

## 1 Variables

### 2 root

|   | var       | symbol  | documentation                | type     | units | eqs |
|---|-----------|---------|------------------------------|----------|-------|-----|
| 8 | $F_{N,A}$ | F_N_A   | fundamental incidence matrix | network  |       |     |
| 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  |
|-----|-------------|----------|--|------------|-------------------------------------|------|
| 9   | $P_{N,A}$   | P_N_A    | projection from node to arc for arc properties   | 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 |                                     |      |
| 162 | $P_{N,NS}$  | P_N_NS   | projection of nodes onto the node species        | projection |                                     |      |
| 10  | $r_{xN}$    | r_x      | x-coordinate                                     | frame      | $m$                                 |      |
| 11  | $r_{yN}$    | r_y      | y-coordinate                                     | frame      | $m$                                 |      |
| 12  | $r_{zN}$    | 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 |
| 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      | $A\,s$                              |      |
| 24  | $A^v$       | Avogadro | Avogadro number                                  | constant   | $mol^{-1}$                          |      |
| 165 | $Boltz_N$   | Boltz    | 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  |

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|    | var        | symbol         | documentation                  | type           | units                       | eqs          |
|----|------------|----------------|--------------------------------|----------------|-----------------------------|--------------|
| 17 | $p_N$      | <b>p</b>       | thermodynamic pressure         | effort         | $kg\,m^{-1}\,s^{-2}$        | <b>6</b>     |
| 18 | $T_N$      | <b>T</b>       | temperature                    | effort         | $K$                         | <b>7</b>     |
| 19 | $\mu_{NS}$ | <b>chemPot</b> | chemical potential             | effort         | $kg\,m^2\,mol^{-1}\,s^{-2}$ | <b>8 136</b> |
| 27 | $Ue_N$     | <b>Ue</b>      | electrical potential – voltage | effort         | $kg\,m^2\,A^{-1}\,s^{-3}$   | <b>14 95</b> |
| 28 | $v_{xN}$   | <b>v_x</b>     | velocity in x-direction        | secondaryState | $ms^{-1}$                   | <b>15</b>    |
| 29 | $v_{yN}$   | <b>v_y</b>     | velocity in y-direction        | secondaryState | $ms^{-1}$                   | <b>16</b>    |
| 30 | $v_{zN}$   | <b>v_z</b>     | velocity in z-direction        | secondaryState | $ms^{-1}$                   | <b>17</b>    |

## 4 control

|     | var             | symbol             | documentation                                   | type      | units                   | eqs                 |
|-----|-----------------|--------------------|---|-----------|-------------------------|---------------------|
| 136 | $x_N$           | <b>x</b>           | state   | state     |                         | <a href="#">111</a> |
| 137 | $x_{oN}$        | <b>xo</b>          | initial state                                   | state     |                         | <a href="#">109</a> |
| 129 | $A_{N,D}$       | <b>A</b>           | dynamic matrix                                  | constant  | $s^{-1}$                |                     |
| 130 | $B_{A,D}$       | <b>B</b>           | input matrix                                    | constant  | $s^{-1}$                |                     |
| 131 | $C_{N,A}$       | <b>C</b>           | measurement matrix                              | constant  |                         |                     |
| 132 | $D_A$           | <b>D</b>           | diagonal event matrix (no dimensional problems) | constant  |                         |                     |
| 133 | $y^o_A$         | <b>setPoint</b>    | set point                                       | constant  |                         | <a href="#">119</a> |
| 134 | $m_A$           | <b>meas</b>        | measurements                                    | constant  |                         |                     |
| 135 | $e_A$           | <b>e</b>           | control error                                   | constant  |                         | <a href="#">108</a> |
| 139 | $1_{N,D}$       | <b>I_N_D</b>       | space transformation D to N                     | constant  |                         |                     |
| 138 | $\dot{x}_D$     | <b>dxdt</b>        | differential state (ABCD) model                 | diffState | $s^{-1}$                | <a href="#">110</a> |
| 141 | $\tilde{I}_N$   | <b>Imeasured</b>   | measured current                                | algebraic | $A$                     | <a href="#">113</a> |
| 143 | $\tilde{U}^e_N$ | <b>UeMeasured</b>  | measured electrical potential                   | algebraic | $kg\,m^2\,A^{-1}s^{-3}$ | <a href="#">115</a> |
| 144 | $\tilde{\xi}$   | <b>addMeasured</b> | measured additive fraction                      | algebraic |                         | <a href="#">116</a> |
| 145 | $R_N$           | <b>RComputed</b>   | measured resistance                             | algebraic | $kg\,m^2\,A^{-2}s^{-3}$ | <a href="#">117</a> |
| 146 | $S$             | <b>store</b>       | quantities to be stored                         | algebraic |                         | <a href="#">118</a> |
| 154 | $y_A$           | <b>y</b>           | output equation                                 | algebraic |                         | <a href="#">126</a> |
| 171 | $s$             | <b>switch</b>      | switches at to                                  | algebraic |                         | <a href="#">138</a> |

## 5 reactions

|     | var              | symbol      | documentation   | type           | units                           | eqs |
|-----|------------------|-------------|---|----------------|---------------------------------|-----|
| 147 | $P_{NK}$         | P_NK        | reactions per node  | projection     |                                 |     |
| 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  |
| 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 |
| 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   |
|-----|---------------|------------|--|----------|-----------------------------|-------|
| 40  | $\lambda_S$   | Mm         | species molecular mass   | constant | $kg\ mol^{-1}$              |       |
| 112 | $\xi$         | additive   | fraction of additives  | constant |                             | 88    |
| 42  | $C_{pN}$      | Cp         | total heat capacity at constant pressure                                   | property | $kg\ m^2\ K^{-1}\ s^{-2}$   | 21    |
| 43  | $C_{VN}$      | Cv         | total heat capacity at constant volume                                     | property | $kg\ m^2\ K^{-1}\ s^{-2}$   | 22    |
| 44  | $k_{xN}^q$    | kq_x       | thermal conductivity in x-direction  | property | $kg\ K^{-1}\ s^{-3}$        | 23    |
| 45  | $k_{yN}^q$    | kq_y       | thermal conductivity in y-direction  | property | $kg\ K^{-1}\ s^{-3}$        | 24    |
| 46  | $k_{zN}^q$    | kq_z       | thermal conductivity in z-direction'                                       | property | $kg\ K^{-1}\ s^{-3}$        | 25    |
| 47  | $k_N^q$       | kq         | thermal conductivity   | property | $kg\ K^{-1}\ s^{-3}$        | 26    |
| 48  | $k_{xN}^c$    | kc_x       | convective mass conductivity in x-direction                                | property | $m^{-1}\ s$                 | 27    |
| 49  | $k_{yN}^c$    | kc_y       | convective mass conductivity in y-direction                                | property | $m^{-1}\ s$                 | 28    |
| 50  | $k_{zN}^c$    | kc_z       | convective mass conductivity in z-direction                                | property | $m^{-1}\ s$                 | 29    |
| 51  | $k_N^c$       | kc         | convective mass conductivity   | property | $m^{-1}\ s$                 | 30    |
| 52  | $k_{xNS}^d$   | kd_x       | diffusional mass conductivity in x-direction                               | property | $kg^{-1}\ m^{-4}\ mol^2\ s$ | 31    |
| 53  | $k_{yNS}^d$   | kd_y       | diffusional mass conductivity in y-direction                               | property | $kg^{-1}\ m^{-4}\ mol^2\ s$ | 32    |
| 54  | $k_{zNS}^d$   | kd_z       | diffusional mass conductivity in z-direction                               | property | $kg^{-1}\ m^{-4}\ mol^2\ s$ | 33    |
| 55  | $k_{NS}^d$    | kd         | diffusional mass conductivity  | property | $kg^{-1}\ m^{-4}\ mol^2\ s$ | 34    |
| 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 | $R_N^e$       | 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 | $kg^{-1}\ m^{-2}\ A^2\ s^3$ | 93    |

## 7 macroscopic

|     | var                           | symbol            | documentation                                    | type               | units           | eqs       |
|-----|-------------------------------|-------------------|--|--------------------|-----------------|-----------|
| 92  | $\hat{V}_A$                   | fV                | volumetric flow                                  | transport          | $m^3 s^{-1}$    | 67<br>140 |
| 93  | $\hat{n}_{AS}^d$              | fnd_AS            | diffusional mass flow in a given stream          | transport          | $mol s^{-1}$    | 68        |
| 94  | $\hat{n}_{NS}^d$              | fnd               | net diffusional mass flow                        | transport          | $mol s^{-1}$    | 69        |
| 95  | $\hat{H}_A^d$                 | fHd_A             | enthalpy flow per diffusional mass stream        | transport          | $kg m^2 s^{-3}$ | 70        |
| 96  | $\hat{H}_N^d$                 | 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  | $\hat{n}_{AS}^c$              | fnc_AS            | molar convectional mass flow in the given stream | transport          | $mol s^{-1}$    | 74        |
| 100 | $\hat{n}_{NS}^c$              | fnc               | net molar convectional mass flow                 | transport          | $mol s^{-1}$    | 75        |
| 102 | $\hat{H}_A^c$                 | fHc_A             | convective enthalpy flow for given stream        | transport          | $kg m^2 s^{-3}$ | 77        |
| 103 | $\hat{H}_N^c$                 | 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 | $\hat{q}_{xA}$                | 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 | $\hat{n}_{AS}^{c,controlled}$ | fnc_AS_controlled | switched flow                                    | transport          | $mol s^{-1}$    | 141       |
| 71  | $A_{yzN}$                     | Ayz               | cross sectional area yz                          | geometry           | $m^2$           | 48        |
| 72  | $A_{xzN}$                     | Axz               | cross sectional area xz                          | geometry           | $m^2$           | 49        |
| 73  | $A_{xyN}$                     | Axy               | cross sectional area xy                          | geometry           | $m^2$           | 50        |
| 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 | $H_N^o$                       | Ho                | initial enthalpy                                 | state              | $kg m^2 s^{-2}$ | 84        |

Continued on next page

|     | var              | symbol             | documentation   | type              | units                  | eqs   |
|-----|------------------|--------------------|---|-------------------|------------------------|---|
| 110 | $n_{NS}^o$       | <b>no</b>          | initial species   | state             | $mol$                  | <a href="#">85</a>  |
| 127 | $1_S$            | <b>one_S</b>       | a vector of ones with the length of the ordinal number of S | constant          |                        |   |
| 57  | $m_N$            | <b>m</b>           | total mass  | secondaryState    | $kg$                   | <a href="#">36</a>  |
| 66  | $c_{NS}$         | <b>c</b>           | molar composition   | secondaryState    | $m^{-3} mol$           | <a href="#">44</a>  |
| 98  | $c_{AS}$         | <b>c_AS</b>        | concentration in convectional flow                          | secondaryState    | $m^{-3} mol$           | <a href="#">73</a>  |
| 126 | $\phi$           | <b>intensities</b> | collected intensities                                       | secondaryState    |                        | <a href="#">106</a>   |
| 128 | $n_N^t$          | <b>nTotal</b>      | total number of moles                                       | secondaryState    | $mol$                  | <a href="#">107</a>   |
| 168 | $n_{tN}$         | <b>nt</b>          | total number of species in a node                           | secondaryState    | $mol$                  | <a href="#">134</a>   |
| 169 | $\xi_{NS}$       | <b>xi</b>          | mole fraction   | secondaryState    |                        | <a href="#">135</a>   |
| 170 | $\tilde{n}_{NS}$ | <b>nProd</b>       | production term   | conversion        | $mol s^{-1}$           | <a href="#">137</a>   |
| 101 | $\dot{n}_{NS}$   | <b>dndt</b>        | differential species balance                                | diffState         | $mol s^{-1}$           | <a href="#">76</a><br><a href="#">142</a>                   |
| 108 | $\dot{H}_N$      | <b>dHdt</b>        | differential enthalpy balance                               | diffState         | $kg m^2 s^{-3}$        | <a href="#">83</a>  |
| 118 | $\dot{U}_N^e$    | <b>dUedt</b>       | Kirkhoffs first law   | diffState         | $kg m^2 A^{-1} s^{-3}$ | <a href="#">96</a> <a href="#">97</a><br><a href="#">98</a> |
| 113 | $I_N$            | <b>i</b>           | electrical current definition                               | internalTransport | $A$                    | <a href="#">89</a>  |



## 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 |
|-----|---------------|------------------------|--|------|-------|-----|
| 124 | $\mapsto \xi$ | <code>_additive</code> | link variable additive to interface material » > control | get  |       | 104 |

## 25 control-macroscopic

|     | var      | symbol               | documentation  | type | units | eqs |
|-----|----------|----------------------|----------------|------|-------|-----|
| 172 | <i>s</i> | <code>_switch</code> | switches at to | get  |       | 139 |

## 26 macroscopic-control

|     | var    | symbol           | documentation  | type | units                   | eqs |
|-----|--------|------------------|--|------|-------------------------|-----|
| 119 | $I_N$  | <code>_i</code>  | link variable i to interface macroscopic »> control  | get  | $A$                     | 99  |
| 125 | $T_N$  | <code>_T</code>  | link variable T to interface macroscopic »> control  | get  | $K$                     | 105 |
| 142 | $Ue_N$ | <code>_Ue</code> | 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 |
|-----|------------------|--------|---|------|---------------|-----|
| 164 | $\tilde{n}_{NS}$ | _nProd | link variable nProd to interface reactions »> macroscopic | get  | $mol\ s^{-1}$ | 131 |

## 30 macroscopic-reactions

|    | var      | symbol          | documentation   | type | units        | eqs |
|----|----------|-----------------|---|------|--------------|-----|
| 67 | $c_{NS}$ | <code>_c</code> | link variable c to interface macroscopic »> reactions | get  | $m^{-3} mol$ | 45  |

### 31 material–macroscopic

|    | var         | symbol   | documentation  | type | units                       | eqs |
|----|-------------|----------|--|------|-----------------------------|-----|
| 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 | $k_{xN}^q$  | _kq_x    | link variable kq x to interface material »> macroscopic    | get  | $kg\,K^{-1}\,s^{-3}$        | 53  |
| 77 | $C_{vN}^v$  | _Cv      | link variable Cv to interface material »> macroscopic      | get  | $kg\,m^2\,K^{-1}\,s^{-2}$   | 54  |
| 78 | $k_{yN}^q$  | _kq_y    | link variable kq y to interface material »> macroscopic    | get  | $kg\,K^{-1}\,s^{-3}$        | 55  |
| 79 | $k_{zN}^q$  | _kq_z    | link variable kq z to interface material »> macroscopic    | get  | $kg\,K^{-1}\,s^{-3}$        | 56  |
| 80 | $k_N^q$     | _kq      | link variable kq to interface material »> macroscopic      | get  | $kg\,K^{-1}\,s^{-3}$        | 57  |
| 81 | $k_{xN}^c$  | _kc_x    | link variable kc x to interface material »> macroscopic    | get  | $m^{-1}\,s$                 | 58  |
| 82 | $C_{pN}$    | _Cp      | link variable Cp to interface material »> macroscopic      | get  | $kg\,m^2\,K^{-1}\,s^{-2}$   | 59  |
| 83 | $k_{yN}^c$  | _kc_y    | link variable kc y to interface material »> macroscopic    | get  | $m^{-1}\,s$                 | 60  |
| 84 | $k_{zN}^c$  | _kc_z    | link variable kc z to interface material »> macroscopic    | get  | $m^{-1}\,s$                 | 61  |
| 85 | $k_N^c$     | _kc      | link variable kc to interface material »> macroscopic      | get  | $m^{-1}\,s$                 | 62  |
| 86 | $k_{xNS}^d$ | _kd_x    | link variable kd x to interface material »> macroscopic    | get  | $kg^{-1}\,m^{-4}\,mol^2\,s$ | 63  |
| 87 | $k_{yNS}^d$ | _kd_y    | link variable kd y to interface material »> macroscopic    | get  | $kg^{-1}\,m^{-4}\,mol^2\,s$ | 64  |
| 88 | $k_{zNS}^d$ | _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 |
|-----|------------|--------------------------|---|------|--------------------------|-----|
| 89  | $k^d_{NS}$ | <code>_kd</code>         | link variable kd to interface material »> macroscopic         | get  | $kg^{-1} m^{-4} mol^2 s$ | 66  |
| 117 | $R^e_N$    | <code>_elConductC</code> | link variable elConductC to interface material »> macroscopic | get  | $kg^{-1} m^{-2} A^2 s^3$ | 94  |
| 140 | $\xi$      | <code>_additive</code>   | link variable additive to interface material »> macroscopic   | get  |                          | 112 |

## 32 macroscopic-material

|     | var   | symbol | documentation  | type | units | eqs |
|-----|-------|--------|--|------|-------|-----|
| 58  | $m_N$ | _m     | link variable m to interface macroscopic »> material | get  | $kg$  | 37  |
| 114 | $I_N$ | _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  | $H_N := U_N - p_N \cdot V_N$  | enthalpy                                 | physical |
| 10 | $A_N := U_N - T_N \cdot S_N$  | Helmholtz energy                         | physical |
| 11 | $G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$                                  | Gibbs free energy                        | physical |
| 14 | $Ue_N := (C_N)^{-1} \cdot U_N$  | electrical potential – voltage           | physical |
| 15 | $v_{xN} := \frac{\partial r_{xN}}{\partial t}$                                | velocity 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 | $k_{xN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}$ | thermal conductivity in x-direction      | material |
| 24 | $k_{yN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{yN}$ | thermal conductivity in y-direction      | material |
| 25 | $k_{zN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{zN}$ | thermal conductivity in z-direction'     | material |
| 26 | $k_N^q := \text{Stack}(k_{xN}^q, k_{yN}^q, k_{zN}^q)$                         | thermal conductivity                     | material |

*Continued on next page*

| no | equation  | documentation                                | layer       |
|----|---|--|-------------|
| 27 | $k_{xN}^c := \left( \lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$ | convective mass conductivity in x-direction  | material    |
| 28 | $k_{yN}^c := \left( \lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$ | convective mass conductivity in y-direction  | material    |
| 29 | $k_{zN}^c := \left( \lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$ | convective mass conductivity in z-direction  | material    |
| 30 | $k_N^c := \text{Stack}(k_{xN}^c, k_{yN}^c, k_{zN}^c)$   | convective mass conductivity                 | material    |
| 31 | $k_{xNS}^d := (\mu_{NS})^{-1} \cdot \left( v_{xN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$       | diffusional mass conductivity in x-direction | material    |
| 32 | $k_{yNS}^d := (\mu_{NS})^{-1} \cdot \left( v_{yN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$       | diffusional mass conductivity in y-direction | material    |
| 33 | $k_{zNS}^d := (\mu_{NS})^{-1} \cdot \left( v_{zN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$       | diffusional mass conductivity in z-direction | material    |
| 34 | $k_{NS}^d := \text{Stack}(k_{xNS}^d, k_{yNS}^d, k_{zNS}^d)$   | diffusional mass conductivity                | material    |
| 35 | $h_{NS} := H_N \odot (n_{NS})^{-1}$   | partial molar enthalpies                     | material    |
| 36 | $m_N := \lambda_S^{S \in NS} \star n_{NS}$  | total mass                                   | macroscopic |
| 38 | $\rho_N := m_N \cdot (V_N)^{-1}$  | density                                      | material    |
| 39 | $T_{NK} := P_{N,NK} \star^N T_N$  | temperature of the reactive system           | reactions   |
| 42 | $K_{NK} := K^o_K \odot \exp((-E^a_{NK}) \cdot (R \cdot T_{NK})^{-1})$   | Arrhenius reaction 'constant'                | reactions   |
| 44 | $c_{NS} := (V_N)^{-1} \odot n_{NS}$   | molar composition                            | macroscopic |
| 48 | $A_{yzN} := r_{yN} \cdot r_{zN}$  | cross sectional area yz                      | macroscopic |

Continued on next page

| no | equation  | documentation                                   | layer       |
|----|---|---|-------------|
| 49 | $A_{xzN} := r_{xN} \cdot r_{zN}$  | cross sectional area xz                         | macroscopic |
| 50 | $A_{xyN} := r_{xN} \cdot r_{yN}$  | cross sectional area xy                         | macroscopic |
| 67 | $\hat{V}_A := (\rho_N)^{-1} \cdot k_{xN}^c \cdot A_{yzN} \cdot D_{N,A} \star^N p_N$         | volumetric flow                                 | macroscopic |
| 68 | $\hat{n}_{AS}^d := A_{yzN} \odot (-k_{xNS}^d) \cdot D_{NS,AS} \star^{NS} \mu_{NS}$          | diffusional mass flow in a given stream         | macroscopic |
| 69 | $\hat{n}_{NS}^d := F_{NS,AS} \star^{AS} \hat{n}_{AS}^d$                                     | net diffusional mass flow                       | macroscopic |
| 70 | $\hat{H}_A^d := \left( F_{NS,AS} \star^{NS} h_{NS} \right) \star^{S \in AS} \hat{n}_{AS}^d$ | enthalpy flow per diffusional mass stream       | macroscopic |
| 71 | $\hat{H}_N^d := F_{N,A} \star^A \hat{H}_A^d$  | net enthaply stream due to diffusion            | macroscopic |
| 72 | $d_A := \text{sign} \left( F_{N,A} \star^N p_N \right)$                                     | flow direction of convectional flow             | macroscopic |
| 73 | $c_{AS} := (0.5 \cdot (F_{NS,AS} - d_A \odot  F_{NS,AS} )) \star^{NS} c_{NS}$               | concentration in convectional flow              | macroscopic |
| 74 | $\hat{n}_{AS}^c := \hat{V}_A \odot c_{AS}$  | molar convetional mass flow in the given stream | macroscopic |
| 75 | $\hat{n}_{NS}^c := F_{NS,AS} \star^{AS} \hat{n}_{AS}^c$                                     | net molar convectional mass flow                | macroscopic |
| 76 | $\dot{n}_{NS} := \hat{n}_{NS}^c + \hat{n}_{NS}^d + \tilde{n}_{NS}$                          | differential species balance                    | macroscopic |
| 77 | $\hat{H}_A^c := \left( F_{NS,AS} \star^{NS} h_{NS} \right) \star^{S \in AS} \hat{n}_{AS}^c$ | convective enthalpy flow for given stream       | macroscopic |
| 78 | $\hat{H}_N^c := F_{N,A} \star^A \hat{H}_A^c$  | net convectional enthalpy stream                | macroscopic |
| 80 | $\hat{w}_N := F_{N,A} \star^A \hat{w}_A$  | net work stream                                 | macroscopic |
| 81 | $\hat{q}_{xA} := A_{yzN} \cdot k_{xN}^q \cdot D_{N,A} \star^N T_N$                          | heat flow in x-direction for given stream       | macroscopic |
| 82 | $\hat{q}_N := F_{N,A} \star^A \hat{q}_{xA}$   | 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  | $I_N := \frac{dC_N}{dt}$   | electrical current definition  | macroscopic |
| 93  | $k^{e,\xi}_N := (R^e_N)^{-1} \cdot \xi$  | simple model for the electrical conductivity as a function of the additive | material    |
| 95  | $Ue_N := (R^e_N)^{-1} \cdot I_N$   | electrical potential – voltage   | macroscopic |
| 96  | $\dot{U}^e_N := 1 \cdot Ue_N$  | Kirkhoff first law   | macroscopic |
| 97  | $\dot{U}^e_N := \text{Root}(Ue_N)$   | 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     |

*Continued on next page*

| no  | equation  | documentation                                  | layer     |
|-----|---|--|-----------|
| 115 | $\check{U}_N^e := U e_N$  | measured electrical potential                  | control   |
| 116 | $\check{\xi} := \mapsto \xi$  | measured additive fraction                     | control   |
| 117 | $R_N := (\check{I}_N)^{-1} \cdot \check{U}_N^e$   | measured resistance                            | control   |
| 118 | $S := \text{MixedStack}(\check{I}_N, \check{U}_N^e, R_N, \check{\xi})$  | quantities to be stored                        | control   |
| 123 | $c_{NK,KS} := P_{NK} \cdot \left( P_{NS,KS} \overset{NS}{\star} c_{NS} \right)$   | var doc :                                      | reactions |
| 125 | $x_{NK,KS} := (c_{NK,KS}^o)^{-1} \cdot c_{NK,KS}$   | matrix of normed, dimensionless mole fractions | reactions |
| 126 | $y_A := C_{N,A} \overset{N}{\star} x_N + D_A \cdot e_A$   | output equation                                | control   |
| 127 | $R := A^v \cdot B$  | 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 | $\tilde{n}_{NS} := V_N \overset{N}{\star} \left( P_{N,NK} \overset{NK}{\star} \left( (K_{NK} \cdot \phi_{NK}) \cdot \left( P_{NS,KS} \overset{KS}{\star} N_{NK,KS} \right) \right) \right)$ | the species production term                    | reactions |
| 132 | $Boltz_N := \text{Instantiate}(S_N, \#)$  | Boltzmann constant                             | physical  |

*Continued on next page*

| no  | equation  | documentation                         | layer                             |
|-----|---|---------------------------------------|-----------------------------------|
| 133 | $R_N := A^v . Boltz_N$  | 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 $\rightarrow$ macroscopic |
| 141 | $\hat{n}^{c,controlled}_{AS} := s . \hat{n}^c_{AS}$   | switched flow                         | macroscopic                       |
| 142 | $\dot{n}_{NS} := F_{NS,AS} \overset{AS}{\star} \text{Stack}(\hat{n}^c_{AS}, \hat{n}^{c,controlled}_{AS})$ | 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     |

*Continued on next page*

| no  | equation   | documentation         | layer     |
|-----|--|-----------------------|-----------|
| 124 | $c^o_{NK,KS} := \text{Instantiate}(c_{NK,KS}, \#)$ | 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 | $k_{xN}^q := k_{xN}^q$   | interface equation | material -> macroscopic  |
| 54 | $C^{v_N} := C^{v_N}$     | interface equation | material -> macroscopic  |
| 55 | $k_{yN}^q := k_{yN}^q$   | interface equation | material -> macroscopic  |
| 56 | $k_{zN}^q := k_{zN}^q$   | interface equation | material -> macroscopic  |
| 57 | $k_N^q := k_N^q$         | interface equation | material -> macroscopic  |
| 58 | $k_{xN}^c := k_{xN}^c$   | interface equation | material -> macroscopic  |

*Continued on next page*

| no  | equation                 | documentation      | layer                  |
|-----|--------------------------|--------------------|------------------------|
| 59  | $CP_N := C_{pN}$         | interface equation | material → macroscopic |
| 60  | $k_{yN}^c := k_{yN}^c$   | interface equation | material → macroscopic |
| 61  | $k_{zN}^c := k_{zN}^c$   | interface equation | material → macroscopic |
| 62  | $k_N^c := k_N^c$         | interface equation | material → macroscopic |
| 63  | $k_{xNS}^d := k_{xNS}^d$ | interface equation | material → macroscopic |
| 64  | $k_{yNS}^d := k_{yNS}^d$ | interface equation | material → macroscopic |
| 65  | $k_{zNS}^d := k_{zNS}^d$ | interface equation | material → macroscopic |
| 66  | $k_{NS}^d := k_{NS}^d$   | interface equation | material → macroscopic |
| 90  | $I_N := I_N$             | interface equation | macroscopic → material |
| 94  | $R_N^e := k_N^{e,\xi}$   | interface equation | material → macroscopic |
| 99  | $I_N := I_N$             | interface equation | macroscopic → control  |
| 104 | $\mapsto \xi := \xi$     | interface equation | material → control     |

*Continued on next page*

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