

## 1 Variables

### 2 root

|   | var       | symbol  | documentation               | type     | units | eqs |
|---|-----------|---------|-----------------------------|----------|-------|-----|
| 8 | $F_{N,A}$ | F_N_A   | fudamental 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 |                                     |      |
| 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   | $mol^{-1}$                          |      |
| 25 | $k^B_N$     | Boltzmann   | Boltzmann constant                               | constant   | $kg\,m^2\,K^{-1}\,s^{-2}$           | 12   |
| 26 | $R_N$       | GasConstant | gas constant                                     | constant   | $kg\,m^2\,mol^{-1}\,K^{-1}\,s^{-2}$ | 13   |
| 17 | $p_N$       | p           | thermodynamic pressure                           | effort     | $kg\,m^{-1}\,s^{-2}$                | 6    |

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|    | var        | symbol         | documentation                  | type           | units                       | eqs          |
|----|------------|----------------|--------------------------------|----------------|-----------------------------|--------------|
| 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</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  |                         |                     |
| 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 | $I_N$       | <b>Imeasured</b>   | measured current                                | algebraic | $A$                     | <a href="#">113</a> |
| 143 | $U^e_N$     | <b>UeMeasured</b>  | measured electrical potential                   | algebraic | $kg\,m^2\,A^{-1}s^{-3}$ | <a href="#">115</a> |
| 144 | $\xi$       | <b>addMeasured</b> | measured additive fraction                      | algebraic |                         | <a href="#">116</a> |
| 145 | $R_N$       | <b>RMeasured</b>   | measured resistance                             | algebraic | $kg\,m^2\,A^{-2}s^{-3}$ | <a href="#">117</a> |
| 146 | $store$     | <b>store</b>       | quantities to be stored                         | algebraic |                         | <a href="#">118</a> |

## 5 reactions

|    | var        | symbol | documentation                            | type           | units                    | eqs |
|----|------------|--------|--|----------------|--------------------------|-----|
| 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  |
| 68 | $c_{KS}$   | c_KS   | concentrations associated with reactions | secondaryState | $m^{-3} mol$             | 46  |
| 69 | $c^o_{KS}$ | co_KS  | norming concentrations                   | secondaryState | $m^{-3} mol$             | 47  |

## 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  |
| 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  | $\hat{H}_{AS}^d$ | 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 convectonal flow                          | transport          |                 | 72  |
| 102 | $\hat{H}_{AS}^c$ | fHc_A   | convective enthalpy flow for given stream                   | transport          | $kg m^2 s^{-3}$ | 77  |
| 103 | $\hat{H}_N^c$    | fHc     | net convectonal 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  |
| 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  |
| 110 | $n_{NS}^o$       | 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           |                 |     |
| 57  | $m_N$            | m       | total mass  | secondaryState     | $kg$            | 36  |

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|     | var              | symbol             | documentation                                   | type              | units                  | eqs   |
|-----|------------------|--------------------|---|-------------------|------------------------|---|
| 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>  |
| 99  | $\hat{n}_{AS}^c$ | <b>fnc_AS</b>      | molar convetional mass flow in the given stream | secondaryState    | $mol s^{-1}$           | <a href="#">74</a>  |
| 100 | $\hat{n}_{NS}^c$ | <b>fnc</b>         | net molar convectional mass flow                | secondaryState    | $mol s^{-1}$           | <a href="#">75</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>   |
| 101 | $\dot{n}_{NS}$   | <b>dndt</b>        | differential species balance                    | diffState         | $mol s^{-1}$           | <a href="#">76</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>       | Kirkhoff 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 | $\xi$ | additive | link variable additive to interface material » > control | get  |       | 104 |

## 25 control-macroscopic

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

## 26 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 | $Ue_N$ | 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 |
|--|-----|--------|---------------|------|-------|-----|
|--|-----|--------|---------------|------|-------|-----|

## 30 macroscopic-reactions

|    | var      | symbol   | documentation   | type | units        | eqs |
|----|----------|----------|---|------|--------------|-----|
| 67 | $c_{NS}$ | <b>c</b> | 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 | $Cv_N$      | 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 | $Cp_N$      | 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  |

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|     | var             | symbol            | documentation   | type | units                    | eqs        |
|-----|-----------------|-------------------|---|------|--------------------------|------------|
| 89  | $k^d_{NS}$      | <b>kd</b>         | link variable kd to interface material »> macroscopic         | get  | $kg^{-1} m^{-4} mol^2 s$ | <b>66</b>  |
| 117 | $R^e_N$         | <b>elConductC</b> | link variable elConductC to interface material »> macroscopic | get  | $kg^{-1} m^{-2} A^2 s^3$ | <b>94</b>  |
| 140 | <i>additive</i> | <b>additive</b>   | link variable additive to interface material »> macroscopic   | get  |                          | <b>112</b> |

## 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    |
|----|--|--------------------------------|----------|
| 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     |
| 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 |
| 12 | $k^B_N := \text{Instantiate}(S_N, \#)$                   | Boltzmann constant             | physical |
| 13 | $R_N := A^v \cdot k^B_N$                                 | gas constant                   | 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 |

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

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| no | equation  | documentation                             | layer       |
|----|---|---|-------------|
| 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 | $\rho_N := m_N \cdot (V_N)^{-1}$  | density                                   | material    |
| 39 | $T_{NK} := P_{N,NK} \overset{N}{\star} T_N$   | temperature of the reactive system        | reactions   |
| 41 | $E^a_{NK} := \text{Instantiate}(P_{N,NK} \overset{N}{\star} R_N \cdot T_{NK}, \#)$                  | Arrhenius activation energy               | reactions   |
| 42 | $K_{NK} := K^o_K \odot \exp((-E^a_{NK}) \cdot (R_N \overset{N}{\star} P_{N,NK} \cdot T_{NK})^{-1})$ | Arrhenius reaction 'constant'             | reactions   |
| 44 | $c_{NS} := (V_N)^{-1} \odot n_{NS}$   | molar composition                         | macroscopic |
| 46 | $c_{KS} := c_{NS} \overset{NS}{\star} P_{NS,KS}$  | concentrations associated with reactions  | reactions   |
| 47 | $c^o_{KS} := \text{Instantiate}(c_{KS}, \#)$  | norming concentrations                    | reactions   |
| 48 | $A_{yzN} := r_{yN} \cdot r_{zN}$  | cross sectional area yz                   | macroscopic |
| 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 | $\hat{V}_A := (\rho_N)^{-1} \cdot k^c_{xN} \cdot A_{yzN} \cdot D_{N,A} \overset{N}{\star} p_N$      | volumetric flow                           | macroscopic |
| 68 | $\hat{n}^d_{AS} := A_{yzN} \odot (-k^d_{xNS}) \cdot D_{NS,AS} \overset{NS}{\star} \mu_{NS}$         | 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 | $\hat{H}^d_A := (F_{NS,AS} \overset{NS}{\star} h_{NS}) \overset{S \in AS}{\star} \hat{n}^d_{AS}$    | 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 |

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| no | equation  | documentation                                   | layer       |
|----|---|---|-------------|
| 72 | $d_A := \text{sign} \left( F_{N,A} \stackrel{N}{\star} p_N \right)$   | flow direction of convectional flow             | macroscopic |
| 73 | $c_{AS} := (0.5 \cdot (F_{NS,AS} - d_A \odot  F_{NS,AS} )) \stackrel{NS}{\star} c_{NS}$                         | 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 | $\hat{n}_{NS}^c := F_{NS,AS} \stackrel{AS}{\star} \hat{n}_{AS}^c$   | net molar convectional mass flow                | macroscopic |
| 76 | $\dot{n}_{NS} := \hat{n}_{NS}^c + \hat{n}_{NS}^d$   | differential species balance                    | macroscopic |
| 77 | $\hat{H}_A^c := \left( F_{NS,AS} \stackrel{NS}{\star} h_{NS} \right) \stackrel{S \in AS}{\star} \hat{n}_{AS}^c$ | convective enthalpy flow for given stream       | macroscopic |
| 78 | $\hat{H}_N^c := F_{N,A} \stackrel{A}{\star} \hat{H}_A^c$  | net convectional enthalpy stream                | macroscopic |
| 79 | $\hat{w}_A := \text{Instantiate}(\hat{H}_A^c, \#)$  | sample work stream                              | macroscopic |
| 80 | $\hat{w}_N := F_{N,A} \stackrel{A}{\star} \hat{w}_A$  | net work stream                                 | macroscopic |
| 81 | $\hat{q}_{xA} := A_{yzN} \cdot k_{xN}^q \cdot D_{N,A} \stackrel{N}{\star} T_N$                                  | heat flow in x-direction for given stream       | macroscopic |
| 82 | $\hat{q}_N := F_{N,A} \stackrel{A}{\star} \hat{q}_{xA}$   | net heat flow                                   | macroscopic |
| 83 | $\dot{H}_N := \hat{H}_N^c + \hat{H}_N^d + \hat{q}_N + \hat{w}_N$  | differential enthalpy balance                   | macroscopic |
| 84 | $H_N^o := \text{Instantiate}(H_N, \#)$  | initial enthalpy                                | macroscopic |
| 85 | $n_{NS}^o := \text{Instantiate}(n_{NS}, \#)$  | initial species                                 | macroscopic |
| 86 | $n_{NS} := \int_{t^o}^{t^e} \dot{n}_{NS} dt$  | fundamental state – molar mass                  | macroscopic |
| 87 | $H_N := \int_{t^o}^{t^e} \dot{H}_N dt$  | enthalpy  | macroscopic |
| 88 | $\xi := \text{Instantiate}(\xi, \#)$  | fraction of additives                           | material    |

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| no  | equation   | documentation  | layer       |
|-----|--|--|-------------|
| 89  | $I_N := \frac{dC_N}{dt}$   | electrical current definition  | macroscopic |
| 91  | $R_N^e := (i_N)^{-1} \cdot U_{eN}$   | electrical resistant   | material    |
| 92  | $R_N^e := \text{Instantiate}(R_N^e, \#)$                                       | electrical resistant   | material    |
| 93  | $k^{e,\xi}_N := (R_N^e)^{-1} \cdot \xi$  | simple model for the electrical conductivity as a function of the additive | material    |
| 95  | $U_{eN} := (R_N^e)^{-1} \cdot I_N$   | electrical potential – voltage   | macroscopic |
| 96  | $\dot{U}_N^e := 1 \cdot U_{eN}$  | Kirkhoff first law   | macroscopic |
| 97  | $\dot{U}_N^e := \text{Root}(U_{eN})$   | Kirkhoff first law   | macroscopic |
| 98  | $\dot{U}_N^e := \text{Instantiate}(\dot{U}_N^e, 0)$                            | Kirkhoff first law   | macroscopic |
| 106 | $\phi := \text{MixedStack}(p_N, T_N, \mu_{NS}, c_{NS}, U_{eN})$                | collected intensities  | macroscopic |
| 107 | $n_N^t := 1_S \overset{S \in NS}{\star} n_{NS}$                                | total number of moles  | macroscopic |
| 108 | $e_A := m_A - y^o_A$   | control error  | control     |
| 109 | $xo_N := \text{Instantiate}(x_N, \#)$  | initial state  | 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     |

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| no  | equation   | documentation                 | layer   |
|-----|--|-------------------------------|---------|
| 113 | $I_N := I_N$                                       | measured current              | control |
| 115 | $U^e_N := Ue_N$                                    | measured electrical potential | control |
| 116 | $\xi := \xi$                                       | measured additive fraction    | control |
| 117 | $R_N := (I_N)^{-1} \cdot U^e_N$                    | measured resistance           | control |
| 118 | $store := \text{MixedStack}(I_N, U^e_N, R_N, \xi)$ | quantities to be stored       | control |



## 35 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 | $Cv_N := Cv_N$           | 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  |

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| no  | equation                 | documentation      | layer                  |
|-----|--------------------------|--------------------|------------------------|
| 59  | $Cp_N := Cp_N$           | 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  | $R_N^e := R_N^e$         | interface equation | material → macroscopic |
| 99  | $I_N := I_N$             | interface equation | macroscopic → control  |
| 104 | $\xi := \xi$             | interface equation | material → control     |

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| no  | equation               | documentation      | layer                  |
|-----|------------------------|--------------------|------------------------|
| 105 | $T_N := T_N$           | interface equation | macroscopic control →  |
| 112 | $additive := additive$ | interface equation | material → macroscopic |
| 114 | $Ue_N := Ue_N$         | interface equation | macroscopic control →  |