1 Variables

2 root

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

3 physical

	var	symbol	documentation	type	units	tokens	eqs
15	$r_{x\,N}$	`r_x`	x-coordinate	frame	m	[]	
16	$r_{y\,N}$	`r_y`	y-coordinate	frame	m	[]	
17	$r_{z\,N}$	`r_z`	z-coordinate	frame	m	[]	
18	$n_{N\,S}$	`n`	foundation state – species mass	state	mol	['mass']	
19	U_N	`U`	foundation state – internal energy	state	$kg\,m^2\,s^{-2}$	['energy']	
20	S_N	`S`	foundation state – entropy	state	$kg\,m^2\,K^{-1}\,s^{-2}$	[]	
21	V_N	`V`	foundation state – volume	state	m^3	[]	
29	H_N	`H`	enthalpy	state	$kg\,m^2\,s^{-2}$	['energy']	13
30	A_N	`A`	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	μ_{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	seconaryState	ms^{-1}	[]	20
37	v_{yN}	v_y	velocity in y-direction	seconaryState	ms^{-1}	[]	21
38	v_{zN}	v_z	velocity in z-direction	seconaryState	ms^{-1}	[]	22
39	v_N	v	velocity vector	seconaryState	ms^{-1}	[]	23

4 control

	var	symbol	documentation	type	units	tokens	eqs

5 reactions

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

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

6 material

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

Continued on next page

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

7 macroscopic

	var	symbol	documentation	type	units	tokens	eqs
78	d_A	d	direction of convective flow	transport		[]	61
80	$A_{y,z\,N}$	Ayz	cross sectional area in x-direction	transport	m^2	[]	63
83	$\hat{V}_A$	fV	convective volumetric flow	transport	$m^3\,s^{-1}$	['mass']	66
84	c_{AS}	c_AS	molar species concentration in convective flow	transport	$m^{-3}\,mol$	['mass']	67
85	$\hat{n}^c_{AS}$	fnc_AS	convective mass flow by stream	transport	$mol\,s^{-1}$	['mass']	68
86	$\hat{n}^c_{NS}$	fnc	net convective mass flow	transport	$mol\,s^{-1}$	['mass']	69
87	$\hat{n}^d_{AS}$	fnd_AS	diffusional mass flow by stream	transport	$mol\,s^{-1}$	['energy']	70
88	$\hat{n}^d_{NS}$	fnd	net diffusional mass flow	transport	$mol\,s^{-1}$	['energy']	71
10	$F_{NS,AS}$	F_NS_AS	blick incidence matrix of directed species graph	network		[]	6
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	$P_N S_K S_{NS,KS}$	P_NS_KS	projection node x species to conversion x species	projection		[]	
92	$one_N K_{NK}$	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	ρ_N	density	density	seconaryState	$kg\,m^{-3}$	['mass']	65
91	$T_N K_{NK}$	T_NK	temperature in reactive systems	conversion	K	['energy']	74
96	$c_K S_{KS}$	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	$N_N S_N K_{NS,NK}$	N_NS_NK	extended stoichiometry	conversion		['energy']	92
114	pn_{NS}	pn	production term	conversion	$mol\,s^{-1}$	['mass']	93

8 solid

	var	symbol	documentation	type	units	tokens	eqs

9 fluid

	var	symbol	documentation	type	units	tokens	eqs

10 liquid

	var	symbol	documentation	type	units	tokens	eqs

11 gas

	var	symbol	documentation	type	units	tokens	eqs

12 control–reactions

	var	symbol	documentation	type	units	tokens	eqs

13 reactions–control

	var	symbol	documentation	type	units	tokens	eqs

14 control–material

	var	symbol	documentation	type	units	tokens	eqs

15 material–control

	var	symbol	documentation	type	units	tokens	eqs

16 control–macroscopic

	var	symbol	documentation	type	units	tokens	eqs

17 macroscopic–control

	var	symbol	documentation	type	units	tokens	eqs

18 reactions–material

	var	symbol	documentation	type	units	tokens	eqs

19 material–reactions

	var	symbol	documentation	type	units	tokens	eqs

20 reactions–macroscopic

	var	symbol	documentation	type	units	tokens	eqs
107	$K_N K_{NK}$	`K_NK`	link	transform	$m^{-3}\,mol\,s^{-1}$	['energy']	86
110	$phi_K S_{KS}$	`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	$T_N K_{NK}$	`T_NK`	temperature of reacive systems	transform	K	['energy']	77
97	$c_K S_{KS}$	`c_KS`	link	transform	$m^{-3}\,mol$	['mass']	79
103	$P_{NN} K_{N,NK}$	`P_N_NK`	link	transform		[]	83

22 material–macroscopic

	var	symbol	documentation	type	units	tokens	eqs
61	λ_S	Mm	link to molar masses	transform	$kg\,mol^{-1}$	[]	44
62	${k^q_x}_N$	kq_x	link	transform	$kg\,K^{-1}\,s^{-3}$	['energy']	45
63	${k^q_y}_N$	kq_y	link	transform	$kg\,K^{-1}\,s^{-3}$	['energy']	46
64	${k^q_z}_N$	kq_z	link	transform	$kg\,K^{-1}\,s^{-3}$	['energy']	47
65	${k^q}_N$	kq	link	transform	$kg\,K^{-1}\,s^{-3}$	['energy']	48
66	${k^c_x}_N$	kc_x	link	transform	$m^{-1}\,s$	['energy', 'mass']	49
67	${k^c_y}_N$	kc_y	link	transform	$m^{-1}\,s$	['energy', 'mass']	50
68	${k^c_z}_N$	kc_z	link	transform	$m^{-1}\,s$	['energy', 'mass']	51
69	${k^c}_N$	kc	link	transform	$m^{-1}\,s$	['energy', 'mass']	52
70	${k^d_x}_{NS}$	kd_x	link	transform	$kg^{-1}\,m^{-4}\,mol^2\,s$	['energy', 'mass']	53
73	${k^d_y}_{NS}$	kd_y	link	transform	$kg^{-1}\,m^{-4}\,mol^2\,s$	['energy', 'mass']	56
74	${k^d_z}_{NS}$	kd_z	link	transform	$kg^{-1}\,m^{-4}\,mol^2\,s$	['energy', 'mass']	57
75	${k^d}_{NS}$	kd	link	transform	$kg^{-1}\,m^{-4}\,mol^2\,s$	['energy', 'mass']	58
76	c_{pS}	cp	link	transform	$m^2\,mol^2\,K^{-1}\,s^{-2}$	['energy', 'mass']	59
77	c_{vS}	cv	link	transform	$m^2\,mol^2\,K^{-1}\,s^{-2}$	['energy', 'mass']	60

23 macroscopic–material

	var	symbol	documentation	type	units	tokens	eqs

24 gas–liquid

	var	symbol	documentation	type	units	tokens	eqs

25 gas–solid

	var	symbol	documentation	type	units	tokens	eqs

26 liquid–solid

	var	symbol	documentation	type	units	tokens	eqs

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	$H_N := U_N + p_N \,.\, V_N$	enthalpy	physical
14	$A_N := U_N - T_N \,.\, S_N$	Helmholtz energy	physical
15	$G_N := U_N + p_N \,.\, V_N - T_N \,.\, S_N$	Gibbs energy	physical
20	$v_{x\,N} := \frac{\partial r_{x\,N}}{\partial t}$	velocity in x-direction	physical
21	$v_{y\,N} := \frac{\partial r_{y\,N}}{\partial t}$	velocity in y-direction	physical
22	$v_{z\,N} := \frac{\partial r_{z\,N}}{\partial t}$	velocity in z-direction	physical
23	$v_N := Stack\left(v_{x\,N}, v_{y\,N}, v_{z\,N}\right)$	velocity vector	physical

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no	equation	documentation	layer
24	$C_{p\,N} := \frac{\partial H_N}{\partial T_N}$	total heat capacity at constant pressure	material
25	$C_{v\,N} := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	material
26	$c_{p\,S} := C_{p\,N} \,.\, (\lambda_S)^{-1} \overset{N \in NS}{\star} n_{NS}$	specific heat capacity at constant pressure	material
27	$c_{v\,S} := C_{v\,N} \,.\, (\lambda_S)^{-1} \overset{N \in NS}{\star} n_{NS}$	specific heat capacity at constant volume	material
28	$k^q_{x\,N} := (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial T_N} \,.\, v_{x\,N}$	thermal conductivity in x-direction	material
29	$k^q_{y\,N} := (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial T_N} \,.\, v_{y\,N}$	thermal conductivity in y-direction	material
30	$k^q_{z\,N} := (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial T_N} \,.\, v_{z\,N}$	thermal conductivity in z-direction	material
31	$k^q{}_N := Stack\left(k^q_{x\,N}, k^q_{y\,N}, k^q_{z\,N}\right)$	Carthesian thermal conductivity vector	material
32	$k^c_{x\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \,.\, (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial p_N} \,.\, v_{x\,N}$	convective mass convectivity in x-direction	material
33	$k^c_{y\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \,.\, (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial p_N} \,.\, v_{y\,N}$	convective mass convectivity in y-direction	material
34	$k^c_{z\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \,.\, (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial p_N} \,.\, v_{z\,N}$	convective mass convectivity in z-direction	material
35	$k^c{}_N := Stack\left(k^c_{x\,N}, k^c_{y\,N}, k^c_{z\,N}\right)$	Cartesian convective mass convectivity vector	material
36	$k^d_{x\,NS} := (\mu_{NS})^{-1} \,.\, \left(v_{x\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in x-direction	material
37	$k^d_{y\,NS} := (\mu_{NS})^{-1} \,.\, \left(v_{y\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in y-direction	material

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no	equation	documentation	layer
38	$k^d_{z\,NS} := (\mu_{NS})^{-1} \,.\, \left(v_{z\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in z-direction	material
39	$k^d{}_{NS} := Stack\left(k^d_{x\,NS}, k^d_{y\,NS}, k^d_{z\,NS}\right)$	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	$k^q_{x\,N} := k^q_{x\,N}$	link	material »> macroscopic
46	$k^q_{y\,N} := k^q_{y\,N}$	link	material »> macroscopic
47	$k^q_{z\,N} := k^q_{z\,N}$	link	material »> macroscopic
48	$k^q{}_N := k^q{}_N$	link	material »> macroscopic
49	$k^c_{x\,N} := k^c_{x\,N}$	link	material »> macroscopic
50	$k^c_{y\,N} := k^c_{y\,N}$	link	material »> macroscopic
51	$k^c_{z\,N} := k^c_{z\,N}$	link	material »> macroscopic

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no	equation	documentation	layer
52	$k^c{}_N := k^c{}_N$	link	material »> macroscopic
53	$k^d_{xNS} := k^d_{xNS}$	link	material »> macroscopic
56	$k^d_{yNS} := k^d_{yNS}$	link	material »> macroscopic
57	$k^d_{zNS} := k^d_{zNS}$	link	material »> macroscopic
58	$k^d{}_{NS} := k^d{}_{NS}$	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	$A_{y,z\,N} := r_{y\,N} \,.\, r_{z\,N}$	cross sectional area in x-direction	macroscopic
64	$m_N := \lambda_S \overset{S \in NS}{\star} n_{NS}$	mass in kg	macroscopic
65	$\rho_N := (V_N)^{-1} \,.\, m_N$	density	macroscopic
66	$\hat{V}_A := (\rho_N)^{-1} \,.\, k^c_{x\,N} \,.\, A_{y,z\,N} \,.\, F_{N,A} \overset{N}{\star} p_N$	convective volumetric flow	macroscopic
67	$c_{AS} := (1/2 \,.\, (F_{NS,AS} - d_A \odot \lvert F_{NS,AS} \rvert)) \overset{NS}{\star} c_{NS}$	molar species concentration in convective flow	macroscopic

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no	equation	documentation	layer
68	$\hat{n}^c_{AS} := \hat{V}_A \odot c_{AS}$	convective mass flow by stream	macroscopic
69	$\hat{n}^c_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^c_{AS}$	net convective mass flow	macroscopic
70	$\hat{n}^d_{AS} := A_{y,z_N} \odot \left(-k^d_{xNS}\right) . F_{NS,AS} \overset{NS}{\star} \mu_{NS}$	diffusional mass flow by stream	macroscopic
71	$\hat{n}^d_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^d_{AS}$	net diffusional mass flow	macroscopic
74	$T_N K_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature in reactive systems	macroscopic
75	$one_N K_{NK} := \left(T_N K_{NK}\right)^{-1} . T_N K_{NK}$	one with energy	macroscopic
77	$T_N K_{NK} := T_N K_{NK}$	temperature of reacive systems	macroscopic »> reactions
78	$c_K S_{KS} := c_{NS} \overset{NS}{\star} P_N S_K S_{NS,KS}$	concentration in the reactive systems	macroscopic
79	$c_K S_{KS} := c_K S_{KS}$	link	macroscopic »> reactions
82	$R_N := Av_N . B_N$	Gas constant	physical
83	$P_{NN} K_{N,NK} := P_{N,NK}$	link	macroscopic »> reactions
84	$Ea_{NK} := Set(P_{NN} K_{N,NK} \overset{N}{\star} R_N . T_N K_{NK}, \#)$	Arrhenius's activation energy	reactions
85	$K_N K_{NK} := Ko_K \odot exp((-Ea_{NK}) . \left(R_N \overset{N}{\star} P_{NN} K_{N,NK} . T_N K_{NK}\right)^{-1})$	Arrhenius reaction constants	reactions
86	$K_N K_{NK} := K_N K_{NK}$	link	reactions »> macroscopic
87	$co_K S_{KS} := Set(c_K S_{KS}, \#)$	standardisation of concentration	reactions
88	$phi_K S_{KS} := \prod \left(c_K S_{KS} . \left(co_K S_{KS}\right)^{-1}\right)$	propabilities to meet	reactions

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no	equation	documentation	layer
89	$phi_K S_{KS} := phi_K S_{KS}$	link	reactions »> macroscopic
90	$N_{S,K} := N_{S,K}$	link	reactions »> macroscopic
91	$xi_{NK} := K_N K_{NK} \,.\, P_{NK,KS} \overset{KS}{\star} phi_K S_{KS}$	extent of reaction	macroscopic
92	$N_N S_N K_{NS,NK} := P_{S,NS} \overset{S}{\star} \left(\left(P_{K,NK} \,.\, T_N K_{NK} \,.\, \left(T_N K_{NK} \right)^{-1} \right) \overset{K}{\star} N_{S,K} \right)$	extended stoichiometry	macroscopic
93	$pn_{NS} := V_N \odot \left(N_N S_N K_{NS,NK} \overset{NK}{\star} xi_{NK} \right)$	production term	macroscopic