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 | Δt | t_interval | time interval | frame | s | 5 |
| 9 | Δ | 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 | ℓ_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 |
| 47 | $h_{N,S}$ | h | partial molar enthalpies | property | $kg m^2 mol^{-1} s^{-2}$ | 38 |
| 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 | λ_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 |
| 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 |
| 38 | k_{xN}^q | kq_x | thermal conductivity in x-direction | property | $kg K^{-1} s^{-3}$ | 29 |
| 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 |

5 macroscopic

| | var | symbol | documentation | type | units | eqs |
|----|-------|--------|---------------|----------------|-------|-----|
| 31 | m_N | m | mass | secondaryState | kg | 23 |

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 | $t^o := \text{Instantiate}(t, 0)$ | 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 |

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| 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 |
| 23 | $m_N := _\lambda_S \star n_{N,S}$ | mass | macroscopic |
| 24 | $B_N := \operatorname{Instantiate}(S_N, \#)$ | Boltzmann constant | physical |
| 25 | $R_N := A^v \cdot B_N$ | Gas constant | physical |
| 26 | $U^e_N := (C_N)^{-1} \cdot U_N$ | 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 | $k_{xN,S}^d := (\mu_{N,S})^{-1} \cdot \left(v_{xN} \cdot \left((V_N)^{-1} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \right) \right)$ | 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- 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- direction | material |

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| no | equation | documentation | layer |
|----|---|---|----------|
| 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 | material |
| 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 | $h_{N,S} := H_N \cdot (n_{N,S})^{-1}$ | 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-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- direction in arc | material |
| 44 | $k_{zA,S}^d := I_{NAN,A} \star k_{zN,S}^d$ | diffusional mass conductivity in z- direction in arc | material |
| 45 | $k_{xA}^q := I_{NAN,A} \star k_{xN}^q$ | thermal conductivity in x-direction in arc | material |
| 46 | $k_{yA}^q := I_{NAN,A} \star k_y^q N$ | thermal conductivity in y-direction in arc | material |

Continued on next page

| no | equation | documentation | layer |
|----|--|--|----------|
| 47 | $k_{zA}^q := I_{NAN,A} \star k_{zN}^q$ | thermal conductivity in z-direction in arc | material |

9 Interface Link Equation

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