1 Variables

2 root

	var	symbol	documentation	type	units	eqs
8	$F_{N,A}$	`F_N_A`	fudamental incidence matrix	network		
5	t	`t`	time	frame	s	
6	t^o	`to`	starting time	frame	s	4
7	t^e	`te`	end time	frame	s	5
1	#	`value`	numerical value	constant		
2	1	`one`	numerical value one	constant		1
3	0	`zero`	numerical value zero	constant		2
4	0.5	`onehalf`	numerical value one half	constant		3

3 physical

	var	symbol	documentation	type	units	eqs
9	$P_{N,A}$	`P_N_A`	projection from node to arc for arc properties	projection		
32	$P_{NS,AS}$	`P_NS_AS`	projection node species to arc species	projection		
33	$P_{K,NK}$	`P_K_NK`	projection of conversion to node conversion	projection		
34	$P_{S,NS}$	`P_S_NS`	projection species to node species	projection		
35	$P_{N,NK}$	`P_N_NK`	projection node to node conversion	projection		
36	$P_{NS,KS}$	`P_NS_KS`	projection node species to conversion species	projection		
37	$P_{A,NS}$	`P_A_NS`	projection arc to node species for conductivity	projection		
65	$P_{NK,KS}$	`P_NK_KS`	projection node conversion to conversion species	projection		
10	r_{xN}	`r_x`	x-coordinate	frame	m	
11	r_{yN}	`r_y`	y-coordinate	frame	m	
12	r_{zN}	`r_z`	z coordinate	frame	m	
13	U_N	`U`	fundamental state – internal energy	state	$kg\,m^2\,s^{-2}$	
14	S_N	`S`	fundamental state – entropy	state	$kg\,m^2\,K^{-1}\,s^{-2}$	
15	V_N	`V`	fundamental state – volume	state	m^3	
16	n_{NS}	`n`	fundamental state – molar mass	state	mol	
20	H_N	`H`	enthalpy	state	$kg\,m^2\,s^{-2}$	9
21	A_N	`A`	Helmholtz energy	state	$kg\,m^2\,s^{-2}$	10
22	G_N	`G`	Gibbs free energy	state	$kg\,m^2\,s^{-2}$	11
23	C_N	`charge`	fundamental state – charge	state	$A\,s$	
24	A^v	`Avogadro`	Avogadro number	constant	mol^{-1}	
25	${k^B}_N$	`Boltzmann`	Boltzmann constant	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	12
26	R_N	`GasConstant`	gas constant	constant	$kg\,m^2\,mol^{-1}\,K^{-1}\,s^{-2}$	13
17	p_N	`p`	thermodynamic pressure	effort	$kg\,m^{-1}\,s^{-2}$	6

Continued on next page

	var	symbol	documentation	type	units	eqs
18	T_N	`T`	temperature	effort	K	7
19	μ_{NS}	`chemPot`	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	8
27	${U^C}_N$	`UC`	electrical potential – voltage	effort	$kg\,m^2\,A^{-1}s^{-3}$	14
28	v_{xN}	`v_x`	velocitiy in x-direction	secondaryState	ms^{-1}	15
29	v_{yN}	`v_y`	velocity in y-direction	secondaryState	ms^{-1}	16
30	v_{zN}	`v_z`	velocity in z-direction	secondaryState	ms^{-1}	17

4 control

	var	symbol	documentation	type	units	eqs

5 reactions

	var	symbol	documentation	type	units	eqs
31	$N_{S,K}$	N	soichiometric matrix	constant		
38	${K^o}_K$	Ko	Arrhenius frequency factor	constant	$m^{-3}\,mol\,s^{-1}$	
62	${E^a}_{NK}$	Ea	Arrhenius activation energy	constant	$kg\,m^2\,mol^{-1}\,s^{-2}$	41
63	K_{NK}	K_NK	Arrhenius reaction 'constant'	constant	$m^{-3}\,mol\,s^{-1}$	42
64	$N_{NS,NK}$	N_NS_NK	soichiometric block matrix node species and node reaction	constant		43
60	T_{NK}	T_NK	temperature of the reactive system	effort	K	39
68	$c_K S_{KS}$	c_KS	concentrations associated with reactions	secondaryState	$m^{-3}\,mol$	46
69	$co_K S_{KS}$	co_KS	norming concentrations	secondaryState	$m^{-3}\,mol$	47

6 material

	var	symbol	documentation	type	units	eqs
40	λ_S	`Mm`	species molecular mass	constant	$kg\,mol^{-1}$	
42	C_{pN}	`Cp`	total heat capacity at constant pressure	property	$kg\,m^2\,K^{-1}\,s^{-2}$	21
43	C_{VN}	`Cv`	total heat capacity at constant volume	property	$kg\,m^2\,K^{-1}\,s^{-2}$	22
44	k^q_{xN}	`kq_x`	thermal conductivity in x-direction	property	$kg\,K^{-1}\,s^{-3}$	23
45	k^q_{yN}	`kq_y`	thermal conductivity in y-direction	property	$kg\,K^{-1}\,s^{-3}$	24
46	k^q_{zN}	`kq_z`	thermal conductivity in z-direction'	property	$kg\,K^{-1}\,s^{-3}$	25
47	kq_N	`kq`	thermal conductivity	property	$kg\,K^{-1}\,s^{-3}$	26
48	k^c_{xN}	`kc_x`	convecitve mass conductivity in x-direction	property	$m^{-1}\,s$	27
49	k^c_{yN}	`kc_y`	convecitve mass conductivity in y-direction	property	$m^{-1}\,s$	28
50	k^c_{zN}	`kc_z`	convecitve mass conductivity in z-direction	property	$m^{-1}\,s$	29
51	$k^c{}_N$	`kc`	convective mass conductivity	property	$m^{-1}\,s$	30
52	k^d_{xNS}	`kd_x`	diffusional mass conductivity in x-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	31
53	k^d_{yNS}	`kd_y`	diffusional mass conductivity in y-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	32
54	k^d_{zNS}	`kd_z`	diffusional mass conductivity in z-direction	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	33
55	$k^d{}_{NS}$	`kd`	diffusional mass condctivity	property	$kg^{-1}\,m^{-4}\,mol^2\,s$	34
56	h_{NS}	`h`	partial molar enthalpies	property	$kg\,m^2\,mol^{-1}\,s^{-2}$	35
59	ρ_N	`density`	density	property	$kg\,m^{-3}$	38

7 macroscopic

	var	symbol	documentation	type	units	eqs
92	$\hat{V}_A$	`fV`	volumetric flow	transport	$m^3\,s^{-1}$	67
93	$\hat{n}^d{}_{AS}$	`fnd_AS`	diffusional mass flow in a given stream	transport	$mol\,s^{-1}$	68
94	$\hat{n}^d{}_{NS}$	`fnd`	net diffusional mass flow	transport	$mol\,s^{-1}$	69
95	$\hat{H}^d{}_A$	`fHd_A`	enthalpy flow per diffusional mass stream	transport	$kg\,m^2\,s^{-3}$	70
96	$\hat{H}^d{}_N$	`fHd`	net enthaply stream due to diffusion	transport	$kg\,m^2\,s^{-3}$	71
97	d_A	`d`	flow direction of convectional flow	transport		72
102	$\hat{H}^c{}_A$	`fHc_A`	convective enthalpy flow for given stream	transport	$kg\,m^2\,s^{-3}$	77
103	$\hat{H}^c{}_N$	`fHc`	net convectional enthalpy stream	transport	$kg\,m^2\,s^{-3}$	78
104	$\hat{w}_A$	`fw_A`	sample work stream	transport	$kg\,m^2\,s^{-3}$	79
105	$\hat{w}_N$	`fHw`	net work stream	transport	$kg\,m^2\,s^{-3}$	80
106	$\hat{q}_{xA}$	`fq_A_x`	heat flow in x-direction for given stream	transport	$kg\,m^2\,s^{-3}$	81
107	$\hat{q}_N$	`fq`	net heat flow	transport	$kg\,m^2\,s^{-3}$	82
71	A_{yzN}	`Ayz`	cross sectional area yz	geometry	m^2	48
72	A_{xzN}	`Axz`	cross sectional area xz	geometry	m^2	49
73	A_{xyN}	`Axy`	cross sectional area xy	geometry	m^2	50
70	$F_{NS,AS}$	`F_NS_AS`	species related incidence matrix	network		
90	$D_{N,A}$	`D`	difference operator	differenceOperator		
91	$D_{NS,AS}$	`D_NS_AS`	difference operator for species topology	differenceOperator		
57	m_N	`m`	total mass	secondaryState	kg	36
66	c_{NS}	`c`	molar composition	secondaryState	$m^{-3}\,mol$	44
98	c_{AS}	`c_AS`	concentration in convectional flow	secondaryState	$m^{-3}\,mol$	73
99	$\hat{n}^c{}_{AS}$	`fnc_AS`	molar convetional mass flow in the given stream	secondaryState	$mol\,s^{-1}$	74
100	$\hat{n}^c{}_{NS}$	`fnc`	net molar convectional mass flow	secondaryState	$mol\,s^{-1}$	75

Continued on next page

	var	symbol	documentation	type	units	eqs
101	$\dot{n}_{NS}$	`dndt`	differential species balance	diffState	$mol\,s^{-1}$	76

8 solid

	var	symbol	documentation	type	units	eqs

9 fluid

	var	symbol	documentation	type	units	eqs

10 liquid

	var	symbol	documentation	type	units	eqs

11 gas

	var	symbol	documentation	type	units	eqs

12 control–control

	var	symbol	documentation	type	units	eqs

13 gas–liquid

	var	symbol	documentation	type	units	eqs

14 gas–gas

	var	symbol	documentation	type	units	eqs

15 liquid–liquid

	var	symbol	documentation	type	units	eqs

16 gas–solid

	var	symbol	documentation	type	units	eqs

17 solid–solid

	var	symbol	documentation	type	units	eqs

18 liquid–solid

	var	symbol	documentation	type	units	eqs

19 material–material

	var	symbol	documentation	type	units	eqs

20 reactions–reactions

	var	symbol	documentation	type	units	eqs

21 control–reactions

	var	symbol	documentation	type	units	eqs

22 reactions–control

	var	symbol	documentation	type	units	eqs

23 control–material

	var	symbol	documentation	type	units	eqs

24 material–control

	var	symbol	documentation	type	units	eqs

25 control–macroscopic

	var	symbol	documentation	type	units	eqs

26 macroscopic–control

	var	symbol	documentation	type	units	eqs

27 reactions–material

	var	symbol	documentation	type	units	eqs

28 material–reactions

	var	symbol	documentation	type	units	eqs

29 reactions–macroscopic

	var	symbol	documentation	type	units	eqs

30 macroscopic–reactions

	var	symbol	documentation	type	units	eqs
67	c_{NS}	c	link variable c to interface macroscopic »> reactions	get	$m^{-3}\,mol$	45

31 material–macroscopic

	var	symbol	documentation	type	units	eqs
41	Mm_S	`Mm`	link variable Mm to interface material »> macroscopic	get	$kg\,mol^{-1}$	20
74	$density_N$	`density`	link variable density to interface material »> macroscopic	get	$kg\,m^{-3}$	51
75	h_{NS}	`h`	link variable h to interface material »> macroscopic	get	$kg\,m^2\,mol^{-1}\,s^{-2}$	52
76	kq_{xN}	`kq_x`	link variable kq x to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	53
77	Cv_N	`Cv`	link variable Cv to interface material »> macroscopic	get	$kg\,m^2\,K^{-1}\,s^{-2}$	54
78	kq_{yN}	`kq_y`	link variable kq y to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	55
79	kq_{zN}	`kq_z`	link variable kq z to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	56
80	kq_N	`kq`	link variable kq to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	57
81	kc_{xN}	`kc_x`	link variable kc x to interface material »> macroscopic	get	$m^{-1}\,s$	58
82	Cp_N	`Cp`	link variable Cp to interface material »> macroscopic	get	$kg\,m^2\,K^{-1}\,s^{-2}$	59
83	kc_{yN}	`kc_y`	link variable kc y to interface material »> macroscopic	get	$m^{-1}\,s$	60
84	kc_{zN}	`kc_z`	link variable kc z to interface material »> macroscopic	get	$m^{-1}\,s$	61
85	kc_N	`kc`	link variable kc to interface material »> macroscopic	get	$m^{-1}\,s$	62
86	kd_{xNS}	`kd_x`	link variable kd x to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	63
87	kd_{yNS}	`kd_y`	link variable kd y to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	64
88	kd_{zNS}	`kd_z`	link variable kd z to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	65

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	var	symbol	documentation	type	units	eqs
89	kd_{NS}	`kd`	link variable kd to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^{2}\,s$	66

32 macroscopic–material

	var	symbol	documentation	type	units	eqs
58	m_N	`m`	link variable m to interface macroscopic »> material	get	kg	37

33 Equations

34 Generic

no	equation	documentation	layer
1	$1 := \text{Instantiate}(\#, \#)$	numerical value 1	root
2	$0 := \text{Instantiate}(\#, \#)$	numerical value zero	root
3	$0.5 := \text{Instantiate}(\#, \#)$	numerical value one half	root
4	$t^o := \text{Instantiate}(t, \#)$	starting time	root
5	$t^e := \text{Instantiate}(t, \#)$	end time	root
6	$p_N := \left(-\frac{\partial U_N}{\partial V_N}\right)$	thermodynamic pressure	physical
7	$T_N := \frac{\partial U_N}{\partial S_N}$	temperature	physical
8	$\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$	chemical potential	physical
9	$H_N := U_N - p_N \,.\, V_N$	enthalpy	physical
10	$A_N := U_N - T_N \,.\, S_N$	Helmholtz energy	physical
11	$G_N := U_N + p_N \,.\, V_N - T_N \,.\, S_N$	Gibbs free energy	physical
12	${k^B}_N := \text{Instantiate}(S_N, \#)$	Boltzmann constant	physical
13	$R_N := A^v \,.\, {k^B}_N$	gas constant	physical
14	${U^C}_N := (C_N)^{-1} \,.\, U_N$	electrical potential – voltage	physical
15	$v_{xN} := \frac{\partial r_{xN}}{\partial t}$	velocitiy in x-direction	physical
16	$v_{yN} := \frac{\partial r_{yN}}{\partial t}$	velocity in y direction	physical

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no	equation	documentation	layer
17	$v_{zN} := \frac{\partial r_{zN}}{\partial t}$	velocity in z-direction	physical
21	$C_{pN} := \frac{\partial H_N}{\partial T_N}$	total heat capacity at constant pressure	material
22	$C_{VN} := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	material
23	$k^q_{xN} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}$	thermal conductivity in x-direction	material
24	$k^q_{yN} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{yN}$	thermal conductivity in y-direction	material
25	$k^q_{zN} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{zN}$	thermal conductivity in z-direction'	material
26	$kq_N := \text{Stack}\left(k^q_{xN}, k^q_{yN}, k^q_{zN}\right)$	thermal conductivity	material
27	$k^c_{xN} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$	convecitve mass conductivity in x-direction	material
28	$k^c_{yN} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$	convecitve mass conductivity in y-direction	material
29	$k^c_{zN} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$	convecitve mass conductivity in z-direction	material
30	$k^c{}_N := \text{Stack}\left(k^c_{xN}, k^c_{yN}, k^c_{zN}\right)$	convective mass conductivity	material
31	$k^d_{xNS} := (\mu_{NS})^{-1} \cdot \left(v_{xN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in x-direction	material
32	$k^d_{yNS} := (\mu_{NS})^{-1} \cdot \left(v_{yN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in y-direction	material
33	$k^d_{zNS} := (\mu_{NS})^{-1} \cdot \left(v_{zN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in z-direction	material
34	$k^d{}_{NS} := \text{Stack}\left(k^d_{xNS}, k^d_{yNS}, k^d_{zNS}\right)$	diffusional mass condctivity	material

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no	equation	documentation	layer
35	$h_{NS} := H_N \odot (n_{NS})^{-1}$	partial molar enthalpies	material
36	$m_N := Mm_S \overset{S \in NS}{\star} n_{NS}$	total mass	macroscopic
38	$\rho_N := m_N \,.\, (V_N)^{-1}$	density	material
39	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature of the reactive system	reactions
41	$E^a{}_{NK} := \text{Instantiate}(P_{N,NK} \overset{N}{\star} R_N \,.\, T_{NK}, \#)$	Arrhenius activation energy	reactions
42	$K_{NK} := K^o{}_K \odot exp((-E^a{}_{NK}) \,.\, \left(R_N \overset{N}{\star} P_{N,NK} \,.\, T_{NK}\right)^{-1})$	Arrhenius reaction 'constant'	reactions
43	$N_{NS,NK} := P_{S,NS} \overset{S}{\star} \left(P_{K,NK} \overset{K}{\star} N_{S,K}\right)$	soichiometric block matrix node species and node reaction	reactions
44	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar composition	macroscopic
46	$c_K S_{KS} := c_{NS} \overset{NS}{\star} P_{NS,KS}$	concentrations associated with reactions	reactions
47	$co_K S_{KS} := \text{Instantiate}(c_K S_{KS}, \#)$	norming concentrations	reactions
48	$A_{yzN} := r_{yN} \,.\, r_{zN}$	cross sectional area yz	macroscopic
49	$A_{xzN} := r_{xN} \,.\, r_{zN}$	cross sectional area xz	macroscopic
50	$A_{xyN} := r_{xN} \,.\, r_{yN}$	cross sectional area xy	macroscopic
67	$\hat{V}_A := (density_N)^{-1} \,.\, kc_{xN} \,.\, A_{yzN} \,.\, D_{N,A} \overset{N}{\star} p_N$	volumetric flow	macroscopic
68	$\hat{n}^d{}_{AS} := A_{yzN} \odot (-kd_{xNS}) \,.\, D_{NS,AS} \overset{NS}{\star} \mu_{NS}$	diffusional mass flow in a given stream	macroscopic
69	$\hat{n}^d{}_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^d{}_{AS}$	net diffusional mass flow	macroscopic

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no	equation	documentation	layer
70	$\hat{H}^d{}_A := \left(F_{NS,AS} \overset{NS}{\star} h_{NS}\right) \overset{S \in AS}{\star} \hat{n}^d{}_{AS}$	enthalpy flow per diffusional mass stream	macroscopic
71	$\hat{H}^d{}_N := F_{N,A} \overset{A}{\star} \hat{H}^d{}_A$	net enthaply stream due to diffusion	macroscopic
72	$d_A := \text{sign}\left(F_{N,A} \overset{N}{\star} p_N\right)$	flow direction of convectional flow	macroscopic
73	$c_{AS} := (0.5\,.\,(F_{NS,AS} - d_A \odot \lvert F_{NS,AS}\rvert)) \overset{NS}{\star} c_{NS}$	concentration in convectional flow	macroscopic
74	$\hat{n}^c{}_{AS} := \hat{V}_A \odot c_{AS}$	molar convetional mass flow in the given stream	macroscopic
75	$\hat{n}^c{}_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^c{}_{AS}$	net molar convectional mass flow	macroscopic
76	$\dot{n}_{NS} := \hat{n}^c{}_{NS} + \hat{n}^d{}_{NS}$	differential species balance	macroscopic
77	$\hat{H}^c{}_A := \left(F_{NS,AS} \overset{NS}{\star} h_{NS}\right) \overset{S \in AS}{\star} \hat{n}^c{}_{AS}$	convective enthalpy flow for given stream	macroscopic
78	$\hat{H}^c{}_N := F_{N,A} \overset{A}{\star} \hat{H}^c{}_A$	net convectional enthalpy stream	macroscopic
79	$\hat{w}_A := \text{Instantiate}(\hat{H}^c{}_A, \#)$	sample work stream	macroscopic
80	$\hat{w}_N := F_{N,A} \overset{A}{\star} \hat{w}_A$	net work stream	macroscopic
81	$\hat{q}_{xA} := A_{yzN}\,.\,kq_{xN}\,.\,D_{N,A} \overset{N}{\star} T_N$	heat flow in x-direction for given stream	macroscopic
82	$\hat{q}_N := F_{N,A} \overset{A}{\star} \hat{q}_{xA}$	net heat flow	macroscopic

35 Interface Link Equation

no	equation	documentation	layer
20	$Mm_S := Mm_S$	interface equation	material –> macroscopic
37	$m_N := m_N$	interface equation	macroscopic –> material
45	$c_{NS} := c_{NS}$	interface equation	macroscopic –> reactions
51	$density_N := density_N$	interface equation	material –> macroscopic
52	$h_{NS} := h_{NS}$	interface equation	material –> macroscopic
53	$kq_{xN} := kq_{xN}$	interface equation	material –> macroscopic
54	$Cv_N := Cv_N$	interface equation	material –> macroscopic
55	$kq_{yN} := kq_{yN}$	interface equation	material –> macroscopic
56	$kq_{zN} := kq_{zN}$	interface equation	material –> macroscopic
57	$kq_N := kq_N$	interface equation	material –> macroscopic
58	$kc_{xN} := kc_{xN}$	interface equation	material –> macroscopic

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no	equation	documentation	layer
59	$Cp_N := Cp_N$	interface equation	material –> macroscopic
60	$kc_{yN} := kc_{yN}$	interface equation	material –> macroscopic
61	$kc_{zN} := kc_{zN}$	interface equation	material –> macroscopic
62	$kc_N := kc_N$	interface equation	material –> macroscopic
63	$kd_{xNS} := kd_{xNS}$	interface equation	material –> macroscopic
64	$kd_{yNS} := kd_{yNS}$	interface equation	material –> macroscopic
65	$kd_{zNS} := kd_{zNS}$	interface equation	material –> macroscopic
66	$kd_{NS} := kd_{NS}$	interface equation	material –> macroscopic