

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 | <i>s</i> | 5 |
| 9 | Δ | pulse | pulse of length time interval | frame | | 7 |
| 5 | t^o | to | time zero | frame | <i>s</i> | 3 |
| 6 | t^e | te | time end | frame | <i>s</i> | 4 |
| 4 | t | t | time | frame | <i>s</i> | |
| 8 | 0.5 | onehalf | numerical one half | constant | | 6 |
| 1 | # | value | numerical value | constant | | |
| 3 | 0 | zero | numerical value zero | constant | | 2 |
| 2 | 1 | one | numerical one | constant | | 1 |

3 physical

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

4 material

| | var | symbol | documentation | type | units | eqs |
|----|---------------------|-----------|---|----------|-----------------------------|-----|
| 26 | λ_S | Mm | species' molecular mass | property | $kg\ mol^{-1}$ | |
| 56 | k_{yA}^q | kq_y_A | thermal conductivity in y-direction in arc | property | $kg\ K^{-1}\ s^{-3}$ | 46 |
| 42 | $k_{yN,S}^d$ | kd_y | diffusional mass conductivity in z-direction | property | $kg^{-1}\ m^{-4}\ mol^2\ s$ | 33 |
| 43 | $k_{zN,S}^d$ | kd_z | diffusional mass conductivity in z-direction | property | $kg^{-1}\ m^{-4}\ mol^2\ s$ | 34 |
| 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 |
| 61 | $k(d, Fick_{xA,S})$ | kd_x_Fick | Fick's diffusivity in arc and x-direction | property | ms^{-1} | 51 |
| 44 | k_{xN}^c | kc_x | convective mass conductivity in x-direction | property | $m^{-1}\ s$ | 35 |
| 51 | k_{zA}^c | kc_z_A | convective mass conductivity in z-direction in arc | property | $m^{-1}\ s$ | 41 |
| 63 | $k(d, Fick_{zA,S})$ | kd_z_Fick | Fick's diffusivity in arc and z-direction | property | ms^{-1} | 53 |
| 38 | k_{xN}^q | kq_x | thermal conductivity in x-direction | property | $kg\ K^{-1}\ s^{-3}$ | 29 |
| 45 | k_{yN}^c | kc_y | convective mass conductivity in y-direction | property | $m^{-1}\ s$ | 36 |
| 47 | $h_{N,S}$ | h | partial molar enthalpies | property | $kg\ m^2\ mol^{-1}\ s^{-2}$ | 38 |
| 37 | C_{vN} | Cv | total heat capacity at constant volume | property | $kg\ m^2\ K^{-1}\ s^{-2}$ | 28 |
| 40 | k_{zN}^q | kq_z | thermal conductivity in z-direction | property | $kg\ K^{-1}\ s^{-3}$ | 31 |
| 60 | v_S | v | molar volume of species | property | $m^3\ mol^{-1}$ | 50 |
| 46 | k_{zN}^c | kc_z | convective mass conductivity in z-direction | property | $m^{-1}\ s$ | 37 |
| 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 |
| 36 | C_{pN} | Cp | total heat capacity at constant pressure | property | $kg\ m^2\ K^{-1}\ s^{-2}$ | 27 |
| 41 | $k_{xN,S}^d$ | kd_x | diffusional mass conductivity in x-direction | property | $kg^{-1}\ m^{-4}\ mol^2\ s$ | 32 |
| 39 | k_{yN}^q | kq_y | thermal conductivity in y-direction | property | $kg\ K^{-1}\ s^{-3}$ | 30 |
| 49 | k_{xA}^c | kc_x_A | convective mass conductivity in x-direction in arc | property | $m^{-1}\ s$ | 39 |
| 59 | ρ_N | density | density | property | $kg\ m^{-3}$ | 49 |
| 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 |

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| | var | symbol | documentation | type | units | eqs |
|----|--------------------|-----------|--|----------|--------------------|-----|
| 62 | $k^d, Fick_{yA,S}$ | kd_y_Fick | Fick's diffusivity in arc and y-direction | property | ms^{-1} | 52 |
| 57 | k_z^q | kq_z_A | thermal conductivity in z-direction in arc | property | $kg K^{-1} s^{-3}$ | 47 |
| 55 | k_x^q | kq_x_A | thermal conductivity in x-direction in arc | property | $kg K^{-1} s^{-3}$ | 45 |
| 58 | m_N | m | mass | property | kg | 48 |
| 50 | k_y^c | kc_y_A | convective mass conductivity in y-direction in arc | property | $m^{-1} s$ | 40 |
| 89 | ρ_A | density_A | density of arc material | property | $kg m^{-3}$ | 78 |

5 macroscopic

| | var | symbol | documentation | type | units | eqs |
|----|-------------------|--------|--|--------------------|-------------------|--------------------|
| 84 | \dot{q}_N | aq | accumulation due to conductive heat flow | transport | $kg\,m^2\,s^{-3}$ | 73 |
| 87 | $c_{A,S}$ | c_A | concentration in convective mass flow | transport | $m^{-3}\,mol$ | 76 |
| 83 | \hat{q}_{xA} | fq_x_A | heat flow in arc and x-direction | transport | $kg\,m^2\,s^{-3}$ | 72 |
| 91 | \dot{V}_A | fV | volumetric flow | transport | $m^3\,s^{-1}$ | 80 |
| 92 | $\hat{n}_{A,S}^c$ | fnc_A | convective mass flow in an arc | transport | $mol\,s^{-1}$ | 81 |
| 93 | $\hat{n}_{N,S}^c$ | anc | accumulation due to convective mass flow | transport | $mol\,s^{-1}$ | 82 |
| 86 | d_A | d | fow direction of convective flow | transport | | 75 |
| 70 | A_{yzA} | A_yz_A | cross sectional area yz of arc | geometry | m^2 | 59 |
| 68 | A_{xyA} | A_xy_A | cross sectional area yz of arc | geometry | m^2 | 57 |
| 66 | A_{xzN} | A_xz | cross sectional area xz | geometry | m^2 | 55 |
| 67 | A_{yzN} | A_yz | cross sectional area yz | geometry | m^2 | 56 |
| 69 | A_{xzA} | A_xz_A | cross sectional area xz of arc | geometry | m^2 | 58 |
| 65 | A_{xyN} | A_xy | cross sectional area xy | geometry | m^2 | 54 |
| 64 | $D_{N,A}$ | D | difference operator | differenceOperator | | |
| 85 | $c_{N,S}$ | c | molar concentration | secondaryState | $m^{-3}\,mol$ | 74 |

6 material–macroscopic

| | var | symbol | documentation | type | units | eqs |
|----|-------------------------|-------------------------|--|------|--------------------------|-----|
| 75 | $k d_{x\text{Fick}A,S}$ | <code>_kd_x_Fick</code> | link variable kd x Fick to interface material »> macroscopic | get | ms^{-1} | 64 |
| 81 | $_{k_y^q A}$ | <code>_kq_y_A</code> | link variable kq y A to interface material »> macroscopic | get | $kg K^{-1} s^{-3}$ | 70 |
| 73 | $_{k_z^c A}$ | <code>_kc_z_A</code> | link variable kc z A to interface material »> macroscopic | get | $m^{-1} s$ | 62 |
| 76 | $k d_{y\text{Fick}A,S}$ | <code>_kd_y_Fick</code> | link variable kd y Fick to interface material »> macroscopic | get | ms^{-1} | 65 |
| 88 | $_{\rho N}$ | <code>_density</code> | link variable density to interface material »> macroscopic | get | $kg m^{-3}$ | 77 |
| 80 | $_{k_x^q A}$ | <code>_kq_x_A</code> | link variable kq x A to interface material »> macroscopic | get | $kg K^{-1} s^{-3}$ | 69 |
| 79 | $k d_{z\text{Fick}A,S}$ | <code>_kd_z_Fick</code> | link variable kd z Fick to interface material »> macroscopic | get | ms^{-1} | 68 |
| 82 | $_{k_z^q A}$ | <code>_kq_z_A</code> | link variable kq z A to interface material »> macroscopic | get | $kg K^{-1} s^{-3}$ | 71 |
| 78 | $_{k_z^d A,S}$ | <code>_kd_z_A</code> | link variable kd z A to interface material »> macroscopic | get | $kg^{-1} m^{-4} mol^2 s$ | 67 |
| 72 | $_{k_y^c A}$ | <code>_kc_y_A</code> | link variable kc y A to interface material »> macroscopic | get | $m^{-1} s$ | 61 |
| 90 | $_{\rho A}$ | <code>_density_A</code> | link variable density A to interface material »> macroscopic | get | $kg m^{-3}$ | 79 |
| 74 | $_{k_x^d A,S}$ | <code>_kd_x_A</code> | link variable kd x A to interface material »> macroscopic | get | $kg^{-1} m^{-4} mol^2 s$ | 63 |
| 71 | $_{k_x^c A}$ | <code>_kc_x_A</code> | link variable kc x A to interface material »> macroscopic | get | $m^{-1} s$ | 60 |
| 30 | $_{\lambda S}$ | <code>_Mm</code> | link variable Mm to interface material »> macroscopic | get | $kg mol^{-1}$ | 22 |

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| | var | symbol | documentation | type | units | eqs |
|----|-----------------|----------------------|---|------|--------------------------|-----|
| 77 | $_{k_y^d A, S}$ | <code>_kd_y_A</code> | link variable kd y A to interface material »> macroscopic | get | $kg^{-1} m^{-4} mol^2 s$ | 66 |

7 Equations

8 Generic

| no | equation | documentation | layer |
|----|--|-------------------------------|----------|
| 1 | $1 := \text{Instantiate}(\#, \#)$ | numerical one | root |
| 2 | $0 := \text{Instantiate}(\#, \#)$ | numerical value zero | root |
| 3 | $t^o := \text{Instantiate}(t, 0)$ | time zero | root |
| 4 | $t^e := \text{Instantiate}(t, \#)$ | time end | root |
| 5 | $\Delta t := \text{Instantiate}(t, \#)$ | time interval | root |
| 6 | $0.5 := \text{Instantiate}(\#, \#)$ | numerical one half | root |
| 7 | $\Delta := \text{sign}(t - t^o) - \text{sign}(t - (t^o - \Delta t))$ | 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 |
| 24 | $B_N := \text{Instantiate}(S_N, \#)$ | Boltzmann constant | physical |
| 25 | $R_N := A^v \cdot B_N$ | Gas constant | physical |
| 26 | $U_N^e := (C_N)^{-1} \cdot U_N$ | electrical potential – voltage | physical |
| 27 | $C_{pN} := \frac{\partial H_N}{\partial T_N}$ | total heat capacity at constant pressure | material |
| 28 | $C_{vN} := \frac{\partial U_N}{\partial T_N}$ | 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 |
| 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 |

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| 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 | $h_{N,S} := H_N \cdot (n_{N,S})^{-1}$ | 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 | $k_{yA}^q := I_{NAN,A} \star k_{yN}^q$ | 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 |

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| no | equation | documentation | layer |
|----|--|---|-------------|
| 49 | $\rho_N := (V_N)^{-1} \cdot m_N$ | density | material |
| 50 | $v_S := V_N \star (n_{N,S})^{-1}$ | molar volume of species | material |
| 51 | $k^{(d, Fick)}_{xA,S} := I_{NAN,A} \star \left(v_{xN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$ | Fick's diffusivity in arc and x-direction | material |
| 52 | $k^{(d, Fick)}_{yA,S} := I_{NAN,A} \star \left(v_{yN} \cdot \frac{\partial U_N}{\partial \mu_{N,S}} \cdot (n_{N,S})^{-1} \right)$ | 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 |
| 57 | $A_{xyA} := I_{NAN,A} \star A_{xyN}$ | cross sectional area yz of arc | macroscopic |
| 58 | $A_{xzA} := I_{NAN,A} \star A_{xzN}$ | cross sectional area xz of arc | macroscopic |
| 59 | $A_{yzA} := I_{NAN,A} \star A_{yzN}$ | cross sectional area yz of arc | macroscopic |
| 72 | $\hat{q}_{xA} := A_{yzA} \cdot _k_{xA}^q \cdot (D_{N,A} \star T_N)$ | heat flow in arc and x-direction | macroscopic |
| 73 | $\dot{q}_N := F_{N,A} \star \hat{q}_{xA}$ | accumulation due to conductive heat flow | macroscopic |
| 74 | $c_{N,S} := (V_N)^{-1} \cdot n_{N,S}$ | molar concentration | macroscopic |
| 75 | $d_A := \text{sign}(D_{N,A} \star p_N)$ | flow direction of convective flow | macroscopic |
| 76 | $c_{A,S} := (0.5 \cdot (D_{N,A} - d_A \cdot D_{N,A})) \star c_{N,S}$ | concentration in convective mass flow | macroscopic |
| 78 | $\rho_A := I_{NAN,A} \star \rho_N$ | density of arc material | material |
| 80 | $\dot{V}_A := (_ \rho_A)^{-1} \cdot _k_{xA}^c \cdot A_{yzA} \cdot (D_{N,A} \star p_N)$ | volumetric flow | macroscopic |

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| no | equation | documentation | layer |
|----|--|--|-------------|
| 81 | $\hat{n}_{A,S}^c := \dot{V}_A \cdot c_{A,S}$ | convective mass flow in an arc | macroscopic |
| 82 | $\dot{n}_{N,S}^c := F_{N,A} \star \hat{n}_{A,S}^c$ | accumulation due to convective mass flow | macroscopic |

9 Interface Link Equation

| no | equation | documentation | layer |
|----|--|--------------------|-------------------------|
| 22 | $_{-}\lambda_S := \lambda_S$ | interface equation | material -> macroscopic |
| 60 | $_{-}k_{xA}^c := k_{xA}^c$ | interface equation | material -> macroscopic |
| 61 | $_{-}k_{yA}^c := k_{yA}^c$ | interface equation | material -> macroscopic |
| 62 | $_{-}k_{zA}^c := k_{zA}^c$ | interface equation | material -> macroscopic |
| 63 | $_{-}k_{xA,S}^d := k_{xA,S}^d$ | interface equation | material -> macroscopic |
| 64 | ${}_kd_{xFick_{A,S}} := k^{(d, Fick_{xA,S}}$ | interface equation | material -> macroscopic |
| 65 | ${}_kd_{yFick_{A,S}} := k^{(d, Fick_{yA,S}}$ | interface equation | material -> macroscopic |
| 66 | $_{-}k_{yA,S}^d := k_{yA,S}^d$ | interface equation | material -> macroscopic |
| 67 | $_{-}k_{zA,S}^d := k_{zA,S}^d$ | interface equation | material -> macroscopic |
| 68 | ${}_kd_{zFick_{A,S}} := k^{(d, Fick_{zA,S}}$ | interface equation | material -> macroscopic |
| 69 | $_{-}k_{xA}^q := k_{xA}^q$ | interface equation | material -> macroscopic |

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| no | equation | documentation | layer |
|----|--------------------------|--------------------|------------------------------------|
| 70 | $_k_{yA}^q := k_{yA}^q$ | interface equation | material \rightarrow macroscopic |
| 71 | $_k_{zA}^q := k_{zA}^q$ | interface equation | material \rightarrow macroscopic |
| 77 | $_\rho_N := \rho_N$ | interface equation | material \rightarrow macroscopic |
| 79 | $_\rho_A := \rho_A$ | interface equation | material \rightarrow macroscopic |