	P_N_NK	projection node to node x conversion	projection		[]	
14	$P_{NK,KS}$	P_NK_KS	projection node x conversion to conversion x species	projection		[]	

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	var	symbol	documentation	type	units	tokens	eqs
95	$P_{NS,KS}$	P_NS_KS	projection node x species to conversion x species	projection		[]	
92	$1_{NK}$	one_NK	one with energy	effort		['energy']	75
79	$c_{NS}$	c	molar concentration	seconaryState	$m^{-3} mol$	['mass']	62
81	$m_N$	m	mass in kg	seconaryState	$kg$	['mass']	64
82	$\rho_N$	density	density	seconaryState	$kg m^{-3}$	['mass']	65
91	$T_{NK}$	T_NK	temperature in reactive systems	conversion	$K$	['energy']	74
96	$c_{KS}$	c_KS	concentration in the reactive systems	conversion	$m^{-3} mol$	['mass']	78
112	$\xi_{NK}$	xi	extent of reaction	conversion	$m^{-3} mol s^{-1}$	['energy', 'mass']	91
113	$N_{NS,NK}$	N_NS_NK	extended stoichiometry	conversion		['energy']	92
114	$\tilde{n}_{NS}$	pn	production term	conversion	$mol s^{-1}$	['mass']	93

## 8 solid

	var	symbol	documentation	type	units	tokens	eqs
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## 9 fluid

	var	symbol	documentation	type	units	tokens	eqs
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## 10 liquid

	var	symbol	documentation	type	units	tokens	eqs
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## 11 gas

	var	symbol	documentation	type	units	tokens	eqs
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## 12 control-reactions

	var	symbol	documentation	type	units	tokens	eqs
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## 13 reactions-control

	var	symbol	documentation	type	units	tokens	eqs
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## 14 control-material

	var	symbol	documentation	type	units	tokens	eqs
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## 15 material-control

	var	symbol	documentation	type	units	tokens	eqs
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## 16 control-macroscopic

	var	symbol	documentation	type	units	tokens	eqs
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## 17 macroscopic-control

	var	symbol	documentation	type	units	tokens	eqs
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## 18 reactions–material

	var	symbol	documentation	type	units	tokens	eqs
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## 19 material–reactions

	var	symbol	documentation	type	units	tokens	eqs
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## 20 reactions–macroscopic

	var	symbol	documentation	type	units	tokens	eqs
107	$K_{NK}$	K_NK	link	transform	$m^{-3} mol s^{-1}$	['energy']	86
110	$\phi_{KS}$	phi_KS	link	transform		['mass']	89
111	$N_{S,K}$	N	link	transform		[]	90

## 21 macroscopic–reactions

	var	symbol	documentation	type	units	tokens	eqs
94	$T_{NK}$	T_NK	temperature of reactive systems	transform	$K$ $m^{-3} mol$	['energy']	77
97	$c_{KS}$	c_KS	link	transform		['mass']	79
103	$P_{N,NK}$	P_N_NK	link	transform		[]	83

## 22 material–macroscopic

	var	symbol	documentation	type	units	tokens	eqs
61	$\lambda_S$	Mm	link to molar masses	transform	$kg\ mol^{-1}$	[]	<a href="#">44</a>
62	$k_{xN}^q$	kq_x	link	transform	$kg\ K^{-1}\ s^{-3}$	['energy']	<a href="#">45</a>
63	$k_{yN}^q$	kq_y	link	transform	$kg\ K^{-1}\ s^{-3}$	['energy']	<a href="#">46</a>
64	$k_{zN}^q$	kq_z	link	transform	$kg\ K^{-1}\ s^{-3}$	['energy']	<a href="#">47</a>
65	$k_N^q$	kq	link	transform	$kg\ K^{-1}\ s^{-3}$	['energy']	<a href="#">48</a>
66	$k_{xN}^c$	kc_x	link	transform	$m^{-1}\ s$	['energy', 'mass']	<a href="#">49</a>
67	$k_{yN}^c$	kc_y	link	transform	$m^{-1}\ s$	['energy', 'mass']	<a href="#">50</a>
68	$k_{zN}^c$	kc_z	link	transform	$m^{-1}\ s$	['energy', 'mass']	<a href="#">51</a>
69	$k_N^c$	kc	link	transform	$m^{-1}\ s$	['energy', 'mass']	<a href="#">52</a>
70	$k_{xNS}^d$	kd_x	link	transform	$kg^{-1}\ m^{-4}\ mol^2\ s$	['energy', 'mass']	<a href="#">53</a>
73	$k_{yNS}^d$	kd_y	link	transform	$kg^{-1}\ m^{-4}\ mol^2\ s$	['energy', 'mass']	<a href="#">56</a>
74	$k_{zNS}^d$	kd_z	link	transform	$kg^{-1}\ m^{-4}\ mol^2\ s$	['energy', 'mass']	<a href="#">57</a>
75	$k_{NS}^d$	kd	link	transform	$kg^{-1}\ m^{-4}\ mol^2\ s$	['energy', 'mass']	<a href="#">58</a>
76	$c_{pS}$	cp	link	transform	$m^2\ mol^2\ K^{-1}\ s^{-2}$	['energy', 'mass']	<a href="#">59</a>
77	$c_{vS}$	cv	link	transform	$m^2\ mol^2\ K^{-1}\ s^{-2}$	['energy', 'mass']	<a href="#">60</a>

## 23 macroscopic-material



	var	symbol	documentation	type	units	tokens	eqs
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24 gas–liquid

	var	symbol	documentation	type	units	tokens	eqs
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25 gas–solid

	var	symbol	documentation	type	units	tokens	eqs
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26 liquid–solid

	var	symbol	documentation	type	units	tokens	eqs
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## 27 Equations

### 27.1 Model equations

no	equation	documentation	layer
1	$1 := Set(\#, \#)$	numerical value 1	root
2	$0 := Set(\#, \#)$	numerical value 1	root
3	$1/2 := Set(\#, \#)$	numerical value 1/2	root
6	$F_{NS,AS} := F_{N,A} \odot P_{NS,AS}$	blick incidence matrix of directed species graph	physical
7	$p_N := \frac{\partial U_N}{\partial V_N}$	thermodynamic pressure	physical
8	$T_N := \frac{\partial U_N}{\partial S_N}$	temperature	physical
9	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	chemical potential	physical
11	$B_N := Set(S_N, \#)$	Boltzmann constant	physical
13	$H_N := U_N + p_N \cdot V_N$	enthalpy	physical
14	$A_N := U_N - T_N \cdot S_N$	Helmholtz energy	physical
15	$G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$	Gibbs energy	physical
20	$v_{xN} := \frac{\partial r_{xN}}{\partial t}$	velocity in x-direction	physical
21	$v_{yN} := \frac{\partial r_{yN}}{\partial t}$	velocity in y-direction	physical
22	$v_{zN} := \frac{\partial r_{zN}}{\partial t}$	velocity in z-direction	physical
23	$v_N := Stack(v_{xN}, v_{yN}, v_{zN})$	velocity vector	physical

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no	equation	documentation	layer
24	$C_{pN} := \frac{\partial H_N}{\partial T_N}$	total heat capacity at constant pressure	material
25	$C_{vN} := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	material
26	$c_{pS} := C_{pN} \cdot (\lambda_S)^{-1} \stackrel{N \in NS}{\star} n_{NS}$	specific heat capacity at constant pressure	material
27	$c_{vS} := C_{vN} \cdot (\lambda_S)^{-1} \stackrel{N \in NS}{\star} n_{NS}$	specific heat capacity at constant volume	material
28	$k_{xN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}$	thermal conductivity in x-direction	material
29	$k_{yN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{yN}$	thermal conductivity in y-direction	material
30	$k_{zN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{zN}$	thermal conductivity in z-direction	material
31	$k_N^q := \text{Stack} \left( k_{xN}^q, k_{yN}^q, k_{zN}^q \right)$	Cartesian thermal conductivity vector	material
32	$k_{xN}^c := \left( \lambda_S \stackrel{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convective mass conductivity in x-direction	material
33	$k_{yN}^c := \left( \lambda_S \stackrel{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$	convective mass conductivity in y-direction	material
34	$k_{zN}^c := \left( \lambda_S \stackrel{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convective mass conductivity in z-direction	material
35	$k_N^c := \text{Stack} \left( k_{xN}^c, k_{yN}^c, k_{zN}^c \right)$	Cartesian convective mass conductivity vector	material
36	$k_{xNS}^d := (\mu_{NS})^{-1} \cdot \left( v_{xN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in x-direction	material
37	$k_{yNS}^d := (\mu_{NS})^{-1} \cdot \left( v_{yN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in y-direction	material

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no	equation	documentation	layer
38	$k_{zNS}^d := (\mu_{NS})^{-1} \cdot \left( v_{zN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$	diffusional mass conductivity in z-direction	material
39	$k_{NS}^d := Stack \left( k_{xNS}^d, k_{yNS}^d, k_{zNS}^d \right)$	Cartesian diffusional mass conductivity vector	material
41	$t^o := Set(t, t)$	starting time	root
42	$t^e := Set(t, t)$	end time	root
43	$h_{NS} := H_N \odot (n_{NS})^{-1}$	partial molar enthalpies	material
44	$\lambda_S := \lambda_S$	link to molar masses	material » macroscopic
45	$k_{xN}^q := k_{xN}^q$	link	material » macroscopic
46	$k_{yN}^q := k_{yN}^q$	link	material » macroscopic
47	$k_{zN}^q := k_{zN}^q$	link	material » macroscopic
48	$k_N^q := k_N^q$	link	material » macroscopic
49	$k_{xN}^c := k_{xN}^c$	link	material » macroscopic
50	$k_{yN}^c := k_{yN}^c$	link	material » macroscopic
51	$k_{zN}^c := k_{zN}^c$	link	material » macroscopic

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no	equation	documentation	layer
52	$k_N^c := k_N^c$	link	material » macroscopic
53	$k_{NS}^d := k_{NS}^d$	link	material » macroscopic
56	$k_{yNS}^d := k_{yNS}^d$	link	material » macroscopic
57	$k_{zNS}^d := k_{zNS}^d$	link	material » macroscopic
58	$k_{NS}^d := k_{NS}^d$	link	material » macroscopic
59	$c_{pS} := c_{pS}$	link	material » macroscopic
60	$c_{vS} := c_{vS}$	link	material » macroscopic
61	$d_A := \text{sign} \left( F_{N,A} \overset{N}{\star} p_N \right)$	direction of convective flow	macroscopic
62	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar concentration	macroscopic
63	$A_{y,zN} := r_{yN} \cdot r_{zN}$	cross sectional area in x-direction	macroscopic
64	$m_N := \lambda_S \overset{S \in NS}{\star} n_{NS}$	mass in kg	macroscopic
65	$\rho_N := (V_N)^{-1} \cdot m_N$	density	macroscopic
66	$\hat{V}_A := (\rho_N)^{-1} \cdot k_{xN}^c \cdot A_{y,zN} \cdot F_{N,A} \overset{N}{\star} p_N$	convective volumetric flow	macroscopic
67	$c_{AS} := (1/2 \cdot (F_{NS,AS} - d_A \odot  F_{NS,AS} )) \overset{NS}{\star} c_{NS}$	molar species concentration in convective flow	macroscopic

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no	equation	documentation	layer
68	$\hat{n}_{AS}^c := \hat{V}_A \odot c_{AS}$	convective mass flow by stream	macroscopic
69	$\hat{n}_{NS}^c := F_{NS,AS} \overset{AS}{\star} \hat{n}_{AS}^c$	net convective mass flow	macroscopic
70	$\hat{n}_{AS}^d := A_{y,z_N} \odot (-k_{x_{NS}}^d) \cdot F_{NS,AS} \overset{NS}{\star} \mu_{NS}$	diffusional mass flow by stream	macroscopic
71	$\hat{n}_{NS}^d := F_{NS,AS} \overset{AS}{\star} \hat{n}_{AS}^d$	net diffusional mass flow	macroscopic
74	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature in reactive systems	macroscopic
75	$1_{NK} := (T_{NK})^{-1} \cdot T_{NK}$	one with energy	macroscopic
77	$T_{NK} := T_{NK}$	temperature of reactive systems	macroscopic »> re- actions
78	$c_{KS} := c_{NS} \overset{NS}{\star} P_{NS,KS}$	concentration in the reactive systems	macroscopic
79	$c_{KS} := c_{KS}$	link	macroscopic »> re- actions
82	$R_N := Av_N \cdot B_N$	Gas constant	physical
83	$P_{N,NK} := P_{N,NK}$	link	macroscopic »> re- actions
84	$E_{a_{NK}} := Set(P_{N,NK} \overset{N}{\star} R_N \cdot T_{NK}, \#)$	Arrhenius's activation energy	reactions
85	$K_{NK} := K^o_K \odot exp((-E_{a_{NK}}) \cdot (R_N \overset{N}{\star} P_{N,NK} \cdot T_{NK})^{-1})$	Arrhenius reaction constants	reactions
86	$K_{NK} := K_{NK}$	link	reactions »> macroscopic
87	$c^o_{KS} := Set(c_{KS}, \#)$	standardisation of concentration	reactions
88	$\phi_{KS} := \prod (c_{KS} \cdot (c^o_{KS})^{-1})$	propabilities to meet	reactions

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no	equation	documentation	layer
89	$\phi_{KS} := \phi_{KS}$	link	reactions »> macroscopic
90	$N_{S,K} := N_{S,K}$	link	reactions »> macroscopic
91	$\xi_{NK} := K_{NK} \cdot P_{NK,KS} \overset{KS}{\star} \phi_{KS}$	extent of reaction	macroscopic
92	$N_{NS,NK} := P_{S,NS} \overset{S}{\star} \left( \left( P_{K,NK} \cdot T_{NK} \cdot (T_{NK})^{-1} \right) \overset{K}{\star} N_{S,K} \right)$	extended stoichiometry	macroscopic
93	$\tilde{n}_{NS} := V_N \odot \left( N_{NS,NK} \overset{NK}{\star} \xi_{NK} \right)$	production term	macroscopic
94	$n_{NS} := Set(n_{NS}, \#)$	foundation state – species mass	physical
95	$U_N := Set(U_N, \#)$	foundation state – internal energy	physical
96	$S_N := Set(S_N, \#)$	foundation state – entropy	physical
97	$V_N := Set(V_N, \#)$	foundation state – volume	physical
98	$t := Set(t, \#)$	time	root
99	$r_{yN} := Set(r_{yN}, \#)$	y-coordinate	physical
100	$r_{zN} := Set(r_{zN}, \#)$	z-coordinate	physical
101	$r_{xN} := Set(r_{xN}, \#)$	x-coordinate	physical