### 1 Variables

### 2 root

|    | var         | symbol     | documentation                         | type       | units | eqs |
|----|-------------|------------|---------------------------------------|------------|-------|-----|
| 10 | $F_{N,A}$   | F          | basic directed graph incidence matrix | network    |       |     |
| 48 | $I_{NAN,A}$ | I_N_A      | project node on arc                   | projection |       |     |
| 7  | $\Delta t$  | t_interval | time interval                         | frame      | s     | 5   |
| 9  | $\Delta$    | pulse      | pulse of length time interval         | frame      |       | 7   |
| 4  | t           | t          | time                                  | frame      | s     |     |
| 5  | $t^o$       | to         | time zero                             | frame      | s     | 3   |
| 6  | $t^e$       | te         | time end                              | frame      | s     | 4   |
| 3  | 0           | zero       | numerical value zero                  | constant   |       | 2   |
| 8  | 0.5         | onehalf    | numerical one half                    | constant   |       | 6   |
| 1  | #           | value      | numerical value                       | constant   |       |     |
| 2  | 1           | one        | numerical one                         | constant   |       | 1   |

# 3 physical

|    | var         | symbol  | documentation                       | type           | units                               | eqs       |
|----|-------------|---------|-------------------------------------|----------------|-------------------------------------|-----------|
| 14 | $r_{zN}$    | r_z     | z-direction                         | frame          | m                                   | 10        |
| 11 | $\ell_N$    | 1       | length                              | frame          | m                                   |           |
| 12 | $r_{xN}$    | r_x     | x-direction                         | frame          | m                                   | 8         |
| 13 | $r_{yN}$    | r_y     | y-direction                         | frame          | m                                   | 9         |
| 17 | $S_N$       | S       | fundamental state - entropy         | state          | $kg  m^2  K^{-1}  s^{-2}$           |           |
| 23 | $A_N$       | A       | Helmholts energy                    | state          | $kgm^2s^{-2}$                       | 17        |
| 16 | $U_N$       | U       | fundamental state - internal energy | state          | $kgm^2s^{-2}$                       |           |
| 24 | $G_N$       | G       | Gibbs free energy                   | state          | $kgm^2s^{-2}$                       | 18        |
| 22 | $H_N$       | Н       | Enthalpy                            | state          | $kgm^2s^{-2}$                       | 15        |
| 18 | $n_{N,S}$   | n       | fundamental state - molar mass      | state          | mol                                 |           |
| 15 | $V_N$       | V       | fundamental state - volume          | state          | $m^3$                               | 11        |
| 25 | $C_N$       | С       | fundamental state - charge          | state          | As                                  |           |
| 33 | $B_N$       | Boltz   | Boltzmann constant                  | constant       | $kg  m^2  K^{-1}  s^{-2}$           | 24        |
| 32 | $A^v$       | Av      | Avogadro number                     | constant       | $mol^{-1}$                          |           |
| 34 | $R_N$       | R       | Gas constant                        | constant       | $kg  m^2  mol^{-1}  K^{-1}  s^{-1}$ | $^2$ $25$ |
| 21 | $\mu_{N,S}$ | chemPot | chemical potential                  | effort         | $kg  m^2  mol^{-1}  s^{-2}$         | 14        |
| 19 | $T_N$       | Т       | temperature                         | effort         | K                                   | 16        |
| 20 | $p_N$       | p       | pressure                            | effort         | $kg  m^{-1}  s^{-2}$                | 13        |
| 35 | $U^e{}_N$   | Ue      | electrical potential – voltage      | effort         | $kg  m^2  A^{-1} s^{-3}$            | 26        |
| 27 | $v_{xN}$    | v_x     | velocity in x-direction             | secondaryState | $ms^{-1}$                           | 19        |
| 29 | $v_{zN}$    | v_z     | velocity in z-direction             | secondaryState | $ms^{-1}$                           | 21        |
| 28 | $v_{yN}$    | v_y     | velocity in y-direction             | secondaryState | $ms^{-1}$                           | 20        |

#### 4 material

|    | var                 | symbol    | documentation                                       | type     | units                       | eqs |
|----|---------------------|-----------|---|----------|-----------------------------|-----|
| 46 | $k_{zN}^c$          | kc_z      | convective mass conductivity in z-direction         | property | $m^{-1} s$                  | 37  |
| 44 | $k_{xN}^c$          | kc_x      | convective mass conductivity in x-direction         | property | $m^{-1} s$                  | 35  |
| 53 | $k_{yA,S}^d$        | kd_y_A    | diffusional mass conductivity in y-direction in arc | property | $kg^{-1} m^{-4} mol^2 s$    | 43  |
| 37 | $C_{vN}$            | Cv        | total heat capacity at constant volume              | property | $kg  m^2  K^{-1}  s^{-2}$   | 28  |
| 43 | $k_{zN,S}^d$        | kd_z      | diffusional mass conductivity in z-direction        | property | $kg^{-1}  m^{-4}  mol^2  s$ | 34  |
| 41 | $k_{xN,S}^d$        | kd_x      | diffusional mass conductivity in x-direction        | property | $kg^{-1} m^{-4} mol^2 s$    | 32  |
| 59 | $density_N$         | density   | density   | property | $kg  m^{-3}$                | 49  |
| 60 | $v_S$               | v         | molar volume of species                             | property | $m^3  mol^{-1}$             | 50  |
| 47 | $h_{N,S}$           | h         | partial molar enthalpies                            | property | $kg  m^2  mol^{-1}  s^{-2}$ | 38  |
| 58 | $m_N$               | m         | mass  | property | kg                          | 48  |
| 54 | $k_{zA,S}^d$        | kd_z_A    | diffusional mass conductivity in z-direction in arc | property | $kg^{-1}  m^{-4}  mol^2  s$ | 44  |
| 36 | $C_{pN}$            | Ср        | total heat capacity at constant pressure            | property | $kg  m^2  K^{-1}  s^{-2}$   | 27  |
| 45 | $k_{yN}^c$          | kc_y      | convective mass conductivity in y-direction         | property | $m^{-1} s$                  | 36  |
| 55 | $k_{xA}^q$          | kq_x_A    | thermal conductivity in x-direction in arc          | property | $kg K^{-1} s^{-3}$          | 45  |
| 26 | $\lambda_S$         | Mm        | species' molecular mass                             | property | $kg  mol^{-1}$              |     |
| 39 | $k_{yN}^q$          | kq_y      | thermal conductivity in y-direction                 | property | $kg  K^{-1}  s^{-3}$        | 30  |
| 62 | $k^(d, Fick_{yA,S}$ | kd_y_Fick | Fick's diffusivity in arc and y-direction           | property | $ms^{-1}$                   | 52  |
| 40 | $k_{zN}^q$          | kq_z      | thermal conductivity in z-direction                 | property | $kg K^{-1} s^{-3}$          | 31  |
| 52 | $k_{xA,S}^d$        | kd_x_A    | diffusional mass conductivity in x-direction in arc | property | $kg^{-1} m^{-4} mol^2 s$    | 42  |
| 49 | $k_{xA}^c$          | kc_x_A    | convective mass conductivity in x-direction in arc  | property | $m^{-1} s$                  | 39  |
| 56 | $k_{yA}^q$          | kq_y_A    | thermal conductivity in y-direction in arc          | property | $kg K^{-1} s^{-3}$          | 46  |
| 57 | $k_{zA}^q$          | kq_z_A    | thermal conductivity in z-direction in arc          | property | $kg  K^{-1}  s^{-3}$        | 47  |
| 42 | $k_{yN,S}^d$        | kd_y      | diffusional mass conductivity in z-direction        | property | $kg^{-1}  m^{-4}  mol^2  s$ | 33  |

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|    | var                 | symbol    | documentation                                      | type     | units              | eqs |
|----|---------------------|-----------|--|----------|--------------------|-----|
| 38 | $k_{xN}^q$          | kq_x      | thermal conductivity in x-direction                | property | $kg K^{-1} s^{-3}$ | 29  |
| 61 | $k^(d, Fick_{xA,S}$ | kd_x_Fick | Fick's diffusivity in arc and x-direction          | property | $ms^{-1}$          | 51  |
| 51 | $k_{zA}^c$          | kc_z_A    | convective mass conductivity in z-direction in arc | property | $m^{-1} s$         | 41  |
| 50 | $k_{yA}^c$          | kc_y_A    | convective mass conductivity in y-direction in arc | property | $m^{-1} s$         | 40  |
| 63 | $k^(d, Fick_{zA,S}$ | kd_z_Fick | Fick's diffusivity in arc and z-direction          | property | $ms^{-1}$          | 53  |

### 5 macroscopic

|    | var       | symbol | documentation           | type                       | units | eqs |
|----|-----------|--------|-------------------------|----------------------------|-------|-----|
| 65 | $A_{xyN}$ | A_xy   | cross sectional area xy | geometry                   | $m^2$ | 54  |
| 67 | $A_{yzN}$ | A_yz   | cross sectional area yz | geometry                   | $m^2$ | 56  |
| 66 | $A_{xzN}$ | A_xz   | cross sectional area xz | geometry                   | $m^2$ | 55  |
| 64 | $D_{N,A}$ | D      | difference operator     | ${ m difference Operator}$ |       |     |

# 6 material-macroscopic

|    | var               | symbol | documentation   | type | units        | eqs |
|----|-------------------|--------|---|------|--------------|-----|
| 30 | $_{-}\lambda_{S}$ | _Mm    | link variable Mm to interface material »> macroscopic | get  | $kgmol^{-1}$ | 22  |

# 7 Equations

### 8 Generic

| no | equation   | documentation                 | layer    |
|----|--|-------------------------------|----------|
| 1  | 1 := Instantiate(#, #)   | numerical one                 | root     |
| 2  | 0 := Instantiate(#, #)   | numerical value zero          | root     |
| 3  | $t^o := \operatorname{Instantiate}(t, 0)$  | time zero                     | root     |
| 4  | $t^e := \text{Instantiate}(t, \#)$   | time end                      | root     |
| 5  | $\Delta t := \operatorname{Instantiate}(t, \#)$  | time interval                 | root     |
| 6  | 0.5 := Instantiate(#, #)   | numerical one half            | root     |
| 7  | $\Delta := \operatorname{sign}(t - t^{o}) - \operatorname{sign}(t - (t^{o} - \Delta t))$ | pulse of length time interval | root     |
| 8  | $r_{xN} := \text{Instantiate}(\ell_N, \#)$   | x-direction                   | physical |
| 9  | $r_{yN} := \text{Instantiate}(\ell_N, \#)$   | y-direction                   | physical |
| 10 | $r_{zN} := \text{Instantiate}(\ell_N, \#)$   | z-direction                   | physical |
| 11 | $V_N := r_{xN} \cdot r_{yN} \cdot r_{zN}$  | volume                        | physical |
| 13 | $p_N := \frac{\partial U_N}{\partial V_N}$   | pressure                      | physical |
| 14 | $\mu_{N,S} := \frac{\partial U_N}{\partial n_{N,S}}$                                     | chemical potential            | physical |
| 15 | $H_N := U_N - p_N \cdot V_N$   | Enthalpy                      | physical |
| 16 | $T_N := \frac{\partial U_N}{\partial S_N}$   | temperature                   | physical |
| 17 | $A_N := U_N - T_N \cdot S_N$   | Helmholts energy              | physical |

Continued on next page

| no | equation   | documentation                                    | layer     |
|----|--|--|-----------|
| 18 | $G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$   | Gibbs free energy                                | physical  |
| 19 | $v_{xN} := (t)^{-1} \cdot r_{xN}$  | velocity in x-direction                          | physical  |
| 20 | $v_{yN} := (t)^{-1} \cdot r_{yN}$  | velocity in y-direction                          | physical  |
| 21 | $v_{zN} := (t)^{-1} \cdot r_{zN}$  | velocity in z-direction                          | physical  |
| 24 | $B_N := \operatorname{Instantiate}(S_N, \#)$   | Boltzmann constant                               | physical  |
| 25 | $R_N := A^v \cdot B_N$   | Gas constant                                     | physical  |
| 26 | $U^e_N := \left(C_N\right)^{-1} . U_N$   | electrical potential – voltage                   | physical  |
| 27 | $C_{pN} := rac{\partial H_N}{\partial T_N}$   | total heat capacity at constant pressure         | material  |
| 28 | $C_{vN} := rac{\partial U_N}{\partial T_N}$   | total heat capacity at constant volume           | material  |
| 29 | $k_{xN}^q := (V_N)^{-1} \cdot C_{pN} \cdot v_{xN}$   | thermal conductivity in x-direction              | material  |
| 30 | $k_{yN}^q := (V_N)^{-1} \cdot C_{pN} \cdot v_{yN}$   | thermal conductivity in y-direction              | material  |
| 31 | $k_{zN}^q := (V_N)^{-1} \cdot C_{pN} \cdot v_{zN}$   | thermal conductivity in z-direction              | material  |
| 32 | $k_{xN,S}^d := \left(\mu_{N,S}\right)^{-1} \cdot \left(v_{xN} \cdot \left(\left(V_N\right)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}}\right)\right)$ | diffusional mass conductivity in x-direction     | material  |
| 33 | $k_{yN,S}^d := (\mu_{N,S})^{-1} \cdot \left( v_{yN} \cdot \left( (V_N)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \right) \right)$                   | diffusional mass conductivity in y-<br>direction | material  |
| 34 | $k_{zN,S}^d := (\mu_{N,S})^{-1} \cdot \left( v_{zN} \cdot \left( (V_N)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \right) \right)$                   | diffusional mass conductivity in z-<br>direction | material  |
| 35 | $k_{xN}^c := \left(\lambda_S \star (\mu_{N,S})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$                            | convective mass conductivity in x-direction      | mat erial |

Continued on next page

| no | equation  | documentation   | layer    |
|----|---|---|----------|
| 36 | $k_{yN}^c := \left(\lambda_S \star (\mu_{N,S})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$ | convective mass conductivity in y-direction             | material |
| 37 | $k_{zN}^c := \left(\lambda_S \star (\mu_{N,S})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$ | convective mass conductivity in z-direction             | material |
| 38 | $\left  \ h_{N,S} := H_N \cdot \left( n_{N,S} \right)^{-1} \right $   | partial molar enthalpies                                | material |
| 39 | $k_{xA}^c := I_{NAN,A} \star k_{xN}^c$  | convective mass conductivity in x-direction in arc      | material |
| 40 | $k_{yA}^c := I_{NAN,A} \star k_{yN}^c$  | convective mass conductivity in y-<br>direction in arc  | material |
| 41 | $k_{zA}^c := I_{NAN,A} \star k_{zN}^c$  | convective mass conductivity in z-direction in arc      | material |
| 42 | $k_{xA,S}^d := I_{NAN,A} \star k_{xN,S}^d$  | diffusional mass conductivity in x-direction in arc     | material |
| 43 | $k_{yA,S}^d := I_{NAN,A} \star k_{yN,S}^d$  | diffusional mass conductivity in z-<br>direction in arc | material |
| 44 | $k_{zA,S}^d := I_{NAN,A} \star k_{zN,S}^d$  | diffusional mass conductivity in z-<br>direction in arc | material |
| 45 | $k_{xA}^q := I_{NAN,A} \star k_{xN}^q$  | thermal conductivity in x-direction in arc              | material |
| 46 | $k_{yA}^q := I_{NAN,A} \star k_{yN}^q$  | thermal conductivity in y-direction in arc              | material |
| 47 | $k_{zA}^q := I_{NAN,A} \star k_{zN}^q$  | thermal conductivity in z-direction in arc              | material |
| 48 | $m_N := \lambda_S \star n_{N,S}$  | mass  | material |

| no | equation   | documentation                             | layer       |
|----|--|---|-------------|
| 49 | $density_N := (V_N)^{-1} \cdot m_N$  | density                                   | material    |
| 50 | $v_S := V_N \star (n_{N,S})^{-1}$  | molar volume of species                   | material    |
| 51 | $k^{(d)} + ick_{xA,S} := I_{NAN,A} \star \left(v_{xN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1}\right)$   | Fick's diffusivity in arc and x-direction | material    |
| 52 | $k^{(d)} + ick_{yA,S} := I_{NAN,A} \star \left( v_{yN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$ | Fick's diffusivity in arc and y-direction | material    |
| 53 | $k^{(d)}, Fick_{zA,S} := I_{NAN,A} \star \left(v_{zN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1}\right)$   | Fick's diffusivity in arc and z-direction | material    |
| 54 | $A_{xyN} := r_{xN} \cdot r_{yN}$   | cross sectional area xy                   | macroscopic |
| 55 | $A_{xzN} := r_{xN} \cdot r_{zN}$   | cross sectional area xz                   | macroscopic |
| 56 | $A_{yzN} := r_{yN} \cdot r_{zN}$   | cross sectional area yz                   | macroscopic |

# 9 Interface Link Equation

| no | equation                       | documentation      | layer                        |
|----|--------------------------------|--------------------|------------------------------|
| 22 | $_{-}\lambda_{S}:=\lambda_{S}$ | interface equation | material -> macro-<br>scopic |