1 Variables

2 root

	var	symbol	documentation	type	units	eqs
V_8	$F_{N,A}$	`F_N_A`	fundamental incidence matrix	network		
V_5	t	`t`	time	frame	s	
V_6	t^o	`to`	starting time	frame	s	4
V_7	t^e	`te`	end time	frame	s	5
V_1	$\#$	`value`	numerical value	constant		
V_2	1	`one`	numerical value one	constant		1
V_3	0	`zero`	numerical value zero	constant		2
V_4	0.5	`onehalf`	numerical value one half	constant		3

3 physical

	var	symbol	documentation	type	units	eqs
V_9	$P_{N,A}$	P_N_A	projection from node to arc for arc properties	projection		
$V_3 2$	$P_{NS,AS}$	P_NS_AS	projection node species to arc species	projection		
$V_3 3$	$P_{K,NK}$	P_K_NK	projection of conversion to node conversion	projection		
$V_3 4$	$P_{S,NS}$	P_S_NS	projection species to node species	projection		
$V_3 5$	$P_{N,NK}$	P_N_NK	projection node to node conversion	projection		
$V_3 6$	$P_{NS,KS}$	P_NS_KS	projection node species to conversion species	projection		
$V_3 7$	$P_{A,NS}$	P_A_NS	projection arc to node species for conductivity	projection		
$V_6 5$	$P_{NK,KS}$	P_NK_KS	projection node conversion to conversion species	projection		
$V_1 62$	$P_{N,NS}$	P_N_NS	projection of nodes onto the node species	projection		
$V_1 0$	r_{xN}	r_x	x-coordinate	frame	m	
$V_1 1$	r_{yN}	r_y	y-coordinate	frame	m	
$V_1 2$	r_{zN}	r_z	z coordinate	frame	m	
$V_1 3$	U_N	U	fundamental state – internal energy	state	$kg\, m^2\, s^{-2}$	
$V_1 4$	S_N	S	fundamental state – entropy	state	$kg\, m^2\, K^{-1}\, s^{-2}$	
$V_1 5$	V_N	V	fundamental state – volume	state	m^3	
$V_1 6$	n_{NS}	n	fundamental state – molar mass	state	mol	86
$V_2 0$	H_N	H	enthalpy	state	$kg\, m^2\, s^{-2}$	9 87
$V_2 1$	A_N	A	Helmholtz energy	state	$kg\, m^2\, s^{-2}$	10
$V_2 2$	G_N	G	Gibbs free energy	state	$kg\, m^2\, s^{-2}$	11
$V_2 3$	C_N	charge	fundamental state – charge	state	$A\, s$	
$V_2 4$	A^v	Avogadro	Avogadro number	constant	mol^{-1}	
$V_1 65$	boz_N	boz	Boltzmann constant	constant	$kg\, m^2\, K^{-1}\, s^{-2}$	132
$V_1 66$	R_N	R	gas constant	constant	$kg\, m^2\, mol^{-1}\, K^{-1}\, s^{-2}$	133

Continued on next page

	var	symbol	documentation	type	units	eqs
V_17	p_N	`p`	thermodynamic pressure	effort	$kg\,m^{-1}\,s^{-2}$	6
V_18	T_N	`T`	temperature	effort	K	7
V_19	μ_{NS}	`chemPot`	chemical potential	effort	$kg\,m^2\,mol^{-1}\,s^{-2}$	8 136
V_27	Ue_N	`Ue`	electrical potential – voltage	effort	$kg\,m^2\,A^{-1}s^{-3}$	14 95
V_28	$v_{x\,N}$	`v_x`	velocity in x-direction	secondaryState	ms^{-1}	15
V_29	$v_{y\,N}$	`v_y`	velocity in y-direction	secondaryState	ms^{-1}	16
V_30	$v_{z\,N}$	`v_z`	velocity in z-direction	secondaryState	ms^{-1}	17

4 control

	var	symbol	documentation	type	units	eqs
V_136	x_N	`x`	state	state		111
V_137	x_{oN}	`xo`	initial state	state		109
V_129	$A_{N,D}$	`A`	dynamic matrix	constant	s^{-1}	
V_130	$B_{A,D}$	`B`	input matrix	constant	s^{-1}	
V_131	$C_{N,A}$	`C`	measurement matrix	constant		
V_132	D_A	`D`	diagonal event matrix (no dimensional problems)	constant		
V_133	$y^o{}_A$	`setPoint`	set point	constant		119
V_134	m_A	`meas`	measurements	constant		
V_135	e_A	`e`	control error	constant		108
V_139	$1_{N,D}$	`I_N_D`	space transformation D to N	constant		
V_138	$\dot{x}_D$	`dxdt`	differential state (ABCD) model	diffState	s^{-1}	110
V_141	$\check{I}_N$	`Imeasured`	measured current	algebraic	A	113
V_143	$\check{U}^e{}_N$	`UeMeasured`	measured electrical potential	algebraic	$kg\,m^2\,A^{-1}s^{-3}$	115
V_144	$\check{\xi}$	`addMeasured`	measured additive fraction	algebraic		116
V_145	R_N	`RComputed`	measured resistance	algebraic	$kg\,m^2\,A^{-2}s^{-3}$	117
V_146	S	`store`	quantities to be stored	algebraic		118
V_154	y_A	`y`	output equation	algebraic		126
V_171	s	`switch`	switches at to	algebraic		138

5 reactions

	var	symbol	documentation	type	units	eqs
$V_1 47$	P_{NK}	P_NK	reactions per node	projection		
$V_3 8$	${K^o}_K$	Ko	Arrhenius frequency factor	constant	$m^{-3}\, mol\, s^{-1}$	
$V_6 2$	${E^a}_{NK}$	Ea	Arrhenius activation energy	constant	$kg\, m^2\, mol^{-1}\, s^{-2}$	41
$V_6 3$	K_{NK}	K_NK	Arrhenius reaction 'constant'	constant	$m^{-3}\, mol\, s^{-1}$	42
$V_1 55$	B	Boltzmann	Boltzmann constant	constant	$kg\, m^2\, K^{-1}\, s^{-2}$	
$V_1 57$	R	GasConstant	gas constant	constant	$kg\, m^2\, mol^{-1}\, K^{-1}\, s^{-2}$	127
$V_1 58$	$N_{K,KS}$	N_K_KS	stoichiometry	constant		
$V_1 59$	$N_{NK,KS}$	N_NK_KS	extended stoichiometric matrix	constant		128
$V_6 0$	T_{NK}	T_NK	temperature of the reactive system	effort	K	39
$V_1 51$	$c_{NK,KS}$	c	concentration matrix reaction per node and species per reaction	secondaryState	$m^{-3}\, mol$	123
$V_1 52$	${c^o}_{NK,KS}$	co	norming concentration	secondaryState	$m^{-3}\, mol$	124
$V_1 53$	$x_{NK,KS}$	x	matrix of normed, dimensionless mole fractions	secondaryState		125
$V_1 60$	ϕ_{NK}	phi	probability function for reactions	secondaryState		129
$V_1 63$	$\tilde{n}_{NS}$	nProd	the species production term	secondaryState	$mol\, s^{-1}$	130

6 material

	var	symbol	documentation	type	units	eqs
V_40	λ_S	`Mm`	species molecular mass	constant	$kg\, mol^{-1}$	
V_112	ξ	`additive`	fraction of additives	constant		88
V_42	$C_{p\,N}$	`Cp`	total heat capacity at constant pressure	property	$kg\, m^2\, K^{-1}\, s^{-2}$	21
V_43	$C_{V\,N}$	`Cv`	total heat capacity at constant volume	property	$kg\, m^2\, K^{-1}\, s^{-2}$	22
V_44	$k^q_{x\,N}$	`kq_x`	thermal conductivity in x-direction	property	$kg\, K^{-1}\, s^{-3}$	23
V_45	$k^q_{y\,N}$	`kq_y`	thermal conductivity in y-direction	property	$kg\, K^{-1}\, s^{-3}$	24
V_46	$k^q_{z\,N}$	`kq_z`	thermal conductivity in z-direction'	property	$kg\, K^{-1}\, s^{-3}$	25
V_47	${k^q}_N$	`kq`	thermal conductivity	property	$kg\, K^{-1}\, s^{-3}$	26
V_48	$k^c_{x\,N}$	`kc_x`	convective mass conductivity in x-direction	property	$m^{-1}\, s$	27
V_49	$k^c_{y\,N}$	`kc_y`	convective mass conductivity in y-direction	property	$m^{-1}\, s$	28
V_50	$k^c_{z\,N}$	`kc_z`	convective mass conductivity in z-direction	property	$m^{-1}\, s$	29
V_51	${k^c}_N$	`kc`	convective mass conductivity	property	$m^{-1}\, s$	30
V_52	$k^d_{x\,N\,S}$	`kd_x`	diffusional mass conductivity in x-direction	property	$kg^{-1}\, m^{-4}\, mol^2\, s$	31
V_53	$k^d_{y\,N\,S}$	`kd_y`	diffusional mass conductivity in y-direction	property	$kg^{-1}\, m^{-4}\, mol^2\, s$	32
V_54	$k^d_{z\,N\,S}$	`kd_z`	diffusional mass conductivity in z-direction	property	$kg^{-1}\, m^{-4}\, mol^2\, s$	33
V_55	${k^d}_{N\,S}$	`kd`	diffusional mass conductivity	property	$kg^{-1}\, m^{-4}\, mol^2\, s$	34
V_56	$h_{N\,S}$	`h`	partial molar enthalpies	property	$kg\, m^2\, mol^{-1}\, s^{-2}$	35
V_59	ρ_N	`density`	density	property	$kg\, m^{-3}$	38
V_115	${R^e}_N$	`elResist`	electrical resistant	property	$kg\, m^2\, A^{-2} s^{-3}$	91 92
V_116	${k^{e,\xi}}_N$	`elConductC`	simple model for the electrical conductivity as a function of the additive	property	$kg^{-1}\, m^{-2}\, A^2 s^3$	93

7 macroscopic

	var	symbol	documentation	type	units	eqs
V_92	$\hat{V}_A$	fV	volumetric flow	transport	$m^3\, s^{-1}$	67 140
V_93	$\hat{n}^d{}_{AS}$	fnd_AS	diffusional mass flow in a given stream	transport	$mol\, s^{-1}$	68
V_94	$\hat{n}^d{}_{NS}$	fnd	net diffusional mass flow	transport	$mol\, s^{-1}$	69
V_95	$\hat{H}^d{}_A$	fHd_A	enthalpy flow per diffusional mass stream	transport	$kg\, m^2\, s^{-3}$	70
V_96	$\hat{H}^d{}_N$	fHd	net enthalpy stream due to diffusion	transport	$kg\, m^2\, s^{-3}$	71
V_97	d_A	d	flow direction of convectional flow	transport		72
V_99	$\hat{n}^c{}_{AS}$	fnc_AS	molar convectional mass flow in the given stream	transport	$mol\, s^{-1}$	74
V_100	$\hat{n}^c{}_{NS}$	fnc	net molar convectional mass flow	transport	$mol\, s^{-1}$	75
V_102	$\hat{H}^c{}_A$	fHc_A	convective enthalpy flow for given stream	transport	$kg\, m^2\, s^{-3}$	77
V_103	$\hat{H}^c{}_N$	fHc	net convectional enthalpy stream	transport	$kg\, m^2\, s^{-3}$	78
V_104	$\hat{w}_A$	fw_A	sample work stream	transport	$kg\, m^2\, s^{-3}$	79
V_105	$\hat{w}_N$	fw	net work stream	transport	$kg\, m^2\, s^{-3}$	80
V_106	$\hat{q}_{x\,A}$	fq_A_x	heat flow in x-direction for given stream	transport	$kg\, m^2\, s^{-3}$	81
V_107	$\hat{q}_N$	fq	net heat flow	transport	$kg\, m^2\, s^{-3}$	82
V_173	$\hat{n}^{c,controlled}{}_{AS}$	fnc_AS_controlled	switched flow	transport	$mol\, s^{-1}$	141
V_71	$A_{yz\,N}$	Ayz	cross sectional area yz	geometry	m^2	48
V_72	$A_{xz\,N}$	Axz	cross sectional area xz	geometry	m^2	49
V_73	$A_{xy\,N}$	Axy	cross sectional area xy	geometry	m^2	50
V_70	$F_{NS,AS}$	F_NS_AS	species related incidence matrix	network		
V_90	$D_{N,A}$	D	difference operator	differenceOperator		
V_91	$D_{NS,AS}$	D_NS_AS	difference operator for species topology	differenceOperator		
V_109	$H^o{}_N$	Ho	initial enthalpy	state	$kg\, m^2\, s^{-2}$	84

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	var	symbol	documentation	type	units	eqs
V_110	${n^o}_{NS}$	`no`	initial species	state	mol	85
V_127	1_S	`one_S`	a vector of ones with the length of the ordinal number of S	constant		
V_57	m_N	`m`	total mass	secondaryState	kg	36
V_66	c_{NS}	`c`	molar composition	secondaryState	$m^{-3}\, mol$	44
V_98	c_{AS}	`c_AS`	concentration in convectional flow	secondaryState	$m^{-3}\, mol$	73
V_126	ϕ	`intensities`	collected intensities	secondaryState		106
V_128	${n^t}_N$	`nTotal`	total number of moles	secondaryState	mol	107
V_168	n_{tN}	`nt`	total number of species in a node	secondaryState	mol	134
V_169	ξ_{NS}	`xi`	mole fraction	secondaryState		135
V_170	$\tilde{n}_{NS}$	`nProd`	production term	conversion	$mol\, s^{-1}$	137
V_101	$\dot{n}_{NS}$	`dndt`	differential species balance	diffState	$mol\, s^{-1}$	76 142
V_108	$\dot{H}_N$	`dHdt`	differential enthalpy balance	diffState	$kg\, m^2\, s^{-3}$	83
V_118	${\dot{U}^e}_N$	`dUedt`	Kirkhoffs first law	diffState	$kg\, m^2\, A^{-1} s^{-3}$	96 97 98
V_113	I_N	`i`	electrical current definition	internalTransport	A	89

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
$V_1 24$	$\mapsto \xi$	`_additive`	link variable additive to interface material »> control	get		104

25 control–macroscopic

	var	symbol	documentation	type	units	eqs
$V_1 72$	s	`_switch`	switches at to	get		139

26 macroscopic–control

	var	symbol	documentation	type	units	eqs
$V_1 19$	I_N	`_i`	link variable i to interface macroscopic »> control	get	A	99
$V_1 25$	T_N	`_T`	link variable T to interface macroscopic »> control	get	K	105
$V_1 42$	Ue_N	`_Ue`	link variable Ue to interface macroscopic »> control	get	$kg\, m^2\, A^{-1} s^{-3}$	114

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
$V_1 64$	$\tilde{n}_{NS}$	`_nProd`	link variable nProd to interface reactions »> macroscopic	get	$mol\, s^{-1}$	131

30 macroscopic–reactions

	var	symbol	documentation	type	units	eqs
V_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
$V_{4}1$	λ_S	`_Mm`	link variable Mm to interface material »> macroscopic	get	$kg\,mol^{-1}$	20
$V_{7}4$	ρ_N	`_density`	link variable density to interface material »> macroscopic	get	$kg\,m^{-3}$	51
$V_{7}5$	h_{NS}	`_h`	link variable h to interface material »> macroscopic	get	$kg\,m^{2}\,mol^{-1}\,s^{-2}$	52
$V_{7}6$	$k^q_{x\,N}$	`_kq_x`	link variable kq x to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	53
$V_{7}7$	cv_N	`_Cv`	link variable Cv to interface material »> macroscopic	get	$kg\,m^{2}\,K^{-1}\,s^{-2}$	54
$V_{7}8$	$k^q_{y\,N}$	`_kq_y`	link variable kq y to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	55
$V_{7}9$	$k^q_{z\,N}$	`_kq_z`	link variable kq z to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	56
$V_{8}0$	$k^q{}_N$	`_kq`	link variable kq to interface material »> macroscopic	get	$kg\,K^{-1}\,s^{-3}$	57
$V_{8}1$	$k^c_{x\,N}$	`_kc_x`	link variable kc x to interface material »> macroscopic	get	$m^{-1}\,s$	58
$V_{8}2$	cp_N	`_Cp`	link variable Cp to interface material »> macroscopic	get	$kg\,m^{2}\,K^{-1}\,s^{-2}$	59
$V_{8}3$	$k^c_{y\,N}$	`_kc_y`	link variable kc y to interface material »> macroscopic	get	$m^{-1}\,s$	60
$V_{8}4$	$k^c_{z\,N}$	`_kc_z`	link variable kc z to interface material »> macroscopic	get	$m^{-1}\,s$	61
$V_{8}5$	$k^c{}_N$	`_kc`	link variable kc to interface material »> macroscopic	get	$m^{-1}\,s$	62
$V_{8}6$	$k^d_{x\,NS}$	`_kd_x`	link variable kd x to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^{2}\,s$	63
$V_{8}7$	$k^d_{y\,NS}$	`_kd_y`	link variable kd y to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^{2}\,s$	64
$V_{8}8$	$k^d_{z\,NS}$	`_kd_z`	link variable kd z to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^{2}\,s$	65

Continued on next page

	var	symbol	documentation	type	units	eqs
V_89	${k^d}_{NS}$	`_kd`	link variable kd to interface material »> macroscopic	get	$kg^{-1}\,m^{-4}\,mol^2\,s$	66
V_117	${R^e}_N$	`_elConductC`	link variable elConductC to interface material »> macroscopic	get	$kg^{-1}\,m^{-2}\,A^2 s^3$	94
V_140	ξ	`_additive`	link variable additive to interface material »> macroscopic	get		112

32 macroscopic–material

	var	symbol	documentation	type	units	eqs
$V_5 8$	m_N	`_m`	link variable m to interface macroscopic »> material	get	kg	37
$V_1 14$	I_N	`_i`	link variable i to interface macroscopic »> material	get	A	90

33 Equations

34 Generic

no	equation	documentation	layer
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
14	$Ue_N := (C_N)^{-1} \,.\, U_N$	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
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	$k^q_{xN} := (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial T_N} \,.\, v_{xN}$	thermal conductivity in x-direction	material
24	$k^q_{yN} := (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial T_N} \,.\, v_{yN}$	thermal conductivity in y-direction	material
25	$k^q_{zN} := (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial T_N} \,.\, v_{zN}$	thermal conductivity in z-direction’	material
26	$k^q{}_N := \text{Stack}\left(k^q_{xN}, k^q_{yN}, k^q_{zN}\right)$	thermal conductivity	material

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no	equation	documentation	layer
27	$k^c_{x\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) . (V_N)^{-1} . \frac{\partial U_N}{\partial p_N} . v_{x\,N}$	convecitve mass conductivity in x-direction	material
28	$k^c_{y\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) . (V_N)^{-1} . \frac{\partial U_N}{\partial p_N} . v_{y\,N}$	convecitve mass conductivity in y-direction	material
29	$k^c_{z\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) . (V_N)^{-1} . \frac{\partial U_N}{\partial p_N} . v_{z\,N}$	convecitve mass conductivity in z-direction	material
30	$k^c{}_N := \mathrm{Stack}\left(k^c_{x\,N}, k^c_{y\,N}, k^c_{z\,N}\right)$	convective mass conductivity	material
31	$k^d_{x\,NS} := (\mu_{NS})^{-1} . \left(v_{x\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in x-direction	material
32	$k^d_{y\,NS} := (\mu_{NS})^{-1} . \left(v_{y\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in y-direction	material
33	$k^d_{z\,NS} := (\mu_{NS})^{-1} . \left(v_{z\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$	diffusional mass conductivity in z-direction	material
34	$k^d{}_{NS} := \mathrm{Stack}\left(k^d_{x\,NS}, k^d_{y\,NS}, k^d_{z\,NS}\right)$	diffusional mass condctivity	material
35	$h_{NS} := H_N \odot (n_{NS})^{-1}$	partial molar enthalpies	material
36	$m_N := \lambda_S \overset{S \in NS}{\star} n_{NS}$	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
42	$K_{NK} := K^o{}_K \odot exp((-E^a{}_{NK}) . (R . T_{NK})^{-1})$	Arrhenius reaction 'constant'	reactions
44	$c_{NS} := (V_N)^{-1} \odot n_{NS}$	molar composition	macroscopic
48	$A_{yz\,N} := r_{y\,N} . r_{z\,N}$	cross sectional area yz	macroscopic

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no	equation	documentation	layer
49	$A_{xz\,N} := r_{x\,N} \,.\, r_{z\,N}$	cross sectional area xz	macroscopic
50	$A_{xy\,N} := r_{x\,N} \,.\, r_{y\,N}$	cross sectional area xy	macroscopic
67	$\hat{V}_A := (\rho_N)^{-1} \,.\, k^c_{x\,N} \,.\, A_{yz\,N} \,.\, D_{N,A} \overset{N}{\star} p_N$	volumetric flow	macroscopic
68	$\hat{n}^d{}_{AS} := A_{yz\,N} \odot \left(-k^d_{x\,NS}\right) \,.\, D_{NS,AS} \overset{NS}{\star} \mu_{NS}$	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
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	$d_A := \mathrm{sign}\left(F_{N,A} \overset{N}{\star} p_N\right)$	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	$\dot{n}_{NS} := \hat{n}^c{}_{NS} + \hat{n}^d{}_{NS} + \tilde{n}_{NS}$	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
80	$\hat{w}_N := F_{N,A} \overset{A}{\star} \hat{w}_A$	net work stream	macroscopic
81	$\hat{q}_{x\,A} := A_{yz\,N} \,.\, k^q_{x\,N} \,.\, D_{N,A} \overset{N}{\star} T_N$	heat flow in x-direction for given stream	macroscopic
82	$\hat{q}_N := F_{N,A} \overset{A}{\star} \hat{q}_{x\,A}$	net heat flow	macroscopic

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no	equation	documentation	layer
83	$\dot{H}_N := \hat{H}^c{}_N + \hat{H}^d{}_N + \hat{q}_N + \hat{w}_N$	differential enthalpy balance	macroscopic
86	$n_{NS} := \int_{t^o}^{t^e} \dot{n}_{NS} \; dt + n^o{}_{NS}$	fundamental state – molar mass	macroscopic
87	$H_N := \int_{t^o}^{t^e} \dot{H}_N \; dt$	enthalpy	macroscopic
89	$I_N := \frac{d\,C_N}{d\,t}$	electrical current definition	macroscopic
93	$k^{e,\xi}{}_N := (R^e{}_N)^{-1} \,.\, \xi$	simple model for the electrical conductivity as a function of the additive	material
95	$Ue_N := (R^e{}_N)^{-1} \,.\, I_N$	electrical potential – voltage	macroscopic
96	$\dot{U}^e{}_N := 1 \,.\, Ue_N$	Kirkhoff first law	macroscopic
97	$\dot{U}^e{}_N := Root\,(Ue_N)$	Kirkhoff first law	macroscopic
106	$\phi := \text{MixedStack}\,(p_N, T_N, \mu_{NS}, c_{NS}, Ue_N)$	collected intensities	macroscopic
107	$n^t{}_N := 1_S \overset{S \in NS}{\star} n_{NS}$	total number of moles	macroscopic
108	$e_A := m_A - y^o{}_A$	control error	control
110	$\dot{x}_D := A_{N,D} \overset{N}{\star} x_N + B_{A,D} \overset{A}{\star} e_A$	differential state (ABCD) model	control
111	$x_N := \int_{t^o}^{t^e} 1_{N,D} \overset{D}{\star} \dot{x}_D \; dt$	state	control
113	$\check{I}_N := I_N$	measured current	control

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no	equation	documentation	layer
115	$\check{U}^{e}{}_{N} := Ue_{N}$	measured electrical potential	control
116	$\check{\xi} := \mapsto \xi$	measured additive fraction	control
117	$R_{N} := \left(\check{I}_{N}\right)^{-1} . \check{U}^{e}{}_{N}$	measured resistance	control
118	$S := \text{MixedStack}\left(\check{I}_{N}, \check{U}^{e}{}_{N}, R_{N}, \check{\xi}\right)$	quantities to be stored	control
123	$c_{NK,KS} := P_{NK} . \left(P_{NS,KS} \overset{NS}{\star} c_{NS}\right)$	var doc :	reactions
125	$x_{NK,KS} := \left(c^{o}{}_{NK,KS}\right)^{-1} . c_{NK,KS}$	matrix of normed, dimensionless mole fractions	reactions
126	$y_{A} := C_{N,A} \overset{N}{\star} x_{N} + D_{A} . e_{A}$	output equation	control
127	$R := A^{v} . B$	gas constant	reactions
128	$N_{NK,KS} := P_{K,NK} \overset{K}{\star} N_{K,KS}$	extended stoichiometrix matrix	reactions
129	$\phi_{NK} := \prod_{KS} x_{NK,KS}{}^{N_{NK,KS}}$	probability function for reactions	reactions
130	$\tilde{n}_{NS} := V_{N} \overset{N}{\star} \left(P_{N,NK} \overset{NK}{\star} \left(\left(K_{NK} . \phi_{NK}\right) . \left(P_{NS,KS} \overset{KS}{\star} N_{NK,KS}\right)\right)\right)$	the species production term	reactions
132	$boz_{N} := \text{Instantiate}(S_{N}, \#)$	Boltzmann constant	physical

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no	equation	documentation	layer
133	$R_N := A^v \,.\, boz_N$	gas constant	physical
134	$n_{tN} := 1_S \overset{S \in NS}{\star} n_{NS}$	total number of species in a node	macroscopic
135	$\xi_{NS} := (n_{tN})^{-1} \odot n_{NS}$	mole fraction	macroscopic
136	$\mu_{NS} := (R_N \,.\, T_N) \odot ln(\xi_{NS})$	chemical potential	macroscopic
137	$\tilde{n}_{NS} := \tilde{n}_{NS}$	production term	macroscopic
138	$s := 0.5 \,.\, (1 + \text{sign}\,(t^o))$	switches at to	control
139	$s := s$	switches at to	control –> macro-scopic
141	$\hat{n}^{c,controlled}{}_{AS} := s \,.\, \hat{n}^c{}_{AS}$	switched flow	macroscopic
142	$\dot{n}_{NS} := F_{NS,AS} \overset{AS}{\star} \text{Stack}\left(\hat{n}^c{}_{AS}, \hat{n}^{c,controlled}{}_{AS}\right)$	differential species balance switched	macroscopic

35 Instantiate

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
41	$E^a{}_{NK} := \text{Instantiate}(R \,.\, T_{NK}, \#)$	Arrhenius activation energy	reactions
79	$\hat{w}_A := \text{Instantiate}(\hat{H}^c{}_A, \#)$	sample work stream	macroscopic
84	$H^o{}_N := \text{Instantiate}(H_N, \#)$	initial enthalpy	macroscopic
85	$n^o{}_{NS} := \text{Instantiate}(n_{NS}, \#)$	initial species	macroscopic
88	$\xi := \text{Instantiate}(\xi, \#)$	fraction of additives	material
91	$R^e{}_N := (I_N)^{-1} \,.\, Ue_N$	electrical resistant	material
92	$R^e{}_N := \text{Instantiate}(R^e{}_N, \#)$	electrical resistant	material
98	$\dot{U}^e{}_N := \text{Instantiate}(\dot{U}^e{}_N, 0)$	Kirkhoff first law	macroscopic
109	$x_{oN} := \text{Instantiate}(x_N, \#)$	initial state	control
119	$y^o{}_A := \text{Instantiate}(y^o{}_A, \#)$	set point	control

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no	equation	documentation	layer
124	${c^o}_{NK,KS} := \mathrm{Instantiate}(c_{NK,KS}, \#)$	norming concentration	reactions

36 Instantiation Equation

no	equation	documentation	layer
140	$\hat{V}_A := \text{Instantiate}(\hat{V}_A, \#)$	instantiation equation	macroscopic

37 Interface Link Equation

no	equation	documentation	layer
20	$\lambda_S := \lambda_S$	interface equation	material –> macroscopic
37	$m_N := m_N$	interface equation	macroscopic –> material
45	$c_{NS} := c_{NS}$	interface equation	macroscopic –> reactions
51	$\rho_N := \rho_N$	interface equation	material –> macroscopic
52	${}_h{}_{NS} := h_{NS}$	interface equation	material –> macroscopic
53	$k^q_{x\,N} := k^q_{x\,N}$	interface equation	material –> macroscopic
54	${}_C v_N := C_{V\,N}$	interface equation	material –> macroscopic
55	$k^q_{y\,N} := k^q_{y\,N}$	interface equation	material –> macroscopic
56	$k^q_{z\,N} := k^q_{z\,N}$	interface equation	material –> macroscopic
57	$k^q{}_N := k^q{}_N$	interface equation	material –> macroscopic
58	$k^c_{x\,N} := k^c_{x\,N}$	interface equation	material –> macroscopic

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no	equation	documentation	layer
59	${}_{C}p_{N} := C_{p\,N}$	interface equation	material -> macroscopic
60	$k^{c}_{y\,N} := k^{c}_{y\,N}$	interface equation	material -> macroscopic
61	$k^{c}_{z\,N} := k^{c}_{z\,N}$	interface equation	material -> macroscopic
62	$k^{c}{}_{N} := k^{c}{}_{N}$	interface equation	material -> macroscopic
63	$k^{d}_{x\,NS} := k^{d}_{x\,NS}$	interface equation	material -> macroscopic
64	$k^{d}_{y\,NS} := k^{d}_{y\,NS}$	interface equation	material -> macroscopic
65	$k^{d}_{z\,NS} := k^{d}_{z\,NS}$	interface equation	material -> macroscopic
66	$k^{d}{}_{NS} := k^{d}{}_{NS}$	interface equation	material -> macroscopic
90	$I_{N} := I_{N}$	interface equation	macroscopic -> material
94	$R^{e}{}_{N} := k^{e,\xi}{}_{N}$	interface equation	material -> macroscopic
99	$I_{N} := I_{N}$	interface equation	macroscopic -> control
104	$\mapsto \xi := \xi$	interface equation	material -> control

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no	equation	documentation	layer
105	$T_N := T_N$	interface equation	macroscopic -> control
112	$\xi := \xi$	interface equation	material -> macroscopic
114	$Ue_N := Ue_N$	interface equation	macroscopic -> control
131	$\tilde{n}_{NS} := \tilde{n}_{NS}$	interface equation	reactions -> macroscopic