1 Variables

2 root

	var	symbol	documentation	type	units	eqs
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		
18	cz_I	cz_I	interface variable macro −> control	network		
19	$A_{N,p,q}$	A_Npq	mapping from inputs to outputs	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		
5	${F^{source}}_{A,I}$	F_AI_source	incidence matrix AI source	network		
11	$I_{t,u}$	I_tu	identity mapping from <t> to <u>	network		
2	$F_{N,A}$	F	incidence matrix	network		
13	$S_{I,q}$	S_Aq	selection matrix arcs to outputs	network		
10	$S_{I,q}$	S_Iq	selection matrix interface to control output	network		
9	$S_{I,p}$	S_Ip	selection matrix interface to control input	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		
21	$u_{N,t,u}$	u_Ntu	input signal in control domain	network		
6	${F^{sink}}_{A,I}$	F_AI_sink	incidence matrix AI sink	network		
22	$y_{N,t,u}$	y_Ntu	output signal in control domain	network		
27	$I_{N,A}$	I_NA	identity mapping from <N> to <A>	network		
20	$A_{N,t,u}$	A_Ntu	mapping from input elements to outputs	network		
12	$S_{A,p}$	S_Ap	selection matrix interface species-related measures	network		
17	cz_N	cz_N	output from control	network		

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	var	symbol	documentation	type	units	eqs
16	mv_I	`mv_I`	interface variable macro −> control	network		
105	t^o	`to`	starting time	frame	s	4
106	t^e	`te`	end time	frame	s	5
107	Δt	`t_interval`	time interval	frame	s	6
1	t	`t`	time	frame	s	
104	0.5	`oneHalf`	numerical value one half	constant		3
199	pi	`pi`		constant		94
102	0	`zero`	numerical value zero	constant		1
103	1	`one`	numerical value one	constant		2
101	$\#$	`value`	numerical value	constant		

3 physical

	var	symbol	documentation	type	units	eqs
24	$r_{y\,N}$	r_y	y-coordinate	frame	m	
23	$r_{x\,N}$	r_x	x-coordinate	frame	m	
25	$r_{z\,N}$	r_z	z-coordinate	frame	m	
109	S_N	S	fundamental state – internal entropy	state	$kg\,m^2\,K^{-1}\,s^{-2}$	
111	$n_{N,S}$	n	fundamental state – molar mass	state	mol	93
110	V_N	V	volume	state	m^3	7 97 98
137	m_N	m	mass	state	kg	30
144	C_N	C	fundamental state – charge	state	$A\,s$	
108	U_N	U	fundamental state – internal energy	state	$kg\,m^2\,s^{-2}$	
123	R	R	gas constant	constant	$kg\,m^2\,mol^{-1}\,K^{-1}\,s^{-2}$	17
122	k^B	Boltz	Boltzmann constant	constant	$kg\,m^2\,K^{-1}\,s^{-2}$	
121	N^A	Avo	Avogadro constant	constant	mol^{-1}	
132	λ_S	Mm	molecular masses	constant	$kg\,mol^{-1}$	
150	$A_{yz\,N}$	Ayz	cross sectional area yz	secondaryState	m^2	42
148	$A_{xy\,N}$	Axy	cross sectional area xy	secondaryState	m^2	40 95
149	$A_{xz\,N}$	Axz	cross sectional are xz	secondaryState	m^2	41
143	ρ_N	rho	density	secondaryState	$kg\,m^{-3}$	36

4 macroscopic

	var	symbol	documentation	type	units	eqs
157	d_A	`d`	flow direction of convective flow	transport		49
194	$\dot{n}_{N,S}$	`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
153	$\hat{q}_{z\,A}$	`fq_z`	heat flow in z-direction	transport	$kg\, m^2\, s^{-3}$	45
152	$\hat{q}_{y\,A}$	`fq_y`	heat flow in y-direction	transport	$kg\, m^2\, s^{-3}$	44
160	$\hat{n}^c_{x\,A,S}$	`fnc_x`	molar convective flow in x-direction	transport	$mol\, s^{-1}$	52
154	$\hat{n}^d_{x\,A,S}$	`fnd_x`	diffusion flow in x-direction	transport	$mol\, s^{-1}$	46 89
156	$\hat{n}^d_{z\,A,S}$	`fnd_z`	diffusion flow in z-direction	transport	$mol\, s^{-1}$	48 91
158	$c_{A,S}$	`c_AS`	concentration in convective event-dynamic flow	transport	$m^{-3}\, mol$	50
195	$\dot{n}^d{}_{N,S}$	`and_x`	accumulation due to diffusion in x-direction	transport	$mol\, s^{-1}$	88
155	$\hat{n}^d_{y\,A,S}$	`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
191	$\hat{k}^{d,Fick}_{y}{}_{A,S}$	`kdAFick_y`	Fick diffusivity in arc and y-direction	properties	ms^{-1}	84
186	$k^q_{x\,A}$	`kqA_x`	thermal conductivity in arc and x-direction	properties	$kg\, K^{-1}\, s^{-3}$	79
180	$k^d_{x\,A,S}$	`kdA_x`	diffusivity in arc and x-direction	properties	$kg^{-1}\, m^{-4}\, mol^2\, s$	73
185	$k^c_{z\,A}$	`kcA_z`	convecive mass conductivity in arc and y-direction	properties	$m^{-1}\, s$	78
181	$k^d_{y\,A,S}$	`kdA_y`	diffusivity in arc and y-direction	properties	$kg^{-1}\, m^{-4}\, mol^2\, s$	74
190	$\hat{k}^{d,Fick}_{x}{}_{A,S}$	`kdAFick_x`	Fick's diffusivity in arc and x-direction	properties	ms^{-1}	83
187	$k^q_{y\,A}$	`kqA_y`	thermal conductivity in arc and y-direction	properties	$kg\, K^{-1}\, s^{-3}$	80
183	$k^c_{x\,A}$	`kcA_x`	convective mass conductivity in arc and x diretion	properties	$m^{-1}\, s$	76
189	ρ_A	`rhoA`	density in arc	properties	$kg\, m^{-3}$	82
188	$k^q_{z\,A}$	`kqA_z`	thermal conductivity in arc and z-direction	properties	$kg\, K^{-1}\, s^{-3}$	81
184	$k^c_{y\,A}$	`kcA_y`	convective mass conductivity in arc and y-direction	properties	$m^{-1}\, s$	77

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	var	symbol	documentation	type	units	eqs
182	${k^d_z}_{A,S}$	kdA_z	diffusivity in arc and z-direction	properties	$kg^{-1}\,m^{-4}\,mol^2\,s$	75
192	${\hat{k}^{d,Fick}_z}_{A,S}$	kdAFick_z	Fick diffusivity in arc and z-direction	properties	ms^{-1}	85
193	$h_{A,S}$	hA	partial molar enthalpiies in arc	properties	$kg\,m^2\,mol^{-1}\,s^{-2}$	86
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
197	${d_x}_N$	d_x	diameter x	constant	m	
161	${\mu^o}_{N,S}$	chemPotStandard	instantiating standard chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	53
113	T_N	T	temperature	effort	K	9
114	$\mu_{N,S}$	chemPot	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	10 54
112	p_N	p	thermodynamic pressure	effort	$kg\,m^{-1}\,s^{-2}$	8
138	$c_{N,S}$	c	molar concentration	secondaryState	$m^{-3}\,mol$	31
141	${c_p}_N$	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
120	${v_z}_N$	v_z	velocity in z-direction	secondaryState	ms^{-1}	16
118	${v_x}_N$	v_x	velocity in x-direction	secondaryState	ms^{-1}	14
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
136	$h_{N,S}$	h	partial molar enthalpies	secondaryState	$kg\,m^2\,mol^{-1}\,s^{-2}$	29
140	$x_{N,S}$	x	mole fraction	secondaryState		33
200	${h_L}_N$	h_L	liquid level cylinder	secondaryState	m	96
119	${v_y}_N$	v_y	velocity in y-direction	secondaryState	ms^{-1}	15
142	${c_V}_N$	cV	specific heat capacity at constant volume	secondaryState	$m^2\,K^{-1}\,s^{-2}$	35
196	$\dot{n}_{N,S}$	an	differential mass balance without reaction	diffState	$mol\,s^{-1}$	92

5 reactions

	var	symbol	documentation	type	units	eqs
26	$N_{S,K}$	`N`	stoichiometric matrix	constant		
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
163	$c_{N,S,p}$	`c`	link variable c to interface reactions	secondaryState	$m^{-3}\,mol$	56
165	$x_{N,S,p}$	`x`	link variable x to interface reactions	secondaryState		58
169	$\xi_{N,K,p}$	`probability`	probability of reaction to take place	conversion		62
168	$f_{N,S,K,p}$	`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
164	$\_x_{I,S}$	`_x`	link variable x to interface macroscopic »> reactions with source:node	get		57
162	$\_c_{I,S}$	`_c`	link variable c to interface macroscopic »> reactions with source:node	get	$m^{-3}\,mol$	55
170	$\_V_I$	`_V`	link variable V to interface macroscopic »> reactions with source:node	get	m^3	63

7 Equations

8 Generic

no	equation	documentation	layer
1	$0 := \textbf{Instantiate}(\#, \#)$	numerical value zero	root
2	$1 := \textbf{Instantiate}(\#, \#)$	numerical value one	root
3	$0.5 := \textbf{Instantiate}(\#, \#)$	numerical value one half	root
4	$t^o := \textbf{Instantiate}(t, \#)$	starting time	root
5	$t^e := \textbf{Instantiate}(t, \#)$	end time	root
6	$\Delta t := \textbf{Instantiate}(t, \#)$	time interval	root
7	$V_N := r_{x\,N} \,.\, r_{y\,N} \,.\, r_{z\,N}$	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	$H_N := U_N - p_N \,.\, V_N$	Enthalpy	macroscopic
12	$A_N := U_N - T_N \,.\, S_N$	Helmholtz energy	macroscopic
13	$G_N := U_N + p_N \,.\, V_N - T_N \,.\, S_N$	Gibbs free energy	macroscopic
14	$v_{x\,N} := \frac{\partial r_{x\,N}}{\partial t}$	velocity in x-direction	macroscopic
15	$v_{y\,N} := \frac{\partial r_{y\,N}}{\partial t}$	velocity in y-direction	macroscopic
16	$v_{z\,N} := \frac{\partial r_{z\,N}}{\partial t}$	velocity in z-direction	macroscopic

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no	equation	documentation	layer
17	$R := N^A \,.\, k^B$	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	$h_{N,S} := H_N \,.\, (n_{N,S})^{-1}$	partial molar enthalpies	macroscopic
30	$m_N := \lambda_S \overset{S}{\star} n_{N,S}$	mass	macroscopic
31	$c_{N,S} := (V_N)^{-1} \,.\, n_{N,S}$	molar concentration	macroscopic
32	$n^t{}_N := \mathbf{reduceSum}\,(n_{N,S}, S)$	total number of moles	macroscopic
33	$x_{N,S} := (n^t{}_N)^{-1} \,.\, n_{N,S}$	mole fraction	macroscopic
34	$c_{p\,N} := Cp_N \,.\, (m_N)^{-1}$	specific heat capacity at constant pressure	physical
35	$c_{V\,N} := CV_N \,.\, (m_N)^{-1}$	specific heat capacity at constant volume	macroscopic
36	$\rho_N := (V_N)^{-1} \,.\, m_N$	density	physical
40	$A_{xy\,N} := r_{x\,N} \,.\, r_{y\,N}$	cross sectional area xy	physical
41	$A_{xz\,N} := r_{x\,N} \,.\, r_{z\,N}$	cross sectional are xz	physical
42	$A_{yz\,N} := r_{y\,N} \,.\, r_{z\,N}$	cross sectional area yz	physical
43	$\hat{q}_{x\,A} := k^q_{x\,A} \,.\, A_{yz\,N} \,.\, F_{N,A} \overset{N}{\star} T_N$	heat flow in x-direction	macroscopic
44	$\hat{q}_{y\,A} := k^q_{y\,A} \,.\, A_{xz\,N} \,.\, F_{N,A} \overset{N}{\star} T_N$	heat flow in y-direction	macroscopic
45	$\hat{q}_{z\,A} := k^q_{z\,A} \,.\, A_{xy\,N} \,.\, F_{N,A} \overset{N}{\star} T_N$	heat flow in z-direction	macroscopic

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no	equation	documentation	layer
46	$\hat{n}^d_{x}{}_{A,S} := \hat{k}^{d,Fick}_{x}{}_{A,S} \,.\, A_{yz}{}_N \,.\, F_{N,A} \overset{N}{\star} c_{N,S}$	Fick diffusion flow in x-direction	macroscopic
47	$\hat{n}^d_{y}{}_{A,S} := \hat{k}^{d,Fick}_{y}{}_{A,S} \,.\, A_{xz}{}_N \,.\, F_{N,A} \overset{N}{\star} c_{N,S}$	Fick diffusion flow in y-direction	macroscopic
48	$\hat{n}^d_{z}{}_{A,S} := \hat{k}^{d,Fick}_{z}{}_{A,S} \,.\, (A_{xy}{}_N \,.\, F_{N,A}) \overset{N}{\star} c_{N,S}$	Fick diffusion flow in z-direction	macroscopic
49	$d_A := \mathbf{sign}\left(F_{N,A} \overset{N}{\star} p_N\right)$	flow direction of convective flow	macroscopic
50	$c_{A,S} := (0.5 \,.\, (F_{N,A} - d_A \,.\, \lvert F_{N,A}\rvert)) \overset{N}{\star} c_{N,S}$	concentration in convective event-dynamic flow	macroscopic
51	$\hat{V}_A := (\rho_A)^{-1} \,.\, k^c_{x}{}_A \,.\, A_{yz}{}_N \,.\, F_{N,A} \overset{N}{\star} p_N$	volumetric flow in x-direction	macroscopic
52	$\hat{n}^c_{x}{}_{A,S} := \hat{V}_A \,.\, c_{A,S}$	molar convective flow in x-direction	macroscopic
53	$\mu^o{}_{N,S} := \mathbf{Instantiate}(\mu_{N,S}, \#)$	instantiating standard chemical potential	macroscopic
54	$\mu_{N,S} := \mu^o{}_{N,S} + R \,.\, T_N \,.\, \mathbf{ln}\,(x_{N,S})$	chemical potential standard model with mole fraction	macroscopic
61	$f_{N,S,K,p} := x_{N,S,p}{}^{((\lvert N_{S,K}\rvert))}$	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	$k^d_{x}{}_{A,S} := I_{N,A} \overset{N}{\star} \left((\mu_{N,S})^{-1} \,.\, \left(v_{x}{}_N \,.\, \left((V_N)^{-1} \,.\, \frac{\partial U_N}{\partial \mu_{N,S}}\right)\right)\right)$	diffusivity in arc and x-direction	macroscopic
74	$k^d_{y}{}_{A,S} := I_{N,A} \overset{N}{\star} \left((\mu_{N,S})^{-1} \,.\, \left(v_{y}{}_N \,.\, \left((V_N)^{-1} \,.\, \frac{\partial U_N}{\partial \mu_{N,S}}\right)\right)\right)$	diffusivity in arc and y-direction	macroscopic
75	$k^d_{z}{}_{A,S} := I_{N,A} \overset{N}{\star} \left((\mu_{N,S})^{-1} \,.\, \left(v_{z}{}_N \,.\, \left((V_N)^{-1} \,.\, \frac{\partial U_N}{\partial \mu_{N,S}}\right)\right)\right)$	diffusivity in arc and z-direction	macroscopic
76	$k^c_{x}{}_A := I_{N,A} \overset{N}{\star} \left(\left(\lambda_S \overset{S}{\star} (\mu_{N,S})^{-1}\right) \,.\, (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial p_N} \,.\, v_{x}{}_N\right)$	convective mass conductivity in arc and x diretion	macroscopic
77	$k^c_{y}{}_A := I_{N,A} \overset{N}{\star} \left(\left(\lambda_S \overset{S}{\star} (\mu_{N,S})^{-1}\right) \,.\, (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial p_N} \,.\, v_{y}{}_N\right)$	convective mass conductivity in arc and y-direction	macroscopic

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no	equation	documentation	layer
78	$k^c_{zA} := I_{N,A} \overset{N}{\star} \left(\left(\lambda_S \overset{S}{\star} (\mu_{N,S})^{-1} \right) . (V_N)^{-1} . \frac{\partial U_N}{\partial p_N} . v_{zN} \right)$	convecive mass conductivity in arc and y-direction	macroscopic
79	$k^q_{xA} := I_{N,A} \overset{N}{\star} \left((V_N)^{-1} . Cp_N . v_{xN} \right)$	thermal conductivity in arc and x-direction	macroscopic
80	$k^q_{yA} := I_{N,A} \overset{N}{\star} \left((V_N)^{-1} . Cp_N . v_{yN} \right)$	thermal conductivity in arc and y-direction	macroscopic
81	$k^q_{zA} := I_{N,A} \overset{N}{\star} \left((V_N)^{-1} . Cp_N . v_{zN} \right)$	thermal conductivity in arc and z-direction	macroscopic
82	$\rho_A := I_{N,A} \overset{N}{\star} \rho_N$	density in arc	macroscopic
83	$\hat{k}^{d,Fick}_x{}_{A,S} := I_{N,A} \overset{N}{\star} \left(v_{xN} . \frac{\partial U_N}{\partial \mu_{N,S}} . (n_{N,S})^{-1} \right)$	Fick's diffusivity in arc and x-direction	macroscopic
84	$\hat{k}^{d,Fick}_y{}_{A,S} := I_{N,A} \overset{N}{\star} \left(v_{yN} . \frac{\partial U_N}{\partial \mu_{N,S}} . (n_{N,S})^{-1} \right)$	Fick diffusivity in arc and y-direction	macroscopic
85	$\hat{k}^{d,Fick}_z{}_{A,S} := I_{N,A} \overset{N}{\star} \left(v_{zN} . \frac{\partial U_N}{\partial \mu_{N,S}} . (n_{N,S})^{-1} \right)$	Fick diffusivity in arc and z-direction	macroscopic
86	$h_{A,S} := I_{N,A} \overset{N}{\star} h_{N,S}$	partial molar enthalpiies in arc	macroscopic
87	$\dot{n}_{N,S} := F_{N,A} \overset{A}{\star} \hat{n}^c_{xA,S}$	accumulation of molar mass due to convection	macroscopic
88	$\dot{n}^d{}_{N,S} := F_{N,A} \overset{A}{\star} \hat{n}^d_{xA,S}$	accumulation due to diffusion in x-direction	macroscopic
89	$\hat{n}^d_{xA,S} := k^d_{xA,S} . (A_{yzN} . F_{N,A}) \overset{N}{\star} \mu_{N,S}$	Fick diffusion flow in x-direction	macroscopic
90	$\hat{n}^d_{yA,S} := k^d_{yA,S} . (A_{yzN} . F_{N,A}) \overset{N}{\star} \mu_{N,S}$	Fick diffusion flow in y-direction	macroscopic
91	$\hat{n}^d_{zA,S} := k^d_{zA,S} . (A_{xyN} . F_{N,A}) \overset{N}{\star} \mu_{N,S}$	mass diffusion flow in z-direction	macroscopic
92	$\dot{n}_{N,S} := \dot{n}_{N,S} + \dot{n}^d{}_{N,S}$	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	$pi := \mathbf{Instantiate}(\#, \#)$		root
95	$A_{xy\,N} := pi \,.\, (0.5 \,.\, d_{x\,N}) \,.\, (0.5 \,.\, d_{x\,N})$	cross sectional area xy	macroscopic
96	$h_{L\,N} := V_N \,.\, (A_{xy\,N})^{-1}$	liquid level cylinder	macroscopic
97	$V_N := \mathbf{Root}\,(\rho_N)$	volume	macroscopic
98	$V_N := m_N \,.\, (\rho_N)^{-1}$	volume	macroscopic

9 Interface Link Equation

no	equation	documentation	layer
55	$\_c_{I,S} := {F^{source}}_{N,I} \overset{N}{\star} c_{N,S}$	interface equation	macroscopic –> reactions
56	$c_{N,S,p} := \left({F^{sink}}_{N,I} \cdot \_c_{I,S}\right) \overset{I}{\star} S_{I,p}$	interface equation	reactions
57	$\_x_{I,S} := {F^{source}}_{N,I} \overset{N}{\star} x_{N,S}$	interface equation	macroscopic –> reactions
58	$x_{N,S,p} := \left({F^{sink}}_{N,I} \cdot \_x_{I,S}\right) \overset{I}{\star} S_{I,p}$	interface equation	reactions
59	$\_T_{I} := {F^{source}}_{N,I} \overset{N}{\star} T_{N}$	interface equation	macroscopic –> reactions
60	$T_{N,p} := \left({F^{sink}}_{N,I} \cdot \_T_{I}\right) \overset{I}{\star} S_{I,p}$	interface equation	reactions
63	$\_V_{I} := {F^{source}}_{N,I} \overset{N}{\star} V_{N}$	interface equation	macroscopic –> reactions
64	$V_{N,p} := \left({F^{sink}}_{N,I} \cdot \_V_{I}\right) \overset{I}{\star} S_{I,p}$	interface equation	reactions