

1 Variables

2 root

| | var | symbol | documentation | type | units | eqs |
|----|------------------|-----------|---|---------|-------|-----|
| 19 | $A_{N,p,q}$ | A_Npq | mapping from inputs to outputs | network | | |
| 8 | $F^{sink}_{N,A}$ | F_NA_sink | incidence matrix NA sink | network | | |
| 18 | cz_I | cz_I | interface variable macro → control | network | | |
| 11 | $I_{t,u}$ | I_tu | identity mapping from <t> to <u> | network | | |
| 10 | $S_{I,q}$ | S_Iq | selection matrix interface to control output | network | | |
| 4 | $F^{sink}_{N,I}$ | F_NI_sink | incidence matrix NI sink | network | | |
| 14 | $S_{N,p,q}$ | S_Npu | selection matrix for stacker | network | | |
| 12 | $S_{A,p}$ | S_Ap | selection matrix interface species-related measures | network | | |
| 17 | cz_N | cz_N | output from control | network | | |
| 20 | $A_{N,t,u}$ | A_Ntu | mapping from input elements to outputs | network | | |
| 16 | mv_I | mv_I | interface variable macro → control | network | | |
| 9 | $S_{I,p}$ | S_Ip | selection matrix interface to control input | network | | |

Continued on next page

| | var | symbol | documentation | type | units | eqs |
|-----|--------------------|-------------|----------------------------------|---------|-------|-----|
| 7 | $F^{source}_{N,A}$ | F_NA_source | incidence matrix NA source | network | | |
| 6 | $F^{sink}_{A,I}$ | F_AI_sink | incidence matrix AI sink | network | | |
| 2 | $F_{N,A}$ | F | incidence matrix | network | | |
| 5 | $F^{source}_{A,I}$ | F_AI_source | incidence matrix AI source | network | | |
| 21 | $u_{N,t,u}$ | u_Ntu | input signal in control domain | network | | |
| 22 | $y_{N,t,u}$ | y_Ntu | output signal in control domain | network | | |
| 27 | $I_{N,A}$ | I_NA | identity mapping from <N> to <A> | network | | |
| 13 | $S_{I,q}$ | S_Aq | selection matrix arcs to outputs | network | | |
| 15 | $S_{N,q,t}$ | S_Nqt | selection matrix or splitter | network | | |
| 3 | $F^{source}_{N,I}$ | F_NI_source | incidence matrix NI source | network | | |
| 105 | t^o | to | starting time | frame | s | 4 |
| 1 | t | t | time | frame | s | |
| 106 | t^e | te | end time | frame | s | 5 |
| 107 | Δt | t_interval | time interval | frame | s | 6 |

Continued on next page

| | var | symbol | documentation | type | units | eqs |
|-----|-----|----------------|--------------------------|----------|-------|-----|
| 101 | # | value | numerical value | constant | | |
| 102 | 0 | zero | numerical value zero | constant | | 1 |
| 103 | 1 | one | numerical value one | constant | | 2 |
| 104 | 0.5 | oneHalf | numerical value one half | constant | | 3 |

3 physical

| | var | symbol | documentation | type | units | eqs |
|-----|-------------|--------------|--------------------------------------|----------|-------------------------------------|-----|
| 24 | r_{yN} | r_y | y-coordinate | frame | m | |
| 25 | r_{zN} | r_z | z-coordinate | frame | m | |
| 23 | r_{xN} | r_x | x-coordinate | frame | m | |
| 109 | S_N | S | fundamental state – internal entropy | state | $kg\,m^2\,K^{-1}\,s^{-2}$ | |
| 111 | $n_{N,S}$ | n | fundamental state – molar mass | state | mol | 93 |
| 144 | C_N | C | fundamental state – charge | state | $A\,s$ | |
| 108 | U_N | U | fundamental state – internal energy | state | $kg\,m^2\,s^{-2}$ | |
| 137 | m_N | m | mass | state | kg | 30 |
| 110 | V_N | V | volume | state | m^3 | 7 |
| 122 | k^B | Boltz | Boltzmann constant | constant | $kg\,m^2\,K^{-1}\,s^{-2}$ | |
| 123 | R | R | gas constant | constant | $kg\,m^2\,mol^{-1}\,K^{-1}\,s^{-2}$ | 17 |
| 132 | λ_S | Mm | molecular masses | constant | $kg\,mol^{-1}$ | |
| 121 | N^A | Avo | Avogadro constant | constant | mol^{-1} | |

Continued on next page

| | var | symbol | documentation | type | units | eqs |
|-----|---|------------|-------------------------|----------------|--------------|-----------|
| 149 | A_{xzN} A_{yzN} A_{xyN} ρ_N | Axz | cross sectional are xz | secondaryState | m^2 | 41 |
| 150 | | Ayz | cross sectional area yz | secondaryState | m^2 | 42 |
| 148 | | Axy | cross sectional area xy | secondaryState | m^2 | 40 |
| 143 | | rho | density | secondaryState | $kg\,m^{-3}$ | 36 |

4 macroscopic

| | var | symbol | documentation | type | units | eqs |
|-----|--------------------|--------------|--|-----------|-------------------|-----------|
| 210 | \dot{q}_{zN} | aq_z | accumulation due to heat flow in z-direction | transport | $kg\,m^2\,s^{-3}$ | 105 |
| 207 | \dot{H}_z^d | aHnd_z | accumulation of enthalpy due to diffusional mass flow in z-direction | transport | $kg\,m^2\,s^{-3}$ | 102 |
| 156 | $\hat{n}_{zA,S}^d$ | fnd_z | diffusion flow in z-direction | transport | $mol\,s^{-1}$ | 48 91 |
| 160 | $\hat{n}_{xA,S}^c$ | fnc_x | molar convective flow in x-direction | transport | $mol\,s^{-1}$ | 52 |
| 211 | \hat{w}_A | fw | a fixed work flow to start with | transport | $kg\,m^2\,s^{-3}$ | 106 |
| 195 | $\dot{n}_{xN,S}^d$ | and_x | accumulation due to diffusion in x-direction | transport | $mol\,s^{-1}$ | 88 |
| 159 | \hat{V}_A | fV | volumetric flow in x-direction | transport | $m^3\,s^{-1}$ | 51 142 |
| 194 | $\dot{n}_{xN,S}^c$ | anc_x | accumulation of molar mass due to convection | transport | $mol\,s^{-1}$ | 87 |
| 213 | $\dot{n}_{zN,S}^d$ | and_z | accumulation due to diffusion in z-direction | transport | $mol\,s^{-1}$ | 108 |
| 151 | \hat{q}_{xA} | fq_x | heat flow in x-direction | transport | $kg\,m^2\,s^{-3}$ | 43 |
| 204 | \dot{H}_{xN}^c | aHnc_x | accumulation of enthalpy due to convective mass flow in x-direction | transport | $kg\,m^2\,s^{-3}$ | 99 |
| 243 | y^{p+}_A | y_p_positive | link variable y p positive to interface macroscopic | transport | | 141 |
| 208 | \dot{q}_{xN} | aq_x | accumulation due to heat flow in x-direction | transport | $kg\,m^2\,s^{-3}$ | 103 |

Continued on next page

| | var | symbol | documentation | type | units | eqs |
|-----|-------------------------|-----------|--|------------|--------------------|-------|
| 158 | $c_{A,S}$ | c_AS | concentration in convective event-dynamic flow | transport | $m^{-3} mol$ | 50 |
| 234 | $\hat{m}_{N,A}$ | fm | convective mass flow | transport | $kg s^{-1}$ | 133 |
| 209 | \dot{q}_{yN} | aq_y | accumulation due to heat flow in y-direction | transport | $kg m^2 s^{-3}$ | 104 |
| 214 | \dot{w}_N | aw | accumulation of enthalpy due to work flow | transport | $kg m^2 s^{-3}$ | 109 |
| 155 | $\hat{n}_{yA,S}^d$ | fnd_y | diffusion flow in y-direction | transport | $mol s^{-1}$ | 47 90 |
| 154 | $\hat{n}_{xA,S}^d$ | fnd_x | diffusion flow in x-direction | transport | $mol s^{-1}$ | 46 89 |
| 212 | $\dot{n}_{yN,S}^d$ | and_y | accumulation due to diffusion in y-direction | transport | $mol s^{-1}$ | 107 |
| 206 | \dot{H}_{yN}^d | aHnd_y | accumulation of enthalpy due to diffusional mass flow in y-direction | transport | $kg m^2 s^{-3}$ | 101 |
| 152 | \hat{q}_{yA} | fq_y | heat flow in y-direction | transport | $kg m^2 s^{-3}$ | 44 |
| 157 | d_A | d | flow direction of convective flow | transport | | 49 |
| 153 | \hat{q}_{zA} | fq_z | heat flow in z-direction | transport | $kg m^2 s^{-3}$ | 45 |
| 205 | \dot{H}_{xN}^d | aHnd_x | accumulation of enthalpy due to diffusional mass flow in x-direction | transport | $kg m^2 s^{-3}$ | 100 |
| 188 | k_{zA}^q | kqA_z | thermal conductivity in arc and z-direction | properties | $kg K^{-1} s^{-3}$ | 81 |
| 192 | $\hat{k}_{zA}^{d,Fick}$ | kdAFick_z | Fick diffusivity in arc and z-direction | properties | ms^{-1} | 85 |

Continued on next page

| | var | symbol | documentation | type | units | eqs |
|-----|---------------------------|-------------|---|------------|--------------------------|-----|
| 182 | $k_{zA,S}^d$ | kdA_z | diffusivity in arc and z-direction | properties | $kg^{-1} m^{-4} mol^2 s$ | 75 |
| 191 | $\hat{k}_{yA,S}^{d,Fick}$ | kdAFick_y | Fick diffusivity in arc and y-direction | properties | ms^{-1} | 84 |
| 186 | k_{xA}^q | kqA_x | thermal conductivity in arc and x-direction | properties | $kg K^{-1} s^{-3}$ | 79 |
| 189 | ρ_A | rhoA | density in arc | properties | $kg m^{-3}$ | 82 |
| 193 | $h_{A,S}$ | hA | partial molar enthalpies in arc | properties | $kg m^2 mol^{-1} s^{-2}$ | 86 |
| 183 | k_{xA}^c | kcA_x | convective mass conductivity in arc and x direction | properties | $m^{-1} s$ | 76 |
| 184 | k_{yA}^c | kcA_y | convective mass conductivity in arc and y-direction | properties | $m^{-1} s$ | 77 |
| 180 | $k_{xA,S}^d$ | kdA_x | diffusivity in arc and x-direction | properties | $kg^{-1} m^{-4} mol^2 s$ | 73 |
| 219 | R_N^e | elResistant | electrical resistant | properties | $kg m^2 A^{-2} s^{-3}$ | 115 |
| 190 | $\hat{k}_{xA,S}^{d,Fick}$ | kdAFick_x | Fick's diffusivity in arc and x-direction | properties | ms^{-1} | 83 |
| 187 | k_{yA}^q | kqA_y | thermal conductivity in arc and y-direction | properties | $kg K^{-1} s^{-3}$ | 80 |
| 185 | k_{zA}^c | kcA_z | convecive mass conductivity in arc and y-direction | properties | $m^{-1} s$ | 78 |
| 181 | $k_{yA,S}^d$ | kdA_y | diffusivity in arc and y-direction | properties | $kg^{-1} m^{-4} mol^2 s$ | 74 |
| 116 | A_N | A | Helmholtz energy | state | $kg m^2 s^{-2}$ | 12 |

Continued on next page

| | var | symbol | documentation | type | units | eqs |
|-----|---------------|-----------------|---|----------------|-----------------------------|-----------|
| 203 | $n^o_{N,S}$ | no | initial mass | state | mol | 98 |
| 115 | H_N | H | Enthalpy | state | $kg\,m^2\,s^{-2}$ | 11 112 |
| 216 | H^o_N | Ho | initial enthalpy | state | $kg\,m^2\,s^{-2}$ | 111 |
| 117 | G_N | G | Gibbs free energy | state | $kg\,m^2\,s^{-2}$ | 13 |
| 217 | U^e_N | Ue | electrical potential – voltage | effort | $kg\,m^2\,A^{-1}\,s^{-3}$ | 113 |
| 161 | $\mu^o_{N,S}$ | chemPotStandard | instantiating standard chemical potential | effort | $kg\,m^2\,mol^{-1}\,s^{-2}$ | 53 |
| 112 | p_N | p | thermodynamic pressure | effort | $kg\,m^{-1}\,s^{-2}$ | 8 |
| 114 | $\mu_{N,S}$ | chemPot | chemical potential | effort | $kg\,m^2\,mol^{-1}\,s^{-2}$ | 10 54 |
| 113 | T_N | T | temperature | effort | K | 9 121 |
| 120 | v_{zN} | v_z | velocity in z-direction | secondaryState | ms^{-1} | 16 |
| 140 | $x_{N,S}$ | x | mole fraction | secondaryState | | 33 |
| 138 | $c_{N,S}$ | c | molar concentration | secondaryState | $m^{-3}\,mol$ | 31 |
| 142 | c_{VN} | cV | specific heat capacity at constant volume | secondaryState | $m^2\,K^{-1}\,s^{-2}$ | 35 |
| 119 | v_{yN} | v_y | velocity in y-direction | secondaryState | ms^{-1} | 15 |

Continued on next page

| | var | symbol | documentation | type | units | eqs |
|-----|-------------------|-----------------------|---|-------------------|-----------------------------|---|
| 136 | $h_{N,S}$ | h | partial molar enthalpies | secondaryState | $kg\,m^2\,mol^{-1}\,s^{-2}$ | 29 |
| 118 | v_{xN} | v_x | velocity in x-direction | secondaryState | ms^{-1} | 14 |
| 222 | T^{ref}_N | T_ref | reference temperature | secondaryState | K | 119 |
| 141 | c_{pN} | cp | specific heat capacity at constant pressure | secondaryState | $m^2\,K^{-1}\,s^{-2}$ | 34 120 |
| 124 | C_{pN} | Cp | total heat capacity at constant pressure | secondaryState | $kg\,m^2\,K^{-1}\,s^{-2}$ | 18 117 |
| 125 | C_{VN} | CV | total heat capacity at constant volume | secondaryState | $kg\,m^2\,K^{-1}\,s^{-2}$ | 19 |
| 139 | n^t_N | nt | total number of moles | secondaryState | mol | 32 |
| 202 | $\tilde{n}_{N,S}$ | np | link variable np to interface macroscopic | conversion | $m^{-3}\,mol\,s^{-1}$ | 97 |
| 196 | $\dot{n}_{N,S}$ | an | differential mass balance without reaction | diffState | $mol\,s^{-1}$ | 92 |
| 220 | \dot{U}^e_A | dUe | Kirkhoffs first law | diffState | $kg\,m^2\,A^{-1}\,s^{-3}$ | 116 |
| 215 | \dot{H}_N | dH | accumulation of enthalpy | diffState | $kg\,m^2\,s^{-3}$ | 110 |
| 218 | I^e_N | current | current definition | internalTransport | A | 114 |
| 224 | \bar{T}_N | T_meas | temperature measurement | observation | | 123 |
| 223 | T^n_N | T_meas_norming | value to norm measurement of temperature | observation | K | 122 |

5 reactions

| | var | symbol | documentation | type | units | eqs |
|-----|---------------------|--------------------|--|----------------|-----------------------------|-----|
| 197 | E^a_K | Ea | Arrhenius activation energy | constant | $kg\ m^2\ mol^{-1}\ s^{-2}$ | |
| 26 | $N_{S,K}$ | N | stoichiometric matrix | constant | | |
| 198 | K^o_K | Ko | Arrhenius frequency factor | constant | $m^{-3}\ mol\ s^{-1}$ | |
| 167 | $T_{N,p}$ | T | link variable T to interface reactions | effort | K | 60 |
| 165 | $x_{N,S,p}$ | x | link variable x to interface reactions | secondaryState | | 58 |
| 163 | $c_{N,S,p}$ | c | link variable c to interface reactions | secondaryState | $m^{-3}\ mol$ | 56 |
| 168 | $f_{N,S,K,p}$ | factor | factor for probability computation | conversion | | 61 |
| 200 | $\tilde{n}_{N,S,q}$ | np | production from reaction set | conversion | $m^{-3}\ mol\ s^{-1}$ | 95 |
| 199 | $K_{N,K,p}$ | K | Arrhenius reaction "constant" | conversion | $m^{-3}\ mol\ s^{-1}$ | 94 |
| 169 | $\xi_{N,K,p}$ | probability | probability of reaction to take place | conversion | | 62 |

6 control

| | var | symbol | documentation | type | units | eqs |
|-----|-------------------|---------------|---|-----------|-------|-----|
| 239 | $y^{p+}_{N,q}$ | y_p_positive | positive signal only | algebraic | | 137 |
| 231 | $e_{N,p}$ | control_error | control error in normed temperature | algebraic | | 130 |
| 237 | $p_{N,p,q}$ | p | controller gain | algebraic | | |
| 227 | $T_{setpointN,p}$ | T_setpoint | setpoint for temperatue | algebraic | | 126 |
| 226 | $\bar{T}_{N,p}$ | T_meas | link variable T meas to interface control | algebraic | | 125 |
| 238 | $y^p_{N,q}$ | y_p_control | output of proportional controller | algebraic | | 136 |

7 control-macroscopic

| | var | symbol | documentation | type | units | eqs |
|-----|---------------|----------------------------|---|------|-------|-----|
| 242 | $_{y^{p+}_I}$ | <code>_y_p_positive</code> | link variable y p positive to interface control »> macroscopic with source:arc | get | | 140 |

8 reactions-macroscopic

| | var | symbol | documentation | type | units | eqs |
|-----|------------|------------|---|------|---------------------|-----|
| 201 | $_{npI,S}$ | _np | link variable np to interface reactions »> macroscopic with source:node | get | $m^{-3} mol s^{-1}$ | 96 |

9 macroscopic-control

| | var | symbol | documentation | type | units | eqs |
|-----|---------------|----------------|--|------|-------|-----|
| 225 | $_T_meas_I$ | _T_meas | link variable T meas to interface macroscopic »> control with source:node | get | | 124 |

10 macroscopic-reactions

| | var | symbol | documentation | type | units | eqs |
|-----|------|--------|--|------|--------------|-----|
| 162 | $_c$ | $_c$ | link variable c to interface macroscopic »> reactions with source:node | get | $m^{-3} mol$ | 55 |
| 166 | $_T$ | $_T$ | link variable T to interface macroscopic »> reactions with source:node | get | K | 59 |
| 164 | $_x$ | $_x$ | link variable x to interface macroscopic »> reactions with source:node | get | | 57 |

11 Equations

12 Generic

| no | equation | documentation | layer |
|----|--|--------------------------|-------------|
| 1 | $0 := \text{Instantiate}(\#, \#)$ | numerical value zero | root |
| 2 | $1 := \text{Instantiate}(\#, \#)$ | numerical value one | 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 | $\Delta t := \text{Instantiate}(t, \#)$ | time interval | root |
| 7 | $V_N := r_{xN} \cdot r_{yN} \cdot r_{zN}$ | volume | physical |
| 8 | $p_N := \frac{\partial U_N}{\partial V_N}$ | thermodynamic pressure | physical |
| 9 | $T_N := \frac{\partial U_N}{\partial S_N}$ | temperature | macroscopic |
| 10 | $\mu_{N,S} := \frac{\partial U_N}{\partial n_{N,S}}$ | chemical potential | macroscopic |
| 11 | $H_N := U_N - p_N \cdot V_N$ | Enthalpy | macroscopic |
| 12 | $A_N := U_N - T_N \cdot S_N$ | Helmholtz energy | macroscopic |
| 13 | $G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$ | Gibbs free energy | macroscopic |
| 14 | $v_{xN} := \frac{\partial r_{xN}}{\partial t}$ | velocity in x-direction | macroscopic |
| 15 | $v_{yN} := \frac{\partial r_{yN}}{\partial t}$ | velocity in y-direction | macroscopic |
| 16 | $v_{zN} := \frac{\partial r_{zN}}{\partial t}$ | velocity in z-direction | macroscopic |

Continued on next page

| no | equation | documentation | layer |
|----|--|---|-------------|
| 17 | $R := N^A \cdot k^B$ | gas constant | physical |
| 18 | $C_{pN} := \frac{\partial H_N}{\partial T_N}$ | total heat capacity at constant pressure | macroscopic |
| 19 | $C_{VN} := \frac{\partial U_N}{\partial T_N}$ | total heat capacity at constant volume | macroscopic |
| 29 | $h_{N,S} := H_N \cdot (n_{N,S})^{-1}$ | partial molar enthalpies | macroscopic |
| 30 | $m_N := \lambda_S^S \star n_{N,S}$ | mass | macroscopic |
| 31 | $c_{N,S} := (V_N)^{-1} \cdot n_{N,S}$ | molar concentration | macroscopic |
| 32 | $n_N^t := \text{reduceSum}(n_{N,S}, S)$ | total number of moles | macroscopic |
| 33 | $x_{N,S} := (n_N^t)^{-1} \cdot n_{N,S}$ | mole fraction | macroscopic |
| 34 | $c_{pN} := C_{pN} \cdot (m_N)^{-1}$ | specific heat capacity at constant pressure | physical |
| 35 | $c_{VN} := C_{VN} \cdot (m_N)^{-1}$ | specific heat capacity at constant volume | macroscopic |
| 36 | $\rho_N := (V_N)^{-1} \cdot m_N$ | density | physical |
| 40 | $A_{xyN} := r_{xN} \cdot r_{yN}$ | cross sectional area xy | physical |
| 41 | $A_{xzN} := r_{xN} \cdot r_{zN}$ | cross sectional area xz | physical |
| 42 | $A_{yzN} := r_{yN} \cdot r_{zN}$ | cross sectional area yz | physical |
| 43 | $\hat{q}_{xA} := k_{xA}^q \cdot A_{yzN} \cdot F_{N,A} \stackrel{N}{\star} T_N$ | heat flow in x-direction | macroscopic |
| 44 | $\hat{q}_{yA} := k_{yA}^q \cdot A_{xzN} \cdot F_{N,A} \stackrel{N}{\star} T_N$ | heat flow in y-direction | macroscopic |
| 45 | $\hat{q}_{zA} := k_{zA}^q \cdot A_{xyN} \cdot F_{N,A} \stackrel{N}{\star} T_N$ | heat flow in z-direction | macroscopic |

Continued on next page

| no | equation | documentation | layer |
|----|---|--|-------------|
| 46 | $\hat{n}_{xA,S}^d := \hat{k}_x^{d,Fick}{}_{A,S} \cdot A_{yzN} \cdot F_{N,A} \star^N c_{N,S}$ | Fick diffusion flow in x-direction | macroscopic |
| 47 | $\hat{n}_{yA,S}^d := \hat{k}_y^{d,Fick}{}_{A,S} \cdot A_{xzN} \cdot F_{N,A} \star^N c_{N,S}$ | Fick diffusion flow in y-direction | macroscopic |
| 48 | $\hat{n}_{zA,S}^d := \hat{k}_z^{d,Fick}{}_{A,S} \cdot (A_{xyN} \cdot F_{N,A}) \star^N c_{N,S}$ | Fick diffusion flow in z-direction | macroscopic |
| 49 | $d_A := \mathbf{sign} \left(F_{N,A} \star^N p_N \right)$ | flow direction of convective flow | macroscopic |
| 50 | $c_{A,S} := (0.5 \cdot (F_{N,A} - d_A \cdot F_{N,A})) \star^N c_{N,S}$ | concentration in convective event-dynamic flow | macroscopic |
| 51 | $\hat{V}_A := (\rho_A)^{-1} \cdot k_{xA}^c \cdot A_{yzN} \cdot F_{N,A} \star^N p_N$ | volumetric flow in x-direction | macroscopic |
| 52 | $\hat{n}_{xA,S}^c := \hat{V}_A \cdot c_{A,S}$ | molar convective flow in x-direction | macroscopic |
| 53 | $\mu_{N,S}^o := \mathbf{Instantiate}(\mu_{N,S}, \#)$ | instantiating standard chemical potential | macroscopic |
| 54 | $\mu_{N,S} := \mu_{N,S}^o + R \cdot T_N \cdot \mathbf{ln}(x_{N,S})$ | chemical potential standard model with mole fraction | macroscopic |
| 61 | $f_{N,S,K,p} := x_{N,S,p}^{((N_S, \kappa))}$ | factor for probability computation | reactions |
| 62 | $\xi_{N,K,p} := \prod_S f_{N,S,K,p}$ | probability of reaction to take place | reactions |
| 73 | $k_{xA,S}^d := I_{N,A} \star^N \left((\mu_{N,S})^{-1} \cdot \left(v_{xN} \cdot \left((V_N)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \right) \right) \right)$ | diffusivity in arc and x-direction | macroscopic |
| 74 | $k_{yA,S}^d := I_{N,A} \star^N \left((\mu_{N,S})^{-1} \cdot \left(v_{yN} \cdot \left((V_N)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \right) \right) \right)$ | diffusivity in arc and y-direction | macroscopic |
| 75 | $k_{zA,S}^d := I_{N,A} \star^N \left((\mu_{N,S})^{-1} \cdot \left(v_{zN} \cdot \left((V_N)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \right) \right) \right)$ | diffusivity in arc and z-direction | macroscopic |
| 76 | $k_{xA}^c := I_{N,A} \star^N \left(\left(\lambda_S \star^S (\mu_{N,S})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN} \right)$ | convective mass conductivity in arc and x direction | macroscopic |
| 77 | $k_{yA}^c := I_{N,A} \star^N \left(\left(\lambda_S \star^S (\mu_{N,S})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN} \right)$ | convective mass conductivity in arc and y-direction | macroscopic |

Continued on next page

| no | equation | documentation | layer |
|----|--|---|-------------|
| 78 | $k_{zA}^c := I_{N,A} \overset{N}{\star} \left(\left(\lambda_S \overset{S}{\star} (\mu_{N,S})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN} \right)$ | convective mass conductivity in arc and y-direction | macroscopic |
| 79 | $k_{xA}^q := I_{N,A} \overset{N}{\star} \left((V_N)^{-1} \cdot C_{pN} \cdot v_{xN} \right)$ | thermal conductivity in arc and x-direction | macroscopic |
| 80 | $k_{yA}^q := I_{N,A} \overset{N}{\star} \left((V_N)^{-1} \cdot C_{pN} \cdot v_{yN} \right)$ | thermal conductivity in arc and y-direction | macroscopic |
| 81 | $k_{zA}^q := I_{N,A} \overset{N}{\star} \left((V_N)^{-1} \cdot C_{pN} \cdot v_{zN} \right)$ | thermal conductivity in arc and z-direction | macroscopic |
| 82 | $\rho_A := I_{N,A} \overset{N}{\star} \rho_N$ | density in arc | macroscopic |
| 83 | $\hat{k}_x^{d,Fick}{}_{A,S} := I_{N,A} \overset{N}{\star} \left(v_{xN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$ | Fick's diffusivity in arc and x-direction | macroscopic |
| 84 | $\hat{k}_y^{d,Fick}{}_{A,S} := I_{N,A} \overset{N}{\star} \left(v_{yN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$ | Fick diffusivity in arc and y-direction | macroscopic |
| 85 | $\hat{k}_z^{d,Fick}{}_{A,S} := I_{N,A} \overset{N}{\star} \left(v_{zN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$ | Fick diffusivity in arc and z-direction | macroscopic |
| 86 | $h_{A,S} := I_{N,A} \overset{N}{\star} h_{N,S}$ | partial molar enthalpies in arc | macroscopic |
| 87 | $\dot{n}_{xN,S}^c := F_{N,A} \overset{A}{\star} \hat{n}_{xA,S}^c$ | accumulation of molar mass due to convection | macroscopic |
| 88 | $\dot{n}_{xN,S}^d := F_{N,A} \overset{A}{\star} \hat{n}_{xA,S}^d$ | accumulation due to diffusion in x-direction | macroscopic |
| 89 | $\hat{n}_{xA,S}^d := k_{xA,S}^d \cdot (A_{yzN} \cdot F_{N,A}) \overset{N}{\star} \mu_{N,S}$ | Fick diffusion flow in x-direction | macroscopic |
| 90 | $\hat{n}_{yA,S}^d := k_{yA,S}^d \cdot (A_{yzN} \cdot F_{N,A}) \overset{N}{\star} \mu_{N,S}$ | Fick diffusion flow in y-direction | macroscopic |
| 91 | $\hat{n}_{zA,S}^d := k_{zA,S}^d \cdot (A_{xyzN} \cdot F_{N,A}) \overset{N}{\star} \mu_{N,S}$ | mass diffusion flow in z-direction | macroscopic |
| 92 | $\dot{n}_{N,S} := \dot{n}_{xN,S}^c + \dot{n}_{xN,S}^d + V_N \cdot \tilde{n}_{N,S}$ | differential mass balance without reaction | macroscopic |

Continued on next page

| no | equation | documentation | layer |
|-----|---|--|-------------|
| 93 | $n_{N,S} := \int_{t^o}^{t^e} \dot{n}_{N,S} dt + n_{N,S}^o$ | fundamental state – molar mass | macroscopic |
| 94 | $K_{N,K,p} := K_K^o \cdot \mathbf{exp} \left((-E_K^a) \cdot (R \cdot T_{N,p})^{-1} \right)$ | Arrhenius reaction "constant" | reactions |
| 95 | $\tilde{n}_{N,S,q} := A_{N,p,q} \overset{p}{\star} \left(N_{S,K} \overset{K}{\star} (K_{N,K,p} \cdot \xi_{N,K,p}) \right)$ | production from reaction set | reactions |
| 98 | $n_{N,S}^o := \mathbf{Instantiate}(n_{N,S}, \#)$ | initial mass | macroscopic |
| 99 | $\dot{H}_{xN}^c := F_{N,A} \overset{A}{\star} \left(\hat{n}_{xA,S}^S \star h_{N,S} \right)$ | enthalpy accumulation due to convective flow in x-direction | macroscopic |
| 100 | $\dot{H}_{xN}^d := F_{N,A} \overset{A}{\star} \left(\hat{n}_{xA,S}^S \star h_{N,S} \right)$ | accumulation of enthalpy due to diffusional mass flow in x-direction | macroscopic |
| 101 | $\dot{H}_{yN}^d := F_{N,A} \overset{A}{\star} \left(\hat{n}_{yA,S}^S \star h_{N,S} \right)$ | accumulation of enthalpy due to diffusional mass flow in y-direction | macroscopic |
| 102 | $\dot{H}_{zN}^d := F_{N,A} \overset{A}{\star} \left(\hat{n}_{zA,S}^S \star h_{N,S} \right)$ | accumulation of enthalpy due to diffusional mass flow in z-direction | macroscopic |
| 103 | $\dot{q}_{xN} := F_{N,A} \overset{A}{\star} \hat{q}_{xA}$ | accumulation due to heat flow in x-direction | macroscopic |
| 104 | $\dot{q}_{yN} := F_{N,A} \overset{A}{\star} \hat{q}_{yA}$ | accumulation due to heat flow in y-direction | macroscopic |
| 105 | $\dot{q}_{zN} := F_{N,A} \overset{A}{\star} \hat{q}_{zA}$ | accumulation due to heat flow in z-direction | macroscopic |
| 106 | $\hat{w}_A := \mathbf{Instantiate}(\hat{q}_{xA}, \#)$ | a fixed work flow to start with | macroscopic |
| 107 | $\dot{n}_{yN,S}^d := F_{N,A} \overset{A}{\star} \hat{n}_{yA,S}^d$ | accumulation due to diffusion in y-direction | macroscopic |
| 108 | $\dot{n}_{zN,S}^d := F_{N,A} \overset{A}{\star} \hat{n}_{zA,S}^d$ | accumulation due to diffusion in z-direction | macroscopic |

Continued on next page

| no | equation | documentation | layer |
|-----|---|--|-------------|
| 109 | $\dot{w}_N := F_{N,A} \overset{A}{\star} \hat{w}_A$ | accumulation of enthalpy due to work flow | macroscopic |
| 110 | $\dot{H}_N := \dot{H}_{xN}^c + \dot{H}_{xN}^d + \dot{H}_{yN}^d + \dot{H}_{zN}^d + \dot{q}_{xN} + \dot{q}_{yN} + \dot{q}_{zN} + \dot{w}_N$ | accumulation of enthalpy | macroscopic |
| 111 | $H_N^o := \mathbf{Instantiate}(H_N, \#)$ | initial enthalpy | macroscopic |
| 112 | $H_N := \int_{t^o}^{t^e} \dot{H}_N dt + H_N^o$ | Enthalpy | macroscopic |
| 113 | $U_N^e := (C_N)^{-1} \cdot U_N$ | electrical potential – voltage | macroscopic |
| 114 | $I_N^e := \frac{dC_N}{dt}$ | current definition | macroscopic |
| 115 | $R_N^e := (I_N^e)^{-1} \cdot U_N^e$ | electrical resistant | macroscopic |
| 116 | $\dot{U}_N^e := F_{N,A} \overset{A}{\star} (R_N^e \cdot I_N^e)$ | Kirkhoffs first law | macroscopic |
| 117 | $C_{pN} := m_N \cdot c_{pN}$ | total heat capacity at constant pressure | macroscopic |
| 119 | $T_N^{ref} := \mathbf{Instantiate}(T_N, \#)$ | reference temperature | macroscopic |
| 120 | $c_{pN} := \mathbf{Instantiate}(c_{pN}, \#)$ | constant specific heat capacity at constant pressure | macroscopic |
| 121 | $T_N := H_N \cdot (C_{pN})^{-1} + T_N^{ref}$ | temperature from constant heat capacity | macroscopic |
| 122 | $T_N^n := \mathbf{Instantiate}(T_N, \#)$ | value to norm measurement of temperature | macroscopic |
| 123 | $\bar{T}_N := T_N \cdot (T_N^n)^{-1}$ | temperature measurement | macroscopic |
| 126 | $T_{setpointN,p} := \mathbf{Instantiate}(\bar{T}_{N,p}, \#)$ | setpoint for temperature | control |
| 130 | $e_{N,p} := T_{setpointN,p} - \bar{T}_{N,p}$ | control error in normed temperature | control |

Continued on next page

| no | equation | documentation | layer |
|-----|---|---|-------------|
| 133 | $\hat{m}_{N,A} := \hat{V}_A \cdot \rho_N$ | convective mass flow | macroscopic |
| 136 | $y^p_{N,q} := (-p_{N,p,q}) \overset{p}{\star} e_{N,p}$ | output of proportional controller | control |
| 137 | $y^{p+}_{N,q} := \mathbf{max}(0 \cdot y^p_{N,q}, y^p_{N,q})$ | positive signal only | control |
| 142 | $\hat{V}_A := y^{p+}_A \cdot (\rho_A)^{-1} \cdot k_{xA}^c \cdot A_{yzN} \cdot F_{N,A} \overset{N}{\star} p_N$ | controlled volumetric flow in x-direction | macroscopic |

13 Interface Link Equation

| no | equation | documentation | layer |
|-----|---|--------------------|--------------------------|
| 55 | $_c_{I,S} := F^{source}_{N,I} \star^N c_{N,S}$ | interface equation | macroscopic -> reactions |
| 56 | $c_{N,S,p} := (F^{sink}_{N,I} \cdot _c_{I,S}) \star^I S_{I,p}$ | interface equation | reactions |
| 57 | $_x_{I,S} := F^{source}_{N,I} \star^N x_{N,S}$ | interface equation | macroscopic -> reactions |
| 58 | $x_{N,S,p} := (F^{sink}_{N,I} \cdot _x_{I,S}) \star^I S_{I,p}$ | interface equation | reactions |
| 59 | $_T_I := F^{source}_{N,I} \star^N T_N$ | interface equation | macroscopic -> reactions |
| 60 | $T_{N,p} := (F^{sink}_{N,I} \cdot _T_I) \star^I S_{I,p}$ | interface equation | reactions |
| 96 | $_np_{I,S} := \text{reduceSum} \left(\left(\left(F^{source}_{N,I} \star^N \tilde{n}_{N,S,q} \right) \cdot S_{I,q} \right), q \right)$ | interface equation | reactions -> macroscopic |
| 97 | $\tilde{n}_{N,S} := F^{source}_{N,I} \star^I _np_{I,S}$ | interface equation | macroscopic |
| 124 | $_T_meas_I := F^{source}_{N,I} \star^N \bar{T}_N$ | interface equation | macroscopic -> control |
| 125 | $\bar{T}_{N,p} := (F^{sink}_{N,I} \cdot _T_meas_I) \star^I S_{I,p}$ | interface equation | control |
| 140 | $_y^{p+}_I := \text{reduceSum} \left(\left(\left(F^{source}_{N,I} \star^N y^{p+}_{N,q} \right) \cdot S_{I,q} \right), q \right)$ | interface equation | control -> macroscopic |
| 141 | $y^{p+}_A := F^{source}_{A,I} \star^I _y^{p+}_I$ | interface equation | macroscopic |