

# 1 Variables

## 2 root

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

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

### 3 physical

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

## 4 macroscopic

	var	symbol	documentation	type	units	eqs
160	$\hat{n}_{x A, S}^c$	fnc_x	molar convective flow in x-direction	transport	$mol\ s^{-1}$	52
194	$\hat{n}_{N, S}$	anc	accumulation of molar mass due to convection	transport	$mol\ s^{-1}$	87
159	$\hat{V}_A$	fV	volumetric flow in x-direction	transport	$m^3\ s^{-1}$	51
195	$\hat{n}_{N, S}^d$	and_x	accumulation due to diffusion in x-direction	transport	$mol\ s^{-1}$	88
152	$\hat{q}_{y A}$	fq_y	heat flow in y-direction	transport	$kg\ m^2\ s^{-3}$	44
155	$\hat{n}_{y A, S}^d$	fnd_y	diffusion flow in y-direction	transport	$mol\ s^{-1}$	47 90
151	$\hat{q}_{x A}$	fq_x	heat flow in x-direction	transport	$kg\ m^2\ s^{-3}$	43
153	$\hat{q}_{z A}$	fq_z	heat flow in z-direction	transport	$kg\ m^2\ s^{-3}$	45
157	$d_A$	d	flow direction of convective flow	transport		49
158	$c_{A, S}$	c_AS	concentration in convective event-dynamic flow	transport	$m^{-3}\ mol$	50
154	$\hat{n}_{x A, S}^d$	fnd_x	diffusion flow in x-direction	transport	$mol\ s^{-1}$	46 89
156	$\hat{n}_{z A, S}^d$	fnd_z	diffusion flow in z-direction	transport	$mol\ s^{-1}$	48 91
192	$\hat{k}_z^{d, Fick}{}_{A, S}$	kdAFick_z	Fick diffusivity in arc and z-direction	properties	$ms^{-1}$	85
180	$k_{x A, S}^d$	kda_x	diffusivity in arc and x-direction	properties	$kg^{-1}\ m^{-4}\ mol^2\ s$	73
188	$k_{z A}^q$	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
185	$k_{z A}^c$	kca_z	convective mass conductivity in arc and y-direction	properties	$m^{-1}\ s$	78
189	$\rho_A$	rhoA	density in arc	properties	$kg\ m^{-3}$	82
191	$\hat{k}_y^{d, Fick}{}_{A, S}$	kdAFick_y	Fick diffusivity in arc and y-direction	properties	$ms^{-1}$	84
184	$k_{y A}^c$	kca_y	convective mass conductivity in arc and y-direction	properties	$m^{-1}\ s$	77
182	$k_{z A, S}^d$	kda_z	diffusivity in arc and z-direction	properties	$kg^{-1}\ m^{-4}\ mol^2\ s$	75
190	$\hat{k}_x^{d, Fick}{}_{A, S}$	kdAFick_x	Fick's diffusivity in arc and x-direction	properties	$ms^{-1}$	83
186	$k_{x A}^q$	kqa_x	thermal conductivity in arc and x-direction	properties	$kg\ K^{-1}\ s^{-3}$	79

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	var	symbol	documentation	type	units	eqs
187	$k_{yA}^q$	kqA_y	thermal conductivity in arc and y-direction	properties	$kg K^{-1} s^{-3}$	80
181	$k_{yA,S}^d$	kdA_y	diffusivity in arc and y-direction	properties	$kg^{-1} m^{-4} mol^2 s$	74
183	$k_{xA}^c$	kcA_x	convective mass conductivity in arc and x direction	properties	$m^{-1} s$	76
115	$H_N$	H	Enthalpy	state	$kg m^2 s^{-2}$	11
116	$A_N$	A	Helmholtz energy	state	$kg m^2 s^{-2}$	12
117	$G_N$	G	Gibbs free energy	state	$kg m^2 s^{-2}$	13
113	$T_N$	T	temperature	effort	$K$	9
112	$p_N$	p	thermodynamic pressure	effort	$kg m^{-1} s^{-2}$	8
114	$\mu_{N,S}$	chemPot	chemical potential	effort	$kg m^2 mol^{-1} s^{-2}$	10 54
161	$\mu_{N,S}^o$	chemPotStandard	instantiating standard chemical potential	effort	$kg m^2 mol^{-1} s^{-2}$	53
119	$v_{yN}$	v_y	velocity in y-direction	secondaryState	$ms^{-1}$	15
120	$v_{zN}$	v_z	velocity in z-direction	secondaryState	$ms^{-1}$	16
124	$Cp_N$	Cp	total heat capacity at constant pressure	secondaryState	$kg m^2 K^{-1} s^{-2}$	18
142	$c_{VN}$	cV	specific heat capacity at constant volume	secondaryState	$m^2 K^{-1} s^{-2}$	35
138	$c_{N,S}$	c	molar concentration	secondaryState	$m^{-3} mol$	31
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
139	$n_N^t$	nt	total number of moles	secondaryState	$mol$	32
140	$x_{N,S}$	x	mole fraction	secondaryState		33
125	$CV_N$	CV	total heat capacity at constant volume	secondaryState	$kg m^2 K^{-1} s^{-2}$	19
118	$v_{xN}$	v_x	velocity in x-direction	secondaryState	$ms^{-1}$	14
196	$\dot{n}_{N,S}$	an	differential mass balance without reaction	diffState	$mol s^{-1}$	92

## 5 reactions

	var	symbol	documentation	type	units	eqs
197	$E^a_K$	<b>Ea</b>	Arrhenius activation energy	constant	$kg\ m^2\ mol^{-1}\ s^{-2}$	
26	$N_{S,K}$	<b>N</b>	stoichiometric matrix	constant		
198	$K^o_K$	<b>Ko</b>	Arrhenius frequency factor	constant	$m^{-3}\ mol\ s^{-1}$	
167	$T_{N,p}$	<b>T</b>	link variable T to interface reactions	effort	$K$	<b>60</b>
165	$x_{N,S,p}$	<b>x</b>	link variable x to interface reactions	secondaryState		<b>58</b>
171	$V_{N,p}$	<b>V</b>	link variable V to interface reactions	secondaryState	$m^3$	<b>64</b>
163	$c_{N,S,p}$	<b>c</b>	link variable c to interface reactions	secondaryState	$m^{-3}\ mol$	<b>56</b>
168	$f_{N,S,K,p}$	<b>factor</b>	factor for probability computation	conversion		<b>61</b>
199	$K_{N,K,p}$	<b>K</b>	Arrhenius reaction "constant"	conversion	$m^{-3}\ mol\ s^{-1}$	<b>94</b>
169	$\xi_{N,K,p}$	<b>probability</b>	probability of reaction to take place	conversion		<b>62</b>
200	$\tilde{n}_{N,S,q}$	<b>np</b>	production from reaction set	conversion	$m^{-3}\ mol\ s^{-1}$	<b>95</b>

## 6 macroscopic-reactions

	var	symbol	documentation	type	units	eqs
162	$_c$	$_c$	link variable c to interface macroscopic »> reactions with source:node	get	$m^{-3} mol$	55
164	$_x$	$_x$	link variable x to interface macroscopic »> reactions with source:node	get		57
166	$_T$	$_T$	link variable T to interface macroscopic »> reactions with source:node	get	$K$	59
170	$_V$	$_V$	link variable V to interface macroscopic »> reactions with source:node	get	$m^3$	63

## 7 Equations

## 8 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	$\mu_{N,S} := \mu_{N,S}^o + R \cdot T_N \cdot \mathbf{ln}(x_{N,S})$	chemical potential standard model with mole fraction	macroscopic
61	$f_{N,S,K,p} := x_{N,S,p}^{(( N_S, \kappa ))}$	factor for probability computation	reactions
62	$\xi_{N,K,p} := \prod_S f_{N,S,K,p}$	probability of reaction to take place	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
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

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

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no	equation	documentation	layer
93	$n_{N,S} := \int_{t^o}^{t^e} \dot{n}_{N,S} \, dt$	fundamental state – molar mass	macroscopic
94	$K_{N,K,p} := K^o_K \cdot \mathbf{exp} \left( (-E^a_K) \cdot (R \cdot T_{N,p})^{-1} \right)$	Arrhenius reaction "constant"	reactions
95	$\tilde{n}_{N,S,q} := A_{N,p,q} \stackrel{p}{\star} \left( N_{S,K} \stackrel{K}{\star} (K_{N,K,p} \cdot \xi_{N,K,p}) \right)$	production from reaction set	reactions

## 9 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