1 Variables

2 root

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

3 physical

| | var | symbol | documentation | type | units | eqs |
|----|-------------|---------|-------------------------------------|----------------|-----------------------------|-----|
| 11 | ℓ_N | 1 | length | frame | m | |
| 13 | r_{yN} | r_y | y-direction | frame | m | 9 |
| 14 | r_{zN} | r_z | z-direction | frame | m | 10 |
| 12 | r_{xN} | r_x | x-direction | frame | $\mid m \mid$ | 8 |
| 24 | G_N | G | Gibbs free energy | state | $kg m^2 s^{-2}$ | 18 |
| 25 | C_N | C | fundamental state - charge | state | As | |
| 22 | H_N | н | Enthalpy | state | $kg m^2 s^{-2}$ | 15 |
| 15 | V_N | V | fundamental state - volume | state | m^3 | 11 |
| 18 | $n_{N,S}$ | n | fundamental state - molar mass | state | mol | |
| 17 | S_N | S | fundamental state - entropy | state | $kg m^2 K^{-1} s^{-2}$ | |
| 16 | U_N | U | fundamental state - internal energy | state | $kg m^2 s^{-2}$ | |
| 23 | A_N | A | Helmholts energy | state | $kg m^2 s^{-2}$ | 17 |
| 20 | p_N | p | pressure | effort | $kg m^{-1} s^{-2}$ | 13 |
| 19 | T_N | Т | temperature | effort | K | 16 |
| 21 | $\mu_{N,S}$ | chemPot | chemical potential | effort | $kg m^2 mol^{-1} s^{-2}$ | 14 |
| 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-macroscopic

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

5 Equations

6 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 |

7 Interface Link Equation

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