

1 Variables

2 root

	var	symbol	documentation	type	units	eqs
6	$F^{sink}_{A,I}$	F_AI_sink	incidence matrix AI sink	network		
5	$F^{source}_{A,I}$	F_AI_source	incidence matrix AI source	network		
15	$S_{N,q,t}$	S_Nqt	selection matrix or splitter	network		
21	$u_{N,t,u}$	u_Ntu	input signal in control domain	network		
14	$S_{N,p,q}$	S_Npu	selection matrix for stacker	network		
4	$F^{sink}_{N,I}$	F_NI_sink	incidence matrix NI sink	network		
10	$S_{I,q}$	S_Iq	selection matrix interface to control output	network		
22	$y_{N,t,u}$	y_Ntu	output signal in control domain	network		
7	$F^{source}_{N,A}$	F_NA_source	incidence matrix NA source	network		
8	$F^{sink}_{N,A}$	F_NA_sink	incidence matrix NA sink	network		
11	$I_{t,u}$	I_tu	identity mapping from <t> to <u>	network		
16	mv_I	mv_I	interface variable macro → control	network		
12	$S_{A,p}$	S_Ap	selection matrix interface species-related measures	network		
2	$F_{N,A}$	F	incidence matrix	network		
18	cz_I	cz_I	interface variable macro → control	network		
20	$A_{N,t,u}$	A_Ntu	mapping from input elements to outputs	network		
3	$F^{source}_{N,I}$	F_NI_source	incidence matrix NI source	network		
27	$I_{N,A}$	I_NA	identity mapping from <N> to <A>	network		
19	$A_{N,p,q}$	A_Npq	mapping from inputs to outputs	network		
9	$S_{I,p}$	S_Ip	selection matrix interface to control input	network		
17	cz_N	cz_N	output from control	network		
13	$S_{I,q}$	S_Aq	selection matrix arcs to outputs	network		

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	var	symbol	documentation	type	units	eqs
1	t	t	time	frame	s	
105	t^o	to	starting time	frame	s	4
107	Δt	t_interval	time interval	frame	s	6
106	t^e	te	end time	frame	s	5
101	$\#$	value	numerical value	constant		
104	0.5	oneHalf	numerical value one half	constant		3
103	1	one	numerical value one	constant		2
102	0	zero	numerical value zero	constant		1

3 physical

	var	symbol	documentation	type	units	eqs
25	r_{zN}	r_z	z-coordinate	frame	m	
24	r_{yN}	r_y	y-coordinate	frame	m	
23	r_{xN}	r_x	x-coordinate	frame	m	
108	U_N	U	fundamental state – internal energy	state	$kg\,m^2\,s^{-2}$	
137	m_N	m	mass	state	kg	30
109	S_N	S	fundamental state – internal entropy	state	$kg\,m^2\,K^{-1}\,s^{-2}$	
144	C_N	C	fundamental state – charge	state	$A\,s$	
111	$n_{N,S}$	n	fundamental state – molar mass	state	mol	93
110	V_N	V	volume	state	m^3	7
132	λ_S	Mm	molecular masses	constant	$kg\,mol^{-1}$	
122	k^B	Boltz	Boltzmann constant	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	
123	R	R	gas constant	constant	$kg\,m^2\,mol^{-1}\,K^{-1}\,s^{-2}$	17
121	N^A	Avo	Avogadro constant	constant	mol^{-1}	
148	A_{xyN}	Axy	cross sectional area xy	secondaryState	m^2	40
149	A_{xzN}	Axz	cross sectional are xz	secondaryState	m^2	41
143	ρ_N	rho	density	secondaryState	$kg\,m^{-3}$	36
150	A_{yzN}	Ayz	cross sectional area yz	secondaryState	m^2	42

4 macroscopic

	var	symbol	documentation	type	units	eqs
151	\hat{q}_{xA}	fq_x	heat flow in x-direction	transport	$kg\,m^2\,s^{-3}$	43
195	$\dot{n}_{N,S}^d$	and_x	accumulation due to diffusion in x-direction	transport	$mol\,s^{-1}$	88
158	$c_{A,S}$	c_AS	concentration in convective event-dynamic flow	transport	$m^{-3}\,mol$	50
157	d_A	d	flow direction of convective flow	transport		49
160	$\hat{n}_{xA,S}^c$	fnc_x	molar convective flow in x-direction	transport	$mol\,s^{-1}$	52
153	\hat{q}_{zA}	fq_z	heat flow in z-direction	transport	$kg\,m^2\,s^{-3}$	45
194	$\dot{n}_{N,S}$	anc	accumulation of molar mass due to convection	transport	$mol\,s^{-1}$	87
155	$\hat{n}_{yA,S}^d$	fnd_y	diffusion flow in y-direction	transport	$mol\,s^{-1}$	47 90
159	\hat{V}_A	fV	volumetric flow in x-direction	transport	$m^3\,s^{-1}$	51
152	\hat{q}_{yA}	fq_y	heat flow in y-direction	transport	$kg\,m^2\,s^{-3}$	44
154	$\hat{n}_{xA,S}^d$	fnd_x	diffusion flow in x-direction	transport	$mol\,s^{-1}$	46 89
156	$\hat{n}_{zA,S}^d$	fnd_z	diffusion flow in z-direction	transport	$mol\,s^{-1}$	48 91
186	k_{xA}^q	kqA_x	thermal conductivity in arc and x-direction	properties	$kg\,K^{-1}\,s^{-3}$	79
187	k_{yA}^q	kqA_y	thermal conductivity in arc and y-direction	properties	$kg\,K^{-1}\,s^{-3}$	80
183	k_{xA}^c	kcA_x	convective mass conductivity in arc and x direction	properties	$m^{-1}\,s$	76
192	$\hat{k}_z^{d,Fick}{}_{A,S}$	kdAFick_z	Fick diffusivity in arc and z-direction	properties	$m\,s^{-1}$	85
191	$\hat{k}_y^{d,Fick}{}_{A,S}$	kdAFick_y	Fick diffusivity in arc and y-direction	properties	$m\,s^{-1}$	84
180	$k_{xA,S}^d$	kdA_x	diffusivity in arc and x-direction	properties	$kg^{-1}\,m^{-4}\,mol^2\,s$	73
185	k_{zA}^c	kcA_z	convective mass conductivity in arc and y-direction	properties	$m^{-1}\,s$	78
188	k_{zA}^q	kqA_z	thermal conductivity in arc and z-direction	properties	$kg\,K^{-1}\,s^{-3}$	81
193	$h_{A,S}$	hA	partial molar enthalpies in arc	properties	$kg\,m^2\,mol^{-1}\,s^{-2}$	86
184	k_{yA}^c	kcA_y	convective mass conductivity in arc and y-direction	properties	$m^{-1}\,s$	77
181	$k_{yA,S}^d$	kdA_y	diffusivity in arc and y-direction	properties	$kg^{-1}\,m^{-4}\,mol^2\,s$	74

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	var	symbol	documentation	type	units	eqs
190	$\hat{k}_x^{d,Fick}{}_{A,S}$	kdAFick_x	Fick's diffusivity in arc and x-direction	properties	ms^{-1}	83
189	ρ_A	rhoA	density in arc	properties	$kg\,m^{-3}$	82
182	$k_z^d{}_{A,S}$	kdA_z	diffusivity in arc and z-direction	properties	$kg^{-1}\,m^{-4}\,mol^2\,s$	75
115	H_N	H	Enthalpy	state	$kg\,m^2\,s^{-2}$	11
117	G_N	G	Gibbs free energy	state	$kg\,m^2\,s^{-2}$	13
116	A_N	A	Helmholtz energy	state	$kg\,m^2\,s^{-2}$	12
161	$\mu^o{}_{N,S}$	chemPotStandard	instantiating standard chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	53
114	$\mu_{N,S}$	chemPot	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	10 54
113	T_N	T	temperature	effort	K	9
112	p_N	p	thermodynamic pressure	effort	$kg\,m^{-1}\,s^{-2}$	8
136	$h_{N,S}$	h	partial molar enthalpies	secondaryState	$kg\,m^2\,mol^{-1}\,s^{-2}$	29
141	c_{pN}	cp	specific heat capacity at constant pressure	secondaryState	$m^2\,K^{-1}\,s^{-2}$	34
125	CV_N	CV	total heat capacity at constant volume	secondaryState	$kg\,m^2\,K^{-1}\,s^{-2}$	19
119	v_{yN}	v_y	velocity in y-direction	secondaryState	ms^{-1}	15
142	c_{VN}	cV	specific heat capacity at constant volume	secondaryState	$m^2\,K^{-1}\,s^{-2}$	35
118	v_{xN}	v_x	velocity in x-direction	secondaryState	ms^{-1}	14
120	v_{zN}	v_z	velocity in z-direction	secondaryState	ms^{-1}	16
140	$x_{N,S}$	x	mole fraction	secondaryState		33
138	$c_{N,S}$	c	molar concentration	secondaryState	$m^{-3}\,mol$	31
139	n^t_N	nt	total number of moles	secondaryState	mol	32
124	Cp_N	Cp	total heat capacity at constant pressure	secondaryState	$kg\,m^2\,K^{-1}\,s^{-2}$	18
179	$pn_{N,S,p}$	pn	link variable pn to interface macroscopic	conversion	$mol\,s^{-1}$	72
196	$\dot{n}_{N,S}$	an	differential mass balance without reaction	diffState	$mol\,s^{-1}$	92

5 reactions

	var	symbol	documentation	type	units	eqs
173	$nt_{N,p}$	nt	link variable nt to interface reactions	state	mol	66
174	$Ea_{N,p}$	Ea	activation energy	constant	$kg\ m^2\ mol^{-1}\ s^{-2}$	67
26	$N_{S,CS}$	N	stoichiometric matrix	constant		
175	$K^o_{N,S}$	Ko	Arrhenius frequency factor	constant	$m^{-3}\ mol\ s^{-1}$	68
167	$T_{N,p}$	T	link variable T to interface reactions	effort	K	60
171	$V_{N,p}$	V	link variable V to interface reactions	secondaryState	m^3	64
165	$x_{N,S,p}$	x	link variable x to interface reactions	secondaryState		58
163	$c_{N,S,p}$	c	link variable c to interface reactions	secondaryState	$m^{-3}\ mol$	56
177	$\tilde{n}_{N,S,p}$	pn	production term	conversion	$mol\ s^{-1}$	70
176	$K_{N,S,p}$	K	Arrhenius reaction "constant"	conversion	$m^{-3}\ mol\ s^{-1}$	69
169	$\xi_{N,CS,p}$	probability	probability of reaction to take place	conversion		62
168	$f_{N,S,CS,p}$	factor	factor for probability computation	conversion		61

6 macroscopic-reactions

	var	symbol	documentation	type	units	eqs
166	$_T_I$	$_T$	link variable T to interface macroscopic »> reactions with source:node	get	K	59
170	$_V_I$	$_V$	link variable V to interface macroscopic »> reactions with source:node	get	m^3	63
172	$_nt_I$	$_nt$	link variable nt to interface macroscopic »> reactions with source:node	get	mol	65
162	$_c_{I,S}$	$_c$	link variable c to interface macroscopic »> reactions with source:node	get	$m^{-3} mol$	55
164	$_x_{I,S}$	$_x$	link variable x to interface macroscopic »> reactions with source:node	get		57

7 reactions-macroscopic

	var	symbol	documentation	type	units	eqs
178	$_{pn_{I,S,p}}$	<code>_pn</code>	link variable pn to interface reactions »> macroscopic with source:node	get	$mol\ s^{-1}$	71

8 Equations

9 Generic

no	equation	documentation	layer
1	$0 := \text{Instantiate}(\#, \#)$	numerical value zero	root
2	$1 := \text{Instantiate}(\#, \#)$	numerical value one	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	$\Delta t := \text{Instantiate}(t, \#)$	time interval	root
7	$V_N := r_{xN} \cdot r_{yN} \cdot r_{zN}$	volume	physical
8	$p_N := \frac{\partial U_N}{\partial V_N}$	thermodynamic pressure	physical
9	$T_N := \frac{\partial U_N}{\partial S_N}$	temperature	macroscopic
10	$\mu_{N,S} := \frac{\partial U_N}{\partial n_{N,S}}$	chemical potential	macroscopic
11	$H_N := U_N - p_N \cdot V_N$	Enthalpy	macroscopic
12	$A_N := U_N - T_N \cdot S_N$	Helmholtz energy	macroscopic
13	$G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$	Gibbs free energy	macroscopic
14	$v_{xN} := \frac{\partial r_{xN}}{\partial t}$	velocity in x-direction	macroscopic
15	$v_{yN} := \frac{\partial r_{yN}}{\partial t}$	velocity in y-direction	macroscopic
16	$v_{zN} := \frac{\partial r_{zN}}{\partial t}$	velocity in z-direction	macroscopic

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no	equation	documentation	layer
17	$R := N^A \cdot k^B$	gas constant	physical
18	$Cp_N := \frac{\partial H_N}{\partial T_N}$	total heat capacity at constant pressure	macroscopic
19	$CV_N := \frac{\partial U_N}{\partial T_N}$	total heat capacity at constant volume	macroscopic
29	$h_{N,S} := H_N \cdot (n_{N,S})^{-1}$	partial molar enthalpies	macroscopic
30	$m_N := \lambda_S \star n_{N,S}$	mass	macroscopic
31	$c_{N,S} := (V_N)^{-1} \cdot n_{N,S}$	molar concentration	macroscopic
32	$n_N^t := \text{reduceSum}(n_{N,S}, S)$	total number of moles	macroscopic
33	$x_{N,S} := (n_N^t)^{-1} \cdot n_{N,S}$	mole fraction	macroscopic
34	$c_{pN} := Cp_N \cdot (m_N)^{-1}$	specific heat capacity at constant pressure	physical
35	$c_{VN} := CV_N \cdot (m_N)^{-1}$	specific heat capacity at constant volume	macroscopic
36	$\rho_N := (V_N)^{-1} \cdot m_N$	density	physical
40	$A_{xyN} := r_{xN} \cdot r_{yN}$	cross sectional area xy	physical
41	$A_{xzN} := r_{xN} \cdot r_{zN}$	cross sectional area xz	physical
42	$A_{yzN} := r_{yN} \cdot r_{zN}$	cross sectional area yz	physical
43	$\hat{q}_{xA} := k_{xA}^q \cdot A_{yzN} \cdot F_{N,A} \star^N T_N$	heat flow in x-direction	macroscopic
44	$\hat{q}_{yA} := k_{yA}^q \cdot A_{xzN} \cdot F_{N,A} \star^N T_N$	heat flow in y-direction	macroscopic
45	$\hat{q}_{zA} := k_{zA}^q \cdot A_{xyN} \cdot F_{N,A} \star^N T_N$	heat flow in z-direction	macroscopic

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no	equation	documentation	layer
46	$\hat{n}_{xA,S}^d := \hat{k}_x^{d,Fick}{}_{A,S} \cdot A_{yzN} \cdot F_{N,A} \star^N c_{N,S}$	Fick diffusion flow in x-direction	macroscopic
47	$\hat{n}_{yA,S}^d := \hat{k}_y^{d,Fick}{}_{A,S} \cdot A_{xzN} \cdot F_{N,A} \star^N c_{N,S}$	Fick diffusion flow in y-direction	macroscopic
48	$\hat{n}_{zA,S}^d := \hat{k}_z^{d,Fick}{}_{A,S} \cdot (A_{xyN} \cdot F_{N,A}) \star^N c_{N,S}$	Fick diffusion flow in z-direction	macroscopic
49	$d_A := \mathbf{sign} \left(F_{N,A} \star^N p_N \right)$	flow direction of convective flow	macroscopic
50	$c_{A,S} := (0.5 \cdot (F_{N,A} - d_A \cdot F_{N,A})) \star^N c_{N,S}$	concentration in convective event-dynamic flow	macroscopic
51	$\hat{V}_A := (\rho_A)^{-1} \cdot k_{xA}^c \cdot A_{yzN} \cdot F_{N,A} \star^N p_N$	volumetric flow in x-direction	macroscopic
52	$\hat{n}_{xA,S}^c := \hat{V}_A \cdot c_{A,S}$	molar convective flow in x-direction	macroscopic
53	$\mu_{N,S}^o := \mathbf{Instantiate}(\mu_{N,S}, \#)$	instantiating standard chemical potential	macroscopic
54	$\mu_{N,S} := \mu_{N,S}^o + R \cdot T_N \cdot \ln(x_{N,S})$	chemical potential standard model with mole fraction	macroscopic
61	$f_{N,S,CS,p} := x_{N,S,p}^{(N_{S,CS})}$	factor for probability computation	reactions
62	$\xi_{N,CS,p} := \prod_S f_{N,S,CS,p}$	probability of reaction to take place	reactions
67	$Ea_{N,p} := \mathbf{Instantiate}(U_N \cdot (nt_{N,p})^{-1}, \#)$	activation energy	reactions
68	$K_{N,S}^o := \mathbf{Instantiate}(\rho_N \cdot (\lambda_S \cdot t)^{-1}, \#)$	Arrhenius frequency factor	reactions
69	$K_{N,S,p} := K_{N,S}^o \cdot \mathbf{exp} \left(Ea_{N,p} \cdot (R \cdot T_{N,p})^{-1} \right)$	Arrhenius reaction "constant"	reactions
70	$\tilde{n}_{N,S,p} := A_{N,p,q} \star^q \left(V_{N,p} \cdot N_{S,CS} \star^{CS} (K_{N,S,p} \cdot \xi_{N,CS,p}) \right)$	production term	reactions
73	$k_{xA,S}^d := I_{N,A} \star^N \left((\mu_{N,S})^{-1} \cdot \left(v_{xN} \cdot \left((V_N)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \right) \right) \right)$	diffusivity in arc and x-direction	macroscopic
74	$k_{yA,S}^d := I_{N,A} \star^N \left((\mu_{N,S})^{-1} \cdot \left(v_{yN} \cdot \left((V_N)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \right) \right) \right)$	diffusivity in arc and y-direction	macroscopic

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no	equation	documentation	layer
75	$k_{zA,S}^d := I_{N,A} \star^N \left((\mu_{N,S})^{-1} \cdot \left(v_{zN} \cdot \left((V_N)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \right) \right) \right)$	diffusivity in arc and z-direction	macroscopic
76	$k_{xA}^c := I_{N,A} \star^N \left(\left(\lambda_S \star^S (\mu_{N,S})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN} \right)$	convective mass conductivity in arc and x direction	macroscopic
77	$k_{yA}^c := I_{N,A} \star^N \left(\left(\lambda_S \star^S (\mu_{N,S})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN} \right)$	convective mass conductivity in arc and y-direction	macroscopic
78	$k_{zA}^c := I_{N,A} \star^N \left(\left(\lambda_S \star^S (\mu_{N,S})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN} \right)$	convective mass conductivity in arc and y-direction	macroscopic
79	$k_{xA}^q := I_{N,A} \star^N \left((V_N)^{-1} \cdot Cp_N \cdot v_{xN} \right)$	thermal conductivity in arc and x-direction	macroscopic
80	$k_{yA}^q := I_{N,A} \star^N \left((V_N)^{-1} \cdot Cp_N \cdot v_{yN} \right)$	thermal conductivity in arc and y-direction	macroscopic
81	$k_{zA}^q := I_{N,A} \star^N \left((V_N)^{-1} \cdot Cp_N \cdot v_{zN} \right)$	thermal conductivity in arc and z-direction	macroscopic
82	$\rho_A := I_{N,A} \star^N \rho_N$	density in arc	macroscopic
83	$\hat{k}_{xA,S}^{d,Fick} := I_{N,A} \star^N \left(v_{xN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$	Fick's diffusivity in arc and x-direction	macroscopic
84	$\hat{k}_{yA,S}^{d,Fick} := I_{N,A} \star^N \left(v_{yN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$	Fick diffusivity in arc and y-direction	macroscopic
85	$\hat{k}_{zA,S}^{d,Fick} := I_{N,A} \star^N \left(v_{zN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$	Fick diffusivity in arc and z-direction	macroscopic
86	$h_{A,S} := I_{N,A} \star^N h_{N,S}$	partial molar enthalpies in arc	macroscopic
87	$\dot{n}_{N,S} := F_{N,A} \star^A \hat{n}_{xA,S}^c$	accumulation of molar mass due to convection	macroscopic
88	$\dot{n}_{N,S}^d := F_{N,A} \star^A \hat{n}_{xA,S}^d$	accumulation due to diffusion in x-direction	macroscopic

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no	equation	documentation	layer
89	$\hat{n}_{xA,S}^d := k_{xA,S}^d \cdot (A_{yzN} \cdot F_{N,A}) \stackrel{N}{\star} \mu_{N,S}$	Fick diffusion flow in x-direction	macroscopic
90	$\hat{n}_{yA,S}^d := k_{yA,S}^d \cdot (A_{yzN} \cdot F_{N,A}) \stackrel{N}{\star} \mu_{N,S}$	Fick diffusion flow in y-direction	macroscopic
91	$\hat{n}_{zA,S}^d := k_{zA,S}^d \cdot (A_{xyN} \cdot F_{N,A}) \stackrel{N}{\star} \mu_{N,S}$	mass diffusion flow in z-direction	macroscopic
92	$\dot{n}_{N,S} := \dot{n}_{N,S} + \dot{n}_{N,S}^d$	differential mass balance without reaction	macroscopic
93	$n_{N,S} := \int_{t^o}^{t^e} \dot{n}_{N,S} dt$	fundamental state – molar mass	macroscopic

10 Interface Link Equation

no	equation	documentation	layer
55	$_c_{I,S} := F^{source}_{N,I} \star^N c_{N,S}$	interface equation	macroscopic \rightarrow reactions
56	$c_{N,S,p} := (F^{sink}_{N,I} \cdot _c_{I,S}) \star^I S_{I,p}$	interface equation	reactions
57	$_x_{I,S} := F^{source}_{N,I} \star^N x_{N,S}$	interface equation	macroscopic \rightarrow reactions
58	$x_{N,S,p} := (F^{sink}_{N,I} \cdot _x_{I,S}) \star^I S_{I,p}$	interface equation	reactions
59	$_T_I := F^{source}_{N,I} \star^N T_N$	interface equation	macroscopic \rightarrow reactions
60	$T_{N,p} := (F^{sink}_{N,I} \cdot _T_I) \star^I S_{I,p}$	interface equation	reactions
63	$_V_I := F^{source}_{N,I} \star^N V_N$	interface equation	macroscopic \rightarrow reactions
64	$V_{N,p} := (F^{sink}_{N,I} \cdot _V_I) \star^I S_{I,p}$	interface equation	reactions
65	$_nt_I := F^{source}_{N,I} \star^N n^t_N$	interface equation	macroscopic \rightarrow reactions
66	$nt_{N,p} := (F^{sink}_{N,I} \cdot _nt_I) \star^I S_{I,p}$	interface equation	reactions
71	$_pn_{I,S,p} := \mathbf{reduceSum} \left(\left(\left(F^{source}_{N,I} \star^N \tilde{n}_{N,S,p} \right) \cdot S_{I,q} \right), q \right)$	interface equation	reactions \rightarrow macroscopic
72	$pn_{N,S,p} := F^{source}_{N,I} \star^I _pn_{I,S,p}$	interface equation	macroscopic