# 1 Variables

# 2 root

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 8 | $F_{N,A}$ | `F_N_A` | fundamental incidence matrix | network | | |
| 216 | $\Delta t$ | `dt_pulse` | lenth of pulse | frame | $s$ | |
| 217 | $pulse$ | `pulse` | pulse function | frame | | 180 |
| 5 | $t$ | `t` | time | frame | $s$ | |
| 6 | $t^o$ | `to` | starting time | frame | $s$ | 4 |
| 7 | $t^e$ | `te` | end time | frame | $s$ | 5 |
| 1 | $\#$ | `value` | numerical value | constant | | |
| 2 | 1 | `one` | numerical value one | constant | | 1 |
| 3 | 0 | `zero` | numerical value zero | constant | | 2 |
| 4 | 0.5 | `onehalf` | numerical value one half | constant | | 3 |

# 3 physical

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 162 | $P_{N,NS}$ | P_N_NS | projection of nodes onto the node species | projection | | |
| 200 | $I_{NS,AS}$ | I_NS_AS | projection species to node species | projection | | |
| 201 | $I_{N,A}$ | I_N_A | projection of nodes and arcs | projection | | |
| 32 | $P_{NS,AS}$ | P_NS_AS | projection node species to arc species | projection | | |
| 33 | $P_{K,NK}$ | P_K_NK | projection of conversion to node conversion | projection | | |
| 34 | $P_{S,NS}$ | P_S_NS | projection species to node species | projection | | |
| 35 | $P_{N,NK}$ | P_N_NK | projection node to node conversion | projection | | |
| 36 | $P_{NS,KS}$ | P_NS_KS | projection node species to conversion species | projection | | |
| 37 | $P_{A,NS}$ | P_A_NS | projection arc to node species for conductivity | projection | | |
| 65 | $P_{NK,KS}$ | P_NK_KS | projection node conversion to conversion species | projection | | |
| 9 | $P_{N,A}$ | P_N_A | projection from node to arc for arc properties | projection | | |
| 10 | $r_{x\,N}$ | r_x | x-coordinate | frame | $m$ | |
| 11 | $r_{y\,N}$ | r_y | y-coordinate | frame | $m$ | |
| 12 | $r_{z\,N}$ | r_z | z coordinate | frame | $m$ | |
| 13 | $U_N$ | U | fundamental state – internal energy | state | $kg\,m^2\,s^{-2}$ | |
| 14 | $S_N$ | S | fundamental state – entropy | state | $kg\,m^2\,K^{-1}\,s^{-2}$ | |
| 15 | $V_N$ | V | fundamental state – volume | state | $m^3$ | |
| 16 | $n_{NS}$ | n | fundamental state – molar mass | state | $mol$ | 86 |
| 20 | $H_N$ | H | enthalpy | state | $kg\,m^2\,s^{-2}$ | 9 87 184 |
| 21 | $A_N$ | A | Helmholtz energy | state | $kg\,m^2\,s^{-2}$ | 10 |
| 22 | $G_N$ | G | Gibbs free energy | state | $kg\,m^2\,s^{-2}$ | 11 |
| 23 | $C_N$ | charge | fundamental state – charge | state | $A\,s$ | |

*Continued on next page*

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 165 | $B_N$ | `boz` | Boltzmann constant | constant | $kg\, m^2\, K^{-1}\, s^{-2}$ | 132 |
| 166 | $R_N$ | `R` | gas constant | constant | $kg\, m^2\, mol^{-1}\, K^{-1}\, s^{-2}$ | 133 |
| 24 | $A^v$ | `Avogadro` | Avogadro number | constant | $mol^{-1}$ | |
| 17 | $p_N$ | `p` | thermodynamic pressure | effort | $kg\, m^{-1}\, s^{-2}$ | 6 |
| 18 | $T_N$ | `T` | temperature | effort | $K$ | 7 185 |
| 19 | $\mu_{NS}$ | `chemPot` | chemical potential | effort | $kg\, m^2\, mol^{-1}\, s^{-2}$ | 8 136 |
| 27 | ${U^e}_N$ | `Ue` | electrical potential – voltage | effort | $kg\, m^2\, A^{-1} s^{-3}$ | 14 95 |
| 28 | ${v_x}_N$ | `v_x` | velocity in x-direction | secondaryState | $ms^{-1}$ | 15 |
| 29 | ${v_y}_N$ | `v_y` | velocity in y-direction | secondaryState | $ms^{-1}$ | 16 |
| 30 | ${v_z}_N$ | `v_z` | velocity in z-direction | secondaryState | $ms^{-1}$ | 17 |

# 4 control

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 136 | $x_N$ | `x` | state | state | | 111 |
| 137 | $x_{oN}$ | `xo` | initial state | state | | 109 |
| 129 | $A_{N,D}$ | `A` | dynamic matrix | constant | $s^{-1}$ | |
| 130 | $B_{A,D}$ | `B` | input matrix | constant | $s^{-1}$ | |
| 131 | $C_{N,A}$ | `C` | measurement matrix | constant | | |
| 132 | $D_A$ | `D` | diagonal event matrix (no dimensional problems) | constant | | |
| 133 | ${y^o}_A$ | `setPoint` | set point | constant | | 119 |
| 134 | $m_A$ | `meas` | measurements | constant | | |
| 135 | $e_A$ | `e` | control error | constant | | 108 |
| 139 | $1_{N,D}$ | `I_N_D` | space transformation D to N | constant | | |
| 219 | $T_norm_N$ | `T_norm` | temprature transmitter constant | constant | $K$ | 186 |
| 138 | $\dot{x}_D$ | `dxdt` | differential state (ABCD) model | diffState | $s^{-1}$ | 110 |
| 141 | $\check{I}_N$ | `Imeasured` | measured current | algebraic | $A$ | 113 |
| 143 | ${\check{U}^e}_N$ | `UeMeasured` | measured electrical potential | algebraic | $kg\,m^2\,A^{-1}s^{-3}$ | 115 |
| 144 | $\check{\xi}$ | `addMeasured` | measured additive fraction | algebraic | | 116 |
| 145 | $R_N$ | `RComputed` | measured resistance | algebraic | $kg\,m^2\,A^{-2}s^{-3}$ | 117 |
| 154 | $y_A$ | `y` | output equation | algebraic | | 126 |
| 171 | $s$ | `switch` | switches at to | algebraic | | 138 |

## 5 reactions

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 147 | $P_{NK}$ | `P_NK` | reactions per node | projection | | |
| 155 | $B$ | `Boltzmann` | Boltzmann constant | constant | $kg\, m^2\, K^{-1}\, s^{-2}$ | |
| 157 | $R$ | `GasConstant` | gas constant | constant | $kg\, m^2\, mol^{-1}\, K^{-1}\, s^{-2}$ | 127 |
| 158 | $N_{K,KS}$ | `N_K_KS` | stoichiometry | constant | | |
| 159 | $N_{NK,KS}$ | `N_NK_KS` | extended stoichiometric matrix | constant | | 128 |
| 38 | ${K^o}_K$ | `Ko` | Arrhenius frequency factor | constant | $m^{-3}\, mol\, s^{-1}$ | |
| 62 | ${E^a}_{NK}$ | `Ea` | Arrhenius activation energy | constant | $kg\, m^2\, mol^{-1}\, s^{-2}$ | 41 |
| 63 | $K_{NK}$ | `K_NK` | Arrhenius reaction 'constant' | constant | $m^{-3}\, mol\, s^{-1}$ | 42 |
| 60 | $T_{NK}$ | `T_NK` | temperature of the reactive system | effort | $K$ | 39 |
| 151 | $c_{NK,KS}$ | `c` | concentration matrix reaction per node and species per reaction | secondaryState | $m^{-3}\, mol$ | 123 |
| 152 | ${c^o}_{NK,KS}$ | `co` | norming concentration | secondaryState | $m^{-3}\, mol$ | 124 |
| 153 | $x_{NK,KS}$ | `x` | matrix of normed, dimensionless mole fractions | secondaryState | | 125 |
| 160 | $\phi_{NK}$ | `phi` | probability function for reactions | secondaryState | | 129 |
| 163 | $\tilde{n}_{NS}$ | `nProd` | the species production term | secondaryState | $mol\, s^{-1}$ | 130 |

# 6 material

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 115 | ${R^e}_N$ | elResist | electrical resistant | property | $kg\,m^2\,A^{-2}s^{-3}$ | 91 92 |
| 116 | ${k^{e,\xi}}_N$ | elConductC | simple model for the electrical conductivity as a function of the additive | property | $kg^{-1}\,m^{-2}\,A^2s^3$ | 93 |
| 183 | ${k^{d,Fick}}_{NS}$ | k_d_Fick | Fick's diffusivity | property | $ms^{-1}$ | |
| 187 | $h_{AS}$ | h_A | partial molar enthalpies (arc) | property | $kg\,m^2\,mol^{-1}\,s^{-2}$ | 153 |
| 188 | ${k^{d,Fick}}_{AS}$ | k_d_Fick_A | Fick's diffusivity (arc) | property | $ms^{-1}$ | 154 |
| 189 | $\rho_A$ | density_A | density (arc) | property | $kg\,m^{-3}$ | 155 |
| 190 | ${k^{e,\xi}}_A$ | elConductC_A | simple model for the electrical conductivity as a function of the additive (arc) | property | $kg^{-1}\,m^{-2}\,A^2s^3$ | 156 |
| 191 | ${k^c_x}_A$ | kc_x_A | convective mass conductivity in x-direction (arc) | property | $m^{-1}\,s$ | 157 |
| 192 | ${k^c_y}_A$ | kc_y_A | convective mass conductivity in y-direction (arc) | property | $m^{-1}\,s$ | 158 |
| 193 | ${k^c_z}_A$ | kc_z_A | convective mass conductivity in z-direction | property | $m^{-1}\,s$ | 159 |
| 194 | ${k^d_x}_{AS}$ | kd_x_A | diffusional mass conductivity in x-direction (arc) | property | $kg^{-1}\,m^{-4}\,mol^2\,s$ | 160 |
| 195 | ${k^d_y}_{AS}$ | kd_y_A | diffusional mass conductivity in y-direction (arc) | property | $kg^{-1}\,m^{-4}\,mol^2\,s$ | 161 |
| 196 | ${k^d_z}_{AS}$ | kd_z_A | diffusional mass conductivity in z-direction (arc) | property | $kg^{-1}\,m^{-4}\,mol^2\,s$ | 162 |
| 197 | ${k^q_x}_A$ | kq_x_A | thermal conductivity in x-direction (arc) | property | $kg\,K^{-1}\,s^{-3}$ | 163 |
| 198 | ${k^q_y}_A$ | kq_y_A | thermal conductivity in y-direction (arc) | property | $kg\,K^{-1}\,s^{-3}$ | 164 |
| 199 | ${k^q_z}_A$ | kq_z_A | thermal conductivity in z-direction (arc) | property | $kg\,K^{-1}\,s^{-3}$ | 165 |
| 42 | ${C_p}_N$ | Cp | total heat capacity at constant pressure | property | $kg\,m^2\,K^{-1}\,s^{-2}$ | 21 |
| 43 | ${C_V}_N$ | Cv | total heat capacity at constant volume | property | $kg\,m^2\,K^{-1}\,s^{-2}$ | 22 |
| 44 | ${k^q_x}_N$ | kq_x | thermal conductivity in x-direction | property | $kg\,K^{-1}\,s^{-3}$ | 23 |
| 45 | ${k^q_y}_N$ | kq_y | thermal conductivity in y-direction | property | $kg\,K^{-1}\,s^{-3}$ | 24 |
| 46 | ${k^q_z}_N$ | kq_z | thermal conductivity in z-direction | property | $kg\,K^{-1}\,s^{-3}$ | 25 |
| 48 | ${k^c_x}_N$ | kc_x | convective mass conductivity in x-direction | property | $m^{-1}\,s$ | 27 |

*Continued on next page*

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 49 | ${k^c_y}_N$ | kc_y | convective mass conductivity in y-direction | property | $m^{-1}\,s$ | 28 |
| 50 | ${k^c_z}_N$ | kc_z | convective mass conductivity in z-direction | property | $m^{-1}\,s$ | 29 |
| 52 | ${k^d_x}_{NS}$ | kd_x | diffusional mass conductivity in x-direction | property | $kg^{-1}\,m^{-4}\,mol^2\,s$ | 31 |
| 53 | ${k^d_y}_{NS}$ | kd_y | diffusional mass conductivity in y-direction | property | $kg^{-1}\,m^{-4}\,mol^2\,s$ | 32 |
| 54 | ${k^d_z}_{NS}$ | kd_z | diffusional mass conductivity in z-direction | property | $kg^{-1}\,m^{-4}\,mol^2\,s$ | 33 |
| 56 | $h_{NS}$ | h | partial molar enthalpies | property | $kg\,m^2\,mol^{-1}\,s^{-2}$ | 35 |
| 59 | $\rho_N$ | density | density | property | $kg\,m^{-3}$ | 38 |
| 115 | ${R^e}_N$ | elResist | electrical resistant | property | $kg\,m^2\,A^{-2}s^{-3}$ | 91 92 |
| 116 | ${k^{e,\xi}}_N$ | elConductC | simple model for the electrical conductivity as a function of the additive | property | $kg^{-1}\,m^{-2}\,A^2s^3$ | 93 |
| 183 | ${k^{d,Fick}}_{NS}$ | k_d_Fick | Fick's diffusivity | property | $ms^{-1}$ | |
| 187 | $h_{AS}$ | h_A | partial molar enthalpies (arc) | property | $kg\,m^2\,mol^{-1}\,s^{-2}$ | 153 |
| 188 | ${k^{d,Fick}}_{AS}$ | k_d_Fick_A | Fick's diffusivity (arc) | property | $ms^{-1}$ | 154 |
| 189 | $\rho_A$ | density_A | density (arc) | property | $kg\,m^{-3}$ | 155 |
| 190 | ${k^{e,\xi}}_A$ | elConductC_A | simple model for the electrical conductivity as a function of the additive (arc) | property | $kg^{-1}\,m^{-2}\,A^2s^3$ | 156 |
| 191 | ${k^c_x}_A$ | kc_x_A | convective mass conductivity in x-direction (arc) | property | $m^{-1}\,s$ | 157 |
| 192 | ${k^c_y}_A$ | kc_y_A | convective mass conductivity in y-direction (arc) | property | $m^{-1}\,s$ | 158 |
| 193 | ${k^c_z}_A$ | kc_z_A | convective mass conductivity in z-direction | property | $m^{-1}\,s$ | 159 |
| 194 | ${k^d_x}_{AS}$ | kd_x_A | diffusional mass conductivity in x-direction (arc) | property | $kg^{-1}\,m^{-4}\,mol^2\,s$ | 160 |
| 195 | ${k^d_y}_{AS}$ | kd_y_A | diffusional mass conductivity in y-direction (arc) | property | $kg^{-1}\,m^{-4}\,mol^2\,s$ | 161 |
| 196 | ${k^d_z}_{AS}$ | kd_z_A | diffusional mass conductivity in z-direction (arc) | property | $kg^{-1}\,m^{-4}\,mol^2\,s$ | 162 |
| 197 | ${k^q_x}_A$ | kq_x_A | thermal conductivity in x-direction (arc) | property | $kg\,K^{-1}\,s^{-3}$ | 163 |
| 198 | ${k^q_y}_A$ | kq_y_A | thermal conductivity in y-direction (arc) | property | $kg\,K^{-1}\,s^{-3}$ | 164 |
| 199 | ${k^q_z}_A$ | kq_z_A | thermal conductivity in z-direction (arc) | property | $kg\,K^{-1}\,s^{-3}$ | 165 |

*Continued on next page*

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 42 | $C_{p\,N}$ | `Cp` | total heat capacity at constant pressure | property | $kg\, m^2\, K^{-1}\, s^{-2}$ | 21 |
| 43 | $C_{V\,N}$ | `Cv` | total heat capacity at constant volume | property | $kg\, m^2\, K^{-1}\, s^{-2}$ | 22 |
| 44 | $k^q_{x\,N}$ | `kq_x` | thermal conductivity in x-direction | property | $kg\, K^{-1}\, s^{-3}$ | 23 |
| 45 | $k^q_{y\,N}$ | `kq_y` | thermal conductivity in y-direction | property | $kg\, K^{-1}\, s^{-3}$ | 24 |
| 46 | $k^q_{z\,N}$ | `kq_z` | thermal conductivity in z-direction | property | $kg\, K^{-1}\, s^{-3}$ | 25 |
| 48 | $k^c_{x\,N}$ | `kc_x` | convective mass conductivity in x-direction | property | $m^{-1}\, s$ | 27 |
| 49 | $k^c_{y\,N}$ | `kc_y` | convective mass conductivity in y-direction | property | $m^{-1}\, s$ | 28 |
| 50 | $k^c_{z\,N}$ | `kc_z` | convective mass conductivity in z-direction | property | $m^{-1}\, s$ | 29 |
| 52 | $k^d_{x\,NS}$ | `kd_x` | diffusional mass conductivity in x-direction | property | $kg^{-1}\, m^{-4}\, mol^2\, s$ | 31 |
| 53 | $k^d_{y\,NS}$ | `kd_y` | diffusional mass conductivity in y-direction | property | $kg^{-1}\, m^{-4}\, mol^2\, s$ | 32 |
| 54 | $k^d_{z\,NS}$ | `kd_z` | diffusional mass conductivity in z-direction | property | $kg^{-1}\, m^{-4}\, mol^2\, s$ | 33 |
| 56 | $h_{NS}$ | `h` | partial molar enthalpies | property | $kg\, m^2\, mol^{-1}\, s^{-2}$ | 35 |
| 59 | $\rho_N$ | `density` | density | property | $kg\, m^{-3}$ | 38 |
| 112 | $\xi$ | `additive` | fraction of additives | constant | | 88 |
| 40 | $\lambda_S$ | `Mm` | species molecular mass | constant | $kg\, mol^{-1}$ | |

# 7 macroscopic

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 100 | $\hat{n}^c{}_{NS}$ | `fnc` | net molar convectional mass flow | transport | $mol\,s^{-1}$ | 75 |
| 102 | $\hat{H}^c{}_A$ | `fHc_A` | convective enthalpy flow for given stream | transport | $kg\,m^2\,s^{-3}$ | 77 |
| 103 | $\hat{H}^c{}_N$ | `fHc` | net convectional enthalpy stream | transport | $kg\,m^2\,s^{-3}$ | 78 |
| 104 | $\hat{w}_A$ | `fw_A` | sample work stream | transport | $kg\,m^2\,s^{-3}$ | 79 |
| 105 | $\hat{w}_N$ | `fw` | net work stream | transport | $kg\,m^2\,s^{-3}$ | 80 |
| 106 | $\hat{q}_{x\,A}$ | `fq_A_x` | heat flow in x-direction for given stream | transport | $kg\,m^2\,s^{-3}$ | 81 |
| 107 | $\hat{q}_N$ | `fq` | net heat flow | transport | $kg\,m^2\,s^{-3}$ | 82 |
| 173 | $\hat{n}^{c,controlled}{}_{AS}$ | `fnc_AS_controlled` | switched flow | transport | $mol\,s^{-1}$ | 141<br>181 |
| 92 | $\hat{V}_A$ | `fV` | volumetric flow | transport | $m^3\,s^{-1}$ | 67<br>140 |
| 93 | $\hat{n}^d{}_{AS}$ | `fnd_AS` | diffusional mass flow in a given stream | transport | $mol\,s^{-1}$ | 68<br>152 |
| 94 | $\hat{n}^d{}_{NS}$ | `fnd` | net diffusional mass flow | transport | $mol\,s^{-1}$ | 69 |
| 95 | $\hat{H}^d{}_A$ | `fHd_A` | enthalpy flow per diffusional mass stream | transport | $kg\,m^2\,s^{-3}$ | 70 |
| 96 | $\hat{H}^d{}_N$ | `fHd` | net enthalpy stream due to diffusion | transport | $kg\,m^2\,s^{-3}$ | 71 |
| 97 | $d_A$ | `d` | flow direction of convectional flow | transport | | 72 |
| 99 | $\hat{n}^c{}_{AS}$ | `fnc_AS` | molar convectional mass flow in the given stream | transport | $mol\,s^{-1}$ | 74 |
| 215 | $A_{yz\,A}$ | `Ayz_A` | cross sectional area yz (arc) | geometry | $m^2$ | 179 |
| 71 | $A_{yz\,N}$ | `Ayz` | cross sectional area yz | geometry | $m^2$ | 48 |
| 70 | $F_{NS,AS}$ | `F_NS_AS` | species related incidence matrix | network | | |
| 90 | $D_{N,A}$ | `D` | difference operator | differenceOperator | | |
| 91 | $D_{NS,AS}$ | `D_NS_AS` | difference operator for species topology | differenceOperator | | |
| 109 | $H^o{}_N$ | `Ho` | initial enthalpy | state | $kg\,m^2\,s^{-2}$ | 84 |

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| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 110 | ${n^o}_{NS}$ | `no` | initial species | state | $mol$ | 85 |
| 127 | $1_S$ | `one_S` | a vector of ones with the length of the ordinal number of S | constant | | |
| 218 | ${T^{ref}}_N$ | `T_ref` | reference temperature | effort | $K$ | 183 |
| 128 | ${n^t}_N$ | `nTotal` | total number of moles | secondaryState | $mol$ | 107 |
| 168 | ${n_t}_N$ | `nt` | total number of species in a node | secondaryState | $mol$ | 134 |
| 169 | $\xi_{NS}$ | `xi` | mole fraction | secondaryState | | 135 |
| 176 | $g_{NS}$ | `g` | | secondaryState | $mol$ | 145 |
| 57 | $m_N$ | `m` | total mass | secondaryState | $kg$ | 36 |
| 66 | $c_{NS}$ | `c` | molar composition | secondaryState | $m^{-3}\, mol$ | 44 |
| 98 | $c_{AS}$ | `c_AS` | concentration in convectional flow | secondaryState | $m^{-3}\, mol$ | 73 |
| 170 | $\tilde{n}_{NS}$ | `nProd` | production term | conversion | $mol\, s^{-1}$ | 137 |
| 101 | $\dot{n}_{NS}$ | `dndt` | differential species balance | diffState | $mol\, s^{-1}$ | 76 182 |
| 108 | $\dot{H}_N$ | `dHdt` | differential enthalpy balance | diffState | $kg\, m^2\, s^{-3}$ | 83 |
| 118 | ${\dot{U}^e}_N$ | `dUedt` | Kirkhoffs first law | diffState | $kg\, m^2\, A^{-1} s^{-3}$ | 96 97 98 |
| 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 energy

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

## 11 liquid

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

## 12 gas

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

# 13 control–control

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

## 14 energy–gas

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

## 15 energy–energy

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

## 16 gas–gas

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

## 17 energy–liquid

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

# 18 liquid–liquid

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

## 19 energy–solid

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

## 20 solid–solid

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

## 21 gas–liquid

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

## 22 gas–solid

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

## 23 liquid–solid

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

## 24 material–material

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

## 25 reactions–reactions

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

## 26 control–reactions

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

## 27 reactions–control

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

# 28 control–material

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

## 29 material–control

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 124 | _$\xi$ | `_additive` | link variable additive to interface material »> control | get | | 104 |

## 30 control–macroscopic

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 172 | $s$ | `_switch` | switches at to | get | | 139 |

# 31 macroscopic–control

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 119 | $\_I_N$ | `_i` | link variable i to interface macroscopic »> control | get | $A$ | 99 |
| 125 | $\_T_N$ | `_T` | link variable T to interface macroscopic »> control | get | $K$ | 105 |
| 142 | $\_{U^e}_N$ | `_Ue` | link variable Ue to interface macroscopic »> control | get | $kg\, m^2\, A^{-1} s^{-3}$ | 114 |

# 32 reactions–material

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

# 33 material–reactions

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|

# 34 reactions–macroscopic

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 164 | $\_\tilde{n}_{NS}$ | `_nProd` | link variable nProd to interface reactions »> macroscopic | get | $mol\,s^{-1}$ | 131 |

## 35 macroscopic–reactions

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 67 | $\_c_{NS}$ | `_c` | link variable c to interface macroscopic »> reactions | get | $m^{-3}\, mol$ | 45 |

# 36 material–macroscopic

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 117 | $\_R^e{}_N$ | `_elConductC` | link variable elConductC to interface material »> macroscopic | get | $kg^{-1}\,m^{-2}\,A^2 s^3$ | 94 |
| 140 | $\_\xi$ | `_additive` | link variable additive to interface material »> macroscopic | get | | 112 |
| 184 | $\_k^{d,Fick}{}_{NS}$ | `_k_d_Fick` | link variable k d Fick to interface material »> macroscopic | get | $ms^{-1}$ | 151 |
| 202 | $\_\rho_A$ | `_density_A` | link variable density A to interface material »> macroscopic | get | $kg\,m^{-3}$ | 166 |
| 203 | $\_R^e{}_A$ | `_elConductC_A` | link variable elConductC A to interface material »> macroscopic | get | $kg^{-1}\,m^{-2}\,A^2 s^3$ | 167 |
| 204 | $\_h_{AS}$ | `_h_A` | link variable h A to interface material »> macroscopic | get | $kg\,m^2\,mol^{-1}\,s^{-2}$ | 168 |
| 205 | $\_k^{d,Fick,A}{}_{AS}$ | `_k_d_Fick_A` | link variable k d Fick A to interface material »> macroscopic | get | $ms^{-1}$ | 169 |
| 206 | $\_k^c_x{}_A$ | `_kc_x_A` | link variable kc x A to interface material »> macroscopic | get | $m^{-1}\,s$ | 170 |
| 207 | $\_k^c_y{}_A$ | `_kc_y_A` | link variable kc y A to interface material »> macroscopic | get | $m^{-1}\,s$ | 171 |
| 208 | $\_k^c_z{}_A$ | `_kc_z_A` | link variable kc z A to interface material »> macroscopic | get | $m^{-1}\,s$ | 172 |
| 209 | $\_k^d_x{}_{AS}$ | `_kd_x_A` | link variable kd x A to interface material »> macroscopic | get | $kg^{-1}\,m^{-4}\,mol^2\,s$ | 173 |
| 210 | $\_k^d_y{}_{AS}$ | `_kd_y_A` | link variable kd y A to interface material »> macroscopic | get | $kg^{-1}\,m^{-4}\,mol^2\,s$ | 174 |
| 211 | $\_k^d_z{}_{AS}$ | `_kd_z_A` | link variable kd z A to interface material »> macroscopic | get | $kg^{-1}\,m^{-4}\,mol^2\,s$ | 175 |
| 212 | $\_k^c_x{}_A$ | `_kq_x_A` | link variable kq x A to interface material »> macroscopic | get | $kg\,K^{-1}\,s^{-3}$ | 176 |

*Continued on next page*

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 213 | $\_k^c_{yA}$ | `_kq_y_A` | link variable kq y A to interface material »> macroscopic | get | $kg\,K^{-1}\,s^{-3}$ | 177 |
| 214 | $\_k^c_{zA}$ | `_kq_z_A` | link variable kq z A to interface material »> macroscopic | get | $kg\,K^{-1}\,s^{-3}$ | 178 |
| 41 | $\_\lambda_S$ | `_Mm` | link variable Mm to interface material »> macroscopic | get | $kg\,mol^{-1}$ | 20 |
| 74 | $\_\rho_N$ | `_density` | link variable density to interface material »> macroscopic | get | $kg\,m^{-3}$ | 51 |
| 75 | $\_h_{NS}$ | `_h` | link variable h to interface material »> macroscopic | get | $kg\,m^2\,mol^{-1}\,s^{-2}$ | 52 |
| 76 | $\_k^q_{xN}$ | `_kq_x` | link variable kq x to interface material »> macroscopic | get | $kg\,K^{-1}\,s^{-3}$ | 53 |
| 77 | $\_Cv_N$ | `_Cv` | link variable Cv to interface material »> macroscopic | get | $kg\,m^2\,K^{-1}\,s^{-2}$ | 54 |
| 78 | $\_k^q_{yN}$ | `_kq_y` | link variable kq y to interface material »> macroscopic | get | $kg\,K^{-1}\,s^{-3}$ | 55 |
| 79 | $\_k^q_{zN}$ | `_kq_z` | link variable kq z to interface material »> macroscopic | get | $kg\,K^{-1}\,s^{-3}$ | 56 |
| 81 | $\_k^c_{xN}$ | `_kc_x` | link variable kc x to interface material »> macroscopic | get | $m^{-1}\,s$ | 58 |
| 82 | $\_Cp_N$ | `_Cp` | link variable Cp to interface material »> macroscopic | get | $kg\,m^2\,K^{-1}\,s^{-2}$ | 59 |
| 83 | $\_k^c_{yN}$ | `_kc_y` | link variable kc y to interface material »> macroscopic | get | $m^{-1}\,s$ | 60 |
| 84 | $\_k^c_{zN}$ | `_kc_z` | link variable kc z to interface material »> macroscopic | get | $m^{-1}\,s$ | 61 |
| 86 | $\_k^d_{xNS}$ | `_kd_x` | link variable kd x to interface material »> macroscopic | get | $kg^{-1}\,m^{-4}\,mol^2\,s$ | 63 |
| 87 | $\_k^d_{yNS}$ | `_kd_y` | link variable kd y to interface material »> macroscopic | get | $kg^{-1}\,m^{-4}\,mol^2\,s$ | 64 |
| 88 | $\_k^d_{zNS}$ | `_kd_z` | link variable kd z to interface material »> macroscopic | get | $kg^{-1}\,m^{-4}\,mol^2\,s$ | 65 |

# 37 macroscopic–material

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 114 | $\_I_N$ | `_i` | link variable i to interface macroscopic »> material | get | $A$ | 90 |
| 58 | $\_m_N$ | `_m` | link variable m to interface macroscopic »> material | get | $kg$ | 37 |

# 38 Equations

# 39 Generic

| no | equation | documentation | layer |
|---|---|---|---|
| 10 | $A_N := U_N - T_N \, . \, S_N$ | Helmholtz energy | physical |
| 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 |
| 11 | $G_N := U_N + p_N \, . \, V_N - T_N \, . \, S_N$ | Gibbs free energy | physical |
| 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 |
| 115 | $\check{U}^e{}_N := \_U^e{}_N$ | measured electrical potential | control |
| 116 | $\check{\xi} := \_\xi$ | measured additive fraction | control |
| 117 | $R_N := \left(\check{I}_N\right)^{-1} . \, \check{U}^e{}_N$ | measured resistance | 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 |

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| no | equation | documentation | layer |
|---|---|---|---|
| 129 | $\phi_{NK} := \prod_{KS} x_{NK,KS}{}^{N_{NK,KS}}$ | probability function for reactions | reactions |
| 130 | $\tilde{n}_{NS} := V_N \overset{N}{\star} \left(P_{N,NK} \overset{NK}{\star} \left((K_{NK} \,.\, \phi_{NK}) \,.\, \left(P_{NS,KS} \overset{KS}{\star} N_{NK,KS}\right)\right)\right)$ | the species production term | reactions |
| 132 | $B_N :=$ Instantiate$(S_N, \#)$ | Boltzmann constant | physical |
| 133 | $R_N := A^v \,.\, B_N$ | 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 |
| 14 | $U^e{}_N := (C_N)^{-1} \,.\, U_N$ | electrical potential – voltage | physical |
| 141 | $\hat{n}^{c,controlled}{}_{AS} := s \,.\, \hat{n}^c{}_{AS}$ | switched flow | macroscopic |
| 145 | $g_{NS} := n_{NS} + n_{NS}$ | | macroscopic |
| 15 | $v_{xN} := \frac{\partial r_{xN}}{\partial t}$ | velocitiy in x-direction | physical |
| 152 | $\hat{n}^d{}_{AS} := A_{yzA} \odot \left(-\_k^{d,Fick,A}{}_{AS}\right) \,.\, D_{NS,AS} \overset{NS}{\star} c_{NS}$ | diffusional mass flow in a given stream | macroscopic |
| 153 | $h_{AS} := I_{NS,AS} \overset{NS}{\star} h_{NS}$ | partial molar enthalpies (arc) | material |
| 154 | $k^{d,Fick}{}_{AS} := I_{NS,AS} \overset{NS}{\star} k^{d,Fick}{}_{NS}$ | Fick's diffusivity (arc) | material |
| 155 | $\rho_A := I_{N,A} \overset{N}{\star} \rho_N$ | density (arc) | material |

*Continued on next page*

| no | equation | documentation | layer |
|---|---|---|---|
| 156 | $k^{e,\xi}{}_{A} := I_{N,A} \overset{N}{\star} k^{e,\xi}{}_{N}$ | simple model for the electrical conductivity as a function of the additive (arc) | material |
| 157 | $k^{c}_{x A} := I_{N,A} \overset{N}{\star} k^{c}_{x N}$ | convective mass conductivity in x-direction (arc) | material |
| 158 | $k^{c}_{y A} := I_{N,A} \overset{N}{\star} k^{c}_{y N}$ | convective mass conductivity in y-direction (arc) | material |
| 159 | $k^{c}_{z A} := I_{N,A} \overset{N}{\star} k^{c}_{z N}$ | convective mass conductivity in z-direction | material |
| 16 | $v_{y N} := \frac{\partial r_{y N}}{\partial t}$ | velocity in y direction | physical |
| 160 | $k^{d}_{x AS} := I_{NS,AS} \overset{NS}{\star} k^{d}_{x NS}$ | diffusional mass conductivity in x-direction (arc) | material |
| 161 | $k^{d}_{y AS} := I_{NS,AS} \overset{NS}{\star} k^{d}_{y NS}$ | diffusional mass conductivity in y-direction (arc) | material |
| 162 | $k^{d}_{z AS} := I_{NS,AS} \overset{NS}{\star} k^{d}_{z NS}$ | diffusional mass conductivity in z-direction (arc) | material |
| 163 | $k^{q}_{x A} := I_{N,A} \overset{N}{\star} k^{q}_{x N}$ | thermal conductivity in x-direction | material |
| 164 | $k^{q}_{y A} := I_{N,A} \overset{N}{\star} k^{q}_{y N}$ | thermal conductivity in y-direction (arc) | material |
| 165 | $k^{q}_{z A} := I_{N,A} \overset{N}{\star} k^{q}_{z N}$ | thermal conductivity in z-direction (arc) | material |
| 17 | $v_{z N} := \frac{\partial r_{z N}}{\partial t}$ | velocity in z-direction | macroscopic |
| 179 | $A_{yz A} := I_{N,A} \overset{N}{\star} A_{yz N}$ | cross sectional area yz (arc) | macroscopic |
| 180 | $pulse := \text{sign}\,(t - t^{o}) - \text{sign}\,(t - (t^{o} + \Delta t))$ | pulse function | root |

*Continued on next page*

| no | equation | documentation | layer |
|---|---|---|---|
| 181 | $\hat{n}^{c,controlled}{}_{AS} := pulse\,.\,\hat{n}^{c}{}_{AS}$ | manipulate flow | macroscopic |
| 182 | $\dot{n}_{NS} := \text{Instantiate}(\dot{n}_{NS}, 0)$ | differential species balance – event dynamic | macroscopic |
| 183 | $T^{ref}{}_{N} := \text{Instantiate}(T_{N}, -)$ | reference temperature | macroscopic |
| 184 | $H_{N} := \_Cp_{N}\,.\,(T_{N} - T^{ref}{}_{N})$ | enthalpy from constant heat capacity | macroscopic |
| 185 | $T_{N} := Root\,(H_{N})$ | temperature | macroscopic |
| 186 | $T_{n}orm_{N} := \text{Instantiate}(\_T_{N}, \#)$ | temprature transmitter constant | control |
| 21 | $C_{p\,N} := \frac{\partial H_{N}}{\partial T_{N}}$ | total heat capacity at constant pressure | material |
| 22 | $C_{V\,N} := \frac{\partial U_{N}}{\partial T_{N}}$ | total heat capacity at constant volume | material |
| 23 | $k^{q}_{x\,N} := (V_{N})^{-1}\,.\,\frac{\partial U_{N}}{\partial T_{N}}\,.\,v_{x\,N}$ | thermal conductivity in x-direction | material |
| 24 | $k^{q}_{y\,N} := (V_{N})^{-1}\,.\,\frac{\partial U_{N}}{\partial T_{N}}\,.\,v_{y\,N}$ | thermal conductivity in y-direction | material |
| 25 | $k^{q}_{z\,N} := (V_{N})^{-1}\,.\,\frac{\partial U_{N}}{\partial T_{N}}\,.\,v_{z\,N}$ | thermal conductivity in z-direction' | material |
| 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 |
| 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 |

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| no | equation | documentation | layer |
|---|---|---|---|
| 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 |
| 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 |
| 6 | $p_N := \left(-\frac{\partial U_N}{\partial V_N}\right)$ | thermodynamic pressure | physical |
| 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 | $\hat{n}^d{}_{AS} := A_{yz\,A} \odot \left(-\_k^d_{x\,AS}\right) \,.\, D_{NS,AS} \overset{NS}{\star} \mu_{NS}$ | 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 |
| 7 | $T_N := \frac{\partial U_N}{\partial S_N}$ | temperature | physical |
| 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 |

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| no | equation | documentation | layer |
|---|---|---|---|
| 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 |
| 8 | $\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$ | chemical potential | physical |
| 80 | $\hat{w}_N := F_{N,A} \overset{A}{\star} \hat{w}_A$ | net work stream | macroscopic |
| 81 | $\hat{q}_{xA} := A_{yzN} \,.\, \_k^q_{xN} \,.\, D_{N,A} \overset{N}{\star} T_N$ | heat flow in x-direction for given stream | macroscopic |
| 82 | $\hat{q}_N := F_{N,A} \overset{A}{\star} \hat{q}_{xA}$ | net heat flow | macroscopic |
| 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 |
| 9 | $H_N := U_N - p_N \,.\, V_N$ | enthalpy | physical |
| 93 | $k^{e,\xi}{}_N := (R^e{}_N)^{-1} \,.\, \xi$ | simple model for the electrical conductivity as a function of the additive | material |
| 95 | $U^e{}_N := (\_R^e{}_N)^{-1} \,.\, I_N$ | electrical potential – voltage | macroscopic |

*Continued on next page*

| no | equation | documentation | layer |
|---|---|---|---|
| 96 | $\dot{U}^{e}{}_{N} := 1 \, . \, U^{e}{}_{N}$ | Kirkhoff first law | macroscopic |
| 97 | $\dot{U}^{e}{}_{N} := Root \left( U^{e}{}_{N} \right)$ | Kirkhoff first law | macroscopic |

## 40 Instantiate

| no | equation | documentation | layer |
|---|---|---|---|
| 1 | $1 := \text{Instantiate}(\#, \#)$ | numerical value 1 | root |
| 109 | $x_{oN} := \text{Instantiate}(x_N, \#)$ | initial state | control |
| 119 | $y^o{}_A := \text{Instantiate}(y^o{}_A, \#)$ | set point | control |
| 124 | $c^o{}_{NK,KS} := \text{Instantiate}(c_{NK,KS}, \#)$ | norming concentration | reactions |
| 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 |
| 41 | $E^a{}_{NK} := \text{Instantiate}(R \,.\, T_{NK}, \#)$ | Arrhenius activation energy | reactions |
| 5 | $t^e := \text{Instantiate}(t, \#)$ | end time | root |
| 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 | $R^e{}_N := (\_I_N)^{-1} \,.\, U^e{}_N$ | 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 |

## 41 Instantiation Equation

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

# 42 Interface Link Equation

| no | equation | documentation | layer |
|---|---|---|---|
| 104 | $\_\xi := \xi$ | interface equation | material -> control |
| 105 | $\_T_N := T_N$ | interface equation | macroscopic -> control |
| 112 | $\_\xi := \xi$ | interface equation | material -> macroscopic |
| 114 | $\_U^e{}_N := U^e{}_N$ | interface equation | macroscopic -> control |
| 131 | $\_\tilde{n}_{NS} := \tilde{n}_{NS}$ | interface equation | reactions -> macroscopic |
| 151 | $\_k^{d,Fick}{}_{NS} := k^{d,Fick}{}_{NS}$ | interface equation | material -> macroscopic |
| 166 | $\_\rho_A := \rho_A$ | interface equation | material -> macroscopic |
| 167 | $\_R^e{}_A := k^{e,\xi}{}_A$ | interface equation | material -> macroscopic |
| 168 | $\_h_{AS} := h_{AS}$ | interface equation | material -> macroscopic |
| 169 | $\_k^{d,Fick,A}{}_{AS} := k^{d,Fick}{}_{AS}$ | interface equation | material -> macroscopic |
| 170 | $\_k^c_{xA} := k^c_{xA}$ | interface equation | material -> macroscopic |

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| no | equation | documentation | layer |
|---|---|---|---|
| 171 | $\_k^c_{yA} := k^c_{yA}$ | interface equation | material –> macroscopic |
| 172 | $\_k^c_{zA} := k^c_{zA}$ | interface equation | material –> macroscopic |
| 173 | $\_k^d_{xAS} := k^d_{xAS}$ | interface equation | material –> macroscopic |
| 174 | $\_k^d_{yAS} := k^d_{yAS}$ | interface equation | material –> macroscopic |
| 175 | $\_k^d_{zAS} := k^d_{zAS}$ | interface equation | material –> macroscopic |
| 176 | $\_k^c_{xA} := k^q_{xA}$ | interface equation | material –> macroscopic |
| 177 | $\_k^c_{yA} := k^q_{yA}$ | interface equation | material –> macroscopic |
| 178 | $\_k^c_{zA} := k^q_{zA}$ | interface equation | material –> macroscopic |
| 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 |

*Continued on next page*

| no | equation | documentation | layer |
|---|---|---|---|
| 52 | $\_h_{NS} := h_{NS}$ | interface equation | material –> macro-scopic |
| 53 | $\_k^q_{x}{}_N := k^q_{x}{}_N$ | interface equation | material –> macro-scopic |
| 54 | $\_Cv_N := C_{V}{}_N$ | interface equation | material –> macro-scopic |
| 55 | $\_k^q_{y}{}_N := k^q_{y}{}_N$ | interface equation | material –> macro-scopic |
| 56 | $\_k^q_{z}{}_N := k^q_{z}{}_N$ | interface equation | material –> macro-scopic |
| 58 | $\_k^c_{x}{}_N := k^c_{x}{}_N$ | interface equation | material –> macro-scopic |
| 59 | $\_Cp_N := C_{p}{}_N$ | interface equation | material –> macro-scopic |
| 60 | $\_k^c_{y}{}_N := k^c_{y}{}_N$ | interface equation | material –> macro-scopic |
| 61 | $\_k^c_{z}{}_N := k^c_{z}{}_N$ | interface equation | material –> macro-scopic |
| 63 | $\_k^d_{x}{}_{NS} := k^d_{x}{}_{NS}$ | interface equation | material –> macro-scopic |
| 64 | $\_k^d_{y}{}_{NS} := k^d_{y}{}_{NS}$ | interface equation | material –> macro-scopic |
| 65 | $\_k^d_{z}{}_{NS} := k^d_{z}{}_{NS}$ | interface equation | material –> macro-scopic |

*Continued on next page*

| no | equation | documentation | layer |
|---|---|---|---|
| 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 |