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	$v_{x\,N}$	`v_x`	velocity in x-direction	seconaryState	ms^{-1}	[]	20
37	$v_{y\,N}$	`v_y`	velocity in y-direction	seconaryState	ms^{-1}	[]	21
38	$v_{z\,N}$	`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	$E_{a\,NK}$	`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	seconaryState	$m^{-3}\, mol\, s^{-1}$	['energy']	85

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	var	symbol	documentation	type	units	tokens	eqs
109	ϕ_{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

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	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
115	$fm_{m\,A}$	`fm_m`	mass flow in arc	transport	$kg\,s^{-1}$	['mass']	94
116	$fnd_{m\,NS,AS}$	`fnd_m`	diffusional mass transfer per arc	transport	$mol\,s^{-1}$	['energy', 'mass']	95
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	$P_{NS,KS}$	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	ρ_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	ξ_{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

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_{NK}	`K_NK`	link	transform	$m^{-3}\,mol\,s^{-1}$	['energy']	86
110	ϕ_{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 reacive systems	transform	K	['energy']	77
97	c_{KS}	`c_KS`	link	transform	$m^{-3}\,mol$	['mass']	79
103	$P_{N,NK}$	`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	$k^d_{x\,N\,S}$	kd_x	link	transform	$kg^{-1}\,m^{-4}\,mol^2\,s$	['energy', 'mass']	53
73	$k^d_{y\,N\,S}$	kd_y	link	transform	$kg^{-1}\,m^{-4}\,mol^2\,s$	['energy', 'mass']	56
74	$k^d_{z\,N\,S}$	kd_z	link	transform	$kg^{-1}\,m^{-4}\,mol^2\,s$	['energy', 'mass']	57
75	${k^d}_{N\,S}$	kd	link	transform	$kg^{-1}\,m^{-4}\,mol^2\,s$	['energy', 'mass']	58
76	${c_p}_S$	cp	link	transform	$m^2\,mol^2\,K^{-1}\,s^{-2}$	['energy', 'mass']	59
77	${c_v}_S$	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	$k^d_{z\,NS} := (\mu_{NS})^{-1} \cdot \left(v_{z\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	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	$k^d_{x\,NS} := k^d_{x\,NS}$	link	material »> macroscopic
56	$k^d_{y\,NS} := k^d_{y\,NS}$	link	material »> macroscopic
57	$k^d_{z\,NS} := k^d_{z\,NS}$	link	material »> macroscopic
58	${k^d}_{NS} := {k^d}_{NS}$	link	material »> macroscopic
59	${c_p}_S := {c_p}_S$	link	material »> macroscopic
60	${c_v}_S := {c_v}_S$	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
74	$T_{NK} := P_{N,NK} \overset{N}{\star} T_N$	temperature in reactive systems	macroscopic
75	$1_{NK} := (T_{NK})^{-1} \,.\, T_{NK}$	one with energy	macroscopic
77	$T_{NK} := T_{NK}$	temperature of reacive systems	macroscopic »> reactions
78	$c_{KS} := c_{NS} \overset{NS}{\star} P_{NS,KS}$	concentration in the reactive systems	macroscopic
79	$c_{KS} := c_{KS}$	link	macroscopic »> reactions
82	$R_N := Av_N \,.\, B_N$	Gas constant	physical
83	$P_{N,NK} := P_{N,NK}$	link	macroscopic »> reactions
84	$E_{a\,NK} := Set(P_{N,NK} \overset{N}{\star} R_N \,.\, T_{NK}, \#)$	Arrhenius's activation energy	reactions
85	$K_{NK} := K^o{}_K \odot exp((-E_{a\,NK}) \,.\, \left(R_N \overset{N}{\star} P_{N,NK} \,.\, T_{NK}\right)^{-1})$	Arrhenius reaction constants	reactions
86	$K_{NK} := K_{NK}$	link	reactions »> macroscopic
87	$c^o{}_{KS} := Set(c_{KS}, \#)$	standardisation of concentration	reactions
88	$\phi_{KS} := \prod \left(c_{KS} \,.\, (c^o{}_{KS})^{-1}\right)$	propabilities to meet	reactions
89	$\phi_{KS} := \phi_{KS}$	link	reactions »> macroscopic

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no	equation	documentation	layer
90	$N_{S,K} := N_{S,K}$	link	reactions »> macroscopic
91	$\xi_{NK} := K_{NK} \,.\, P_{NK,KS} \overset{KS}{\star} \phi_{KS}$	extent of reaction	macroscopic
92	$N_{NS,NK} := P_{S,NS} \overset{S}{\star} \left(\left(P_{K,NK} \,.\, T_{NK} \,.\, (T_{NK})^{-1}\right) \overset{K}{\star} N_{S,K}\right)$	extended stoichiometry	macroscopic
93	$\tilde{n}_{NS} := V_N \odot \left(N_{NS,NK} \overset{NK}{\star} \xi_{NK}\right)$	production term	macroscopic
94	$fm_{m\,A} := \lambda_S \overset{S \in AS}{\star} \hat{n}^c_{AS}$	mass flow in arc	macroscopic
95	$fnd_{m\,NS,AS} := A_{y,z\,N} \odot \left(-k^d_{x\,NS}\right) \,.\, \left(F_{NS,AS} \overset{NS}{\star} \mu_{NS}\right)$	diffusional mass transfer per arc	macroscopic