

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 | | |
| 162 | $P_{NN}S_{N,NS}$ | 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} | |
| 17 | p_N | p | thermodynamic pressure | effort | $kg\,m^{-1}\,s^{-2}$ | 6 |
| 18 | T_N | T | temperature | effort | K | 7 |

Continued on next page

| | var | symbol | documentation | type | units | eqs |
|----|------------|----------------|--------------------------------|----------------|-----------------------------|--------------|
| 19 | μ_{NS} | chemPot | chemical potential | effort | $kg\,m^2\,mol^{-1}\,s^{-2}$ | 8 |
| 27 | Ue_N | Ue | electrical potential – voltage | effort | $kg\,m^2\,A^{-1}\,s^{-3}$ | 14 95 |
| 28 | v_{xN} | v_x | velocity in x-direction | secondaryState | ms^{-1} | 15 |
| 29 | v_{yN} | v_y | velocity in y-direction | secondaryState | ms^{-1} | 16 |
| 30 | v_{zN} | 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 | | |
| 138 | \dot{x}_D | dxdt | differential state (ABCD) model | diffState | s^{-1} | 110 |
| 141 | \tilde{I}_N | Imeasured | measured current | algebraic | A | 113 |
| 143 | \tilde{U}^e_N | UeMeasured | measured electrical potential | algebraic | $kg\,m^2\,A^{-1}s^{-3}$ | 115 |
| 144 | $\tilde{\xi}$ | addMeasured | measured additive fraction | algebraic | | 116 |
| 145 | $RComputed_N$ | RComputed | measured resistance | algebraic | $kg\,m^2\,A^{-2}s^{-3}$ | 117 |
| 146 | $store$ | store | quantities to be stored | algebraic | | 118 |
| 154 | y_A | y | output equation | algebraic | | 126 |

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 stoichiometrix 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 | ϕ_{NK} | phi | probability function for reactions | secondaryState | | 129 |
| 163 | $nProd_{NS}$ | nProd | the species production term | secondaryState | $mol s^{-1}$ | 130 |

6 material

| | var | symbol | documentation | type | units | eqs |
|-----|---------------|------------|--|----------|-----------------------------|-------|
| 40 | λ_S | Mm | species molecular mass | constant | $kg\ mol^{-1}$ | |
| 112 | ξ | 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 | ρ_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 enthaply stream due to diffusion | transport | $kg m^2 s^{-3}$ | 71 |
| 97 | d_A | d | flow direction of convectional 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 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 |
| 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 |

Continued on next page

| | var | symbol | documentation | type | units | eqs |
|-----|------------------|--------------------|---|-------------------|------------------------|---|
| 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 |
| 99 | \hat{n}_{AS}^c | fnc_AS | molar convetional mass flow in the given stream | secondaryState | $mol s^{-1}$ | 74 |
| 100 | \hat{n}_{NS}^c | fnc | net molar convectional mass flow | secondaryState | $mol s^{-1}$ | 75 |
| 126 | ϕ | intensities | collected intensities | secondaryState | | 106 |
| 128 | n_N^t | nTotal | total number of moles | secondaryState | mol | 107 |
| 101 | \dot{n}_{NS} | dndt | differential species balance | diffState | $mol s^{-1}$ | 76 |
| 108 | \dot{H}_N | dHdt | differential enthalpy balance | diffState | $kg m^2 s^{-3}$ | 83 |
| 118 | \dot{U}_N^e | dUedt | Kirkhoff 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 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 | ξ | <code>_additive</code> | 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 | <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 |
|--|-----|--------|---------------|------|-------|-----|
|--|-----|--------|---------------|------|-------|-----|

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 | λ_S | _Mm | link variable Mm to interface material »> macroscopic | get | $kg\,mol^{-1}$ | 20 |
| 74 | ρ_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 |

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 | <i>additive</i> | <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 |
|----|--|--|----------|
| 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 |
| 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 |

Continued on next page

| no | equation | documentation | layer |
|----|--|--|-------------|
| 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 | $k_{xN}^c := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$ | convective mass conductivity in x-direction | material |
| 28 | $k_{yN}^c := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$ | convective mass conductivity in y-direction | material |
| 29 | $k_{zN}^c := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$ | 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 | $m_N := \lambda_S \overset{S \in NS}{\star} n_{NS}$ | total mass | macroscopic |

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| no | equation | documentation | layer |
|----|---|---|-------------|
| 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 | $E^a_{NK} := \text{Instantiate}(R.T_{NK}, \#)$ | Arrhenius activation energy | reactions |
| 42 | $K_{NK} := K^o_K \odot \exp((-E^a_{NK}) \cdot (R.T_{NK})^{-1})$ | 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 |
| 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 | $\hat{H}^d_A := \left(F_{NS,AS} \overset{NS}{\star} h_{NS} \right) \overset{S \in AS}{\star} \hat{n}^d_{AS}$ | 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 | $d_A := \text{sign} \left(F_{N,A} \overset{N}{\star} p_N \right)$ | flow direction of convectonal flow | macroscopic |
| 73 | $c_{AS} := (0.5 \cdot (F_{NS,AS} - d_A \odot F_{NS,AS})) \overset{NS}{\star} c_{NS}$ | concentration in convectonal 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 convectonal mass flow | macroscopic |

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|----|--|--|-------------|
| 76 | $\dot{n}_{NS} := \hat{n}_{NS}^c + \hat{n}_{NS}^d$ | differential species balance | macroscopic |
| 77 | $\hat{H}_{\text{A}}^c := \left(F_{NS,AS} \overset{NS}{\star} h_{NS} \right) \overset{S \in AS}{\star} \hat{n}_{AS}^c$ | convective enthalpy flow for given stream | macroscopic |
| 78 | $\hat{H}_{\text{N}}^c := F_{N,A} \overset{A}{\star} \hat{H}_{\text{A}}^c$ | net convectional enthalpy stream | macroscopic |
| 79 | $\hat{w}_{\text{A}} := \text{Instantiate}(\hat{H}_{\text{A}}^c, \#)$ | sample work stream | macroscopic |
| 80 | $\hat{w}_{\text{N}} := F_{N,A} \overset{A}{\star} \hat{w}_{\text{A}}$ | net work stream | macroscopic |
| 81 | $\hat{q}_{xA} := A_{yzN} \cdot k_{xN}^q \cdot D_{N,A} \overset{N}{\star} T_N$ | heat flow in x-direction for given stream | macroscopic |
| 82 | $\hat{q}_{\text{N}} := F_{N,A} \overset{A}{\star} \hat{q}_{xA}$ | net heat flow | macroscopic |
| 83 | $\dot{H}_{\text{N}} := \hat{H}_{\text{N}}^c + \hat{H}_{\text{N}}^d + \hat{q}_{\text{N}} + \hat{w}_{\text{N}}$ | differential enthalpy balance | macroscopic |
| 84 | $H_{\text{N}}^o := \text{Instantiate}(H_{\text{N}}, \#)$ | 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 | $H_{\text{N}} := \int_{t^o}^{t^e} \dot{H}_{\text{N}} dt$ | enthalpy | macroscopic |
| 88 | $\xi := \text{Instantiate}(\xi, \#)$ | fraction of additives | material |
| 89 | $I_{\text{N}} := \frac{dC_{\text{N}}}{dt}$ | electrical current definition | macroscopic |
| 91 | $R_{\text{N}}^e := (i_{\text{N}})^{-1} \cdot U e_{\text{N}}$ | electrical resistant | material |
| 92 | $R_{\text{N}}^e := \text{Instantiate}(R_{\text{N}}^e, \#)$ | electrical resistant | material |
| 93 | $k^{e,\xi}_{\text{N}} := (R_{\text{N}}^e)^{-1} \cdot \xi$ | simple model for the electrical conductivity as a function of the additive | material |

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|-----|--|---------------------------------|-------------|
| 95 | $Ue_N := (R^e_N)^{-1} \cdot I_N$ | electrical potential – voltage | macroscopic |
| 96 | $\dot{U}^e_N := 1 \cdot Ue_N$ | Kirchhoff first law | macroscopic |
| 97 | $\dot{U}^e_N := \text{Root}(Ue_N)$ | Kirchhoff first law | macroscopic |
| 98 | $\dot{U}^e_N := \text{Instantiate}(\dot{U}^e_N, 0)$ | Kirchhoff 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 |
| 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 |
| 113 | $\check{I}_N := I_N$ | measured current | control |
| 115 | $\check{U}^e_N := Ue_N$ | measured electrical potential | control |
| 116 | $\check{\xi} := \xi$ | measured additive fraction | control |

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|-----|---|--|-----------|
| 117 | $RComputed_N := (\check{I}_N)^{-1} \cdot \check{U}^e_N$ | measured resistance | control |
| 118 | $store := \text{MixedStack}(\check{I}_N, \check{U}^e_N, RComputed_N, \check{\xi})$ | quantities to be stored | control |
| 119 | $y^o_A := \text{Instantiate}(y^o_A, \#)$ | set point | control |
| 123 | $c_{NK,KS} := P_{NK} \cdot \left(P_{NS,KS} \overset{NS}{\star} c_{NS} \right)$ | var doc : | reactions |
| 124 | $c^o_{NK,KS} := \text{Instantiate}(c_{NK,KS}, \#)$ | norming concentration | reactions |
| 125 | $x_{NK,KS} := (c^o_{NK,KS})^{-1} \cdot c_{NK,KS}$ | 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 | $nProd_{NS} := V_N \overset{N}{\star} \left(P_{N,NK} \overset{NK}{\star} \left((K_{NK} \cdot \phi_{NK}) \cdot \left(P_{NS,KS} \overset{KS}{\star} N_{NK,KS} \right) \right) \right)$ | the species production term | reactions |

35 Interface Link Equation

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|----|--------------------------|--------------------|--------------------------|
| 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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|-----|--------------------------|--------------------|------------------------|
| 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 | $\xi := \xi$ | interface equation | material → control |

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|-----|-------------------|--------------------|------------------------|
| 105 | $T_N := T_N$ | interface equation | macroscopic control → |
| 112 | $additive := \xi$ | interface equation | material → macroscopic |
| 114 | $Ue_N := Ue_N$ | interface equation | macroscopic control → |