

1 Variables

2 root

| | var | symbol | documentation | type | units | tokens | eqs |
|---|-------|----------------|--------------------------------------|----------|-------|--------|-----|
| 5 | F | F | incidence matrix of a directed graph | network | | [] | |
| 6 | t | t | time | frame | s | [] | |
| 7 | t_o | to | starting time | frame | s | [] | 4 |
| 8 | t_e | te | end time | frame | s | [] | 5 |
| 1 | $\#$ | value | numerical value | constant | | [] | |
| 2 | 0 | zero | numerical value zero | constant | | [] | 1 |
| 3 | 1 | one | numerical value one | constant | | [] | 2 |
| 4 | 0.5 | onehalf | numerical value one half | constant | | [] | 3 |

3 physical

| | var | symbol | documentation | type | units | tokens | eqs |
|----|------------|--------------------|------------------------------------|----------------|-------------------------------------|--------|-----|
| 9 | r_{xN} | r_x | x-coordinate | frame | m | [] | |
| 10 | r_{yN} | r_y | y-coordinate | frame | m | [] | |
| 23 | r_{zN} | r_z | z-coordinate | frame | m | [] | |
| 11 | U_N | U | foundation state – internal energy | state | $kg\ m^2\ s^{-2}$ | [] | |
| 12 | S_N | S | foundation state – entropy | state | $kg\ m^2\ K^{-1}\ s^{-2}$ | [] | |
| 13 | V_N | V | foundation state – volume | state | m^3 | [] | |
| 18 | H_N | H | enthalpy | state | $kg\ m^2\ s^{-2}$ | [] | 9 |
| 19 | A_N | A | Helmholtz energy | state | $kg\ m^2\ s^{-2}$ | [] | 10 |
| 20 | G_N | G | Gibbs energy | state | $kg\ m^2\ s^{-2}$ | [] | 11 |
| 42 | n_{NS} | n | species molar mass | state | mol | [] | |
| 26 | A^v | Avogadro | Avogadro number | constant | mol^{-1} | [] | |
| 27 | Bo_N | Boltzmann | Boltzmann constant | constant | $kg\ m^2\ K^{-1}\ s^{-2}$ | [] | 16 |
| 28 | R_N | GasConstant | Gas constant | constant | $kg\ m^2\ mol^{-1}\ K^{-1}\ s^{-2}$ | [] | 17 |
| 15 | p_N | p | thermodynamic pressure | effort | $kg\ m^{-1}\ s^{-2}$ | [] | 6 |
| 16 | T_N | T | temperature | effort | K | [] | 7 |
| 45 | μ_{NS} | chem_pot | chemical potential | effort | $kg\ m^2\ mol^{-1}\ s^{-2}$ | [] | 32 |
| 21 | v_{xN} | v_x | velocity in x-direction | secondaryState | ms^{-1} | [] | 12 |
| 22 | v_{yN} | v_y | velocity in y direction | secondaryState | ms^{-1} | [] | 13 |
| 24 | v_{zN} | v_z | velocity in z-direction | secondaryState | ms^{-1} | [] | 14 |
| 25 | v_N | v | velocity vector | secondaryState | ms^{-1} | [] | 15 |

4 control

| | var | symbol | documentation | type | units | tokens | eqs |
|--|-----|--------|---------------|------|-------|--------|-----|
|--|-----|--------|---------------|------|-------|--------|-----|

5 reactions

| | var | symbol | documentation | type | units | tokens | eqs |
|--|-----|--------|---------------|------|-------|--------|-----|
|--|-----|--------|---------------|------|-------|--------|-----|

6 material

| | var | symbol | documentation | type | units | tokens | eqs |
|----|-------------|--------|-----------------------------------------------|---------------|------------------------------|--------|-----|
| 29 | S | Mm | species molecular masses | constant | $kg\ mol^{-1}$ | [] | |
| 46 | C_{pN} | C_p | total heat capacity at constant pressure | seconaryState | $kg\ m^2\ K^{-1}\ s^{-2}$ | [] | 33 |
| 47 | C_{vN} | C_v | specific heat capacity at constant volume | seconaryState | $kg\ m^2\ K^{-1}\ s^{-2}$ | [] | 34 |
| 48 | c_{pS} | cp | specific heat capacity at constant pressure | seconaryState | $m^2\ mol^2\ K^{-1}\ s^{-2}$ | [] | 35 |
| 49 | c_{vS} | cv | specific heat capacity at constant volume | seconaryState | $m^2\ mol^2\ K^{-1}\ s^{-2}$ | [] | 36 |
| 30 | C_{pN} | Cp | total heat capacity at constant pressure | property | $kg\ m^2\ K^{-1}\ s^{-2}$ | [] | 18 |
| 31 | C_{vN} | Cv | total heat capacity at constant volume | property | $kg\ m^2\ K^{-1}\ s^{-2}$ | [] | 19 |
| 34 | k_{xN}^q | kq_x | thermal conductivity in x-direction | property | $kg\ K^{-1}\ s^{-3}$ | [] | 22 |
| 35 | k_{yN}^q | kq_y | thermal conductivity in y-direction | property | $kg\ K^{-1}\ s^{-3}$ | [] | 23 |
| 36 | k_{zN}^q | kq_z | thermal conductivity in z-direction | property | $kg\ K^{-1}\ s^{-3}$ | [] | 24 |
| 37 | k_N^q | kq | Cartesian thermal conductivity vector | property | $kg\ K^{-1}\ s^{-3}$ | [] | 25 |
| 50 | k_{xN}^c | kc_x | convective mass convectivity in x-direction | property | $m^{-1}\ s$ | [] | 37 |
| 51 | k_{yN}^c | kc_y | convective mass convectivity in y-direction | property | $m^{-1}\ s$ | [] | 38 |
| 52 | k_{zN}^c | kc_z | convective mass convectivity in z-direction | property | $m^{-1}\ s$ | [] | 39 |
| 53 | k_N^c | kc | Cartesian convective mass convectivity vector | property | $m^{-1}\ s$ | [] | 40 |
| 54 | k_{xNS}^d | kd_x | diffusional mass conductivity in x-direction | property | $kg^{-1}\ m^{-4}\ mol^2\ s$ | [] | 41 |
| 55 | k_{yNS}^d | kd_y | diffusional mass conductivity in y-direction | property | $kg^{-1}\ m^{-4}\ mol^2\ s$ | [] | 42 |
| 56 | k_{zNS}^d | kd_z | diffusional mass conductivity in z-direction | property | $kg^{-1}\ m^{-4}\ mol^2\ s$ | [] | 43 |
| 57 | k_{NS}^d | kd | Cartesian dffusional mass conductivity vector | property | $kg^{-1}\ m^{-4}\ mol^2\ s$ | [] | 44 |
| 58 | h_{NS} | h | partial molar enthalpies | property | $kg\ m^2\ mol^{-1}\ s^{-2}$ | [] | 45 |

7 macroscopic

| | var | symbol | documentation | type | units | tokens | eqs |
|--|-----|--------|---------------|------|-------|--------|-----|
|--|-----|--------|---------------|------|-------|--------|-----|

8 solid

| | var | symbol | documentation | type | units | tokens | eqs |
|--|-----|--------|---------------|------|-------|--------|-----|
|--|-----|--------|---------------|------|-------|--------|-----|

9 fluid

| | var | symbol | documentation | type | units | tokens | eqs |
|--|-----|--------|---------------|------|-------|--------|-----|
|--|-----|--------|---------------|------|-------|--------|-----|

10 liquid

| | var | symbol | documentation | type | units | tokens | eqs |
|--|-----|--------|---------------|------|-------|--------|-----|
|--|-----|--------|---------------|------|-------|--------|-----|

11 gas

| | var | symbol | documentation | type | units | tokens | eqs |
|--|-----|--------|---------------|------|-------|--------|-----|
|--|-----|--------|---------------|------|-------|--------|-----|

12 control-control

| | var | symbol | documentation | type | units | tokens | eqs |
|--|-----|--------|---------------|------|-------|--------|-----|
|--|-----|--------|---------------|------|-------|--------|-----|

13 gas–liquid

| | var | symbol | documentation | type | units | tokens | eqs |
|--|-----|--------|---------------|------|-------|--------|-----|
|--|-----|--------|---------------|------|-------|--------|-----|

14 gas–gas

| | var | symbol | documentation | type | units | tokens | eqs |
|--|-----|--------|---------------|------|-------|--------|-----|
|--|-----|--------|---------------|------|-------|--------|-----|

15 liquid–liquid

| | var | symbol | documentation | type | units | tokens | eqs |
|--|-----|--------|---------------|------|-------|--------|-----|
|--|-----|--------|---------------|------|-------|--------|-----|

16 gas-solid

| | var | symbol | documentation | type | units | tokens | eqs |
|--|-----|--------|---------------|------|-------|--------|-----|
|--|-----|--------|---------------|------|-------|--------|-----|

17 solid–solid

| | var | symbol | documentation | type | units | tokens | eqs |
|--|-----|--------|---------------|------|-------|--------|-----|
|--|-----|--------|---------------|------|-------|--------|-----|

18 liquid–solid

| | var | symbol | documentation | type | units | tokens | eqs |
|--|-----|--------|---------------|------|-------|--------|-----|
|--|-----|--------|---------------|------|-------|--------|-----|

19 material–material

| | var | symbol | documentation | type | units | tokens | eqs |
|--|-----|--------|---------------|------|-------|--------|-----|
|--|-----|--------|---------------|------|-------|--------|-----|

20 reactions-reactions

| | var | symbol | documentation | type | units | tokens | eqs |
|--|-----|--------|---------------|------|-------|--------|-----|
|--|-----|--------|---------------|------|-------|--------|-----|

21 Equations

22 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 | $p_N := \left(-\frac{\partial U_N}{\partial V_N}\right)$ | thermodynamic pressure | physical |
| 7 | $T_N := \frac{\partial U_N}{\partial S_N}$ | temperature | physical |
| 9 | $H_N := U_N - p_N \cdot V_N$ | enthalpy | physical |
| 10 | $A_N := U_N - T_N \cdot S_N$ | Helmholtz energy | physical |
| 11 | $G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$ | Gibbs energy | physical |
| 12 | $v_{xN} := \frac{\partial r_{xN}}{\partial t}$ | velocity in x-direction | physical |
| 13 | $v_{yN} := \frac{\partial r_{yN}}{\partial t}$ | velocity in y direction | physical |
| 14 | $v_{zN} := \frac{\partial r_{zN}}{\partial t}$ | velocity in z-direction | physical |
| 15 | $v_N := \text{Stack}(v_{xN}, v_{yN}, v_{zN})$ | velocity vector | physical |
| 16 | $Bo_N := \text{Instantiate}(S_N, \#)$ | Boltzmann constant | physical |
| 17 | $R_N := A^v \cdot Bo_N$ | Gas constant | physical |

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| no | equation | documentation | layer |
|----|-------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------|----------|
| 18 | $C_{pN} := \frac{\partial H_N}{\partial T_N}$ | total heat capacity | material |
| 19 | $C_{vN} := \frac{\partial U_N}{\partial T_N}$ | total heat capacity at constant volume | material |
| 22 | $k_{xN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}$ | thermal conductivity in x-direction | material |
| 23 | $k_{yN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{yN}$ | thermal conductivity in y-direction | material |
| 24 | $k_{zN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{zN}$ | thermal conductivity in z-direction | material |
| 25 | $k_N^q := \text{Stack}(k_{xN}^q, k_{yN}^q, k_{zN}^q)$ | Cartesian thermal conductivity vector | material |
| 32 | $\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$ | chemical potential | physical |
| 33 | $C_{pN} := \frac{\partial H_N}{\partial T_N}$ | total heat capacity at constant pressure | material |
| 34 | $C_{vN} := \frac{\partial U_N}{\partial T_N}$ | specic heat capacity at constant volume | material |
| 35 | $c_{pS} := C_{pN} \cdot (S)^{-1} \stackrel{N \in NS}{\star} n_{NS}$ | specific heat capacity at constant pressure | material |
| 36 | $c_{vS} := C_{vN} \cdot (S)^{-1} \stackrel{N \in NS}{\star} n_{NS}$ | specific heat capacity at constant volume | material |
| 37 | $k_{xN}^c := \left(S \stackrel{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$ | convective mass convectivity in x-direction | material |
| 38 | $k_{yN}^c := \left(S \stackrel{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$ | convective mass convectivity in y-direction | material |
| 39 | $k_{zN}^c := \left(S \stackrel{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$ | convective mass convectivity in z-direction | material |
| 40 | $k_N^c := \text{Stack}(k_{xN}^c, k_{yN}^c, k_{zN}^c)$ | Cartesian convective mass convectivity vector | material |

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| no | equation | documentation | layer |
|----|-----------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------|----------|
| 41 | $k_{xNS}^d := (\mu_{NS})^{-1} \cdot \left(v_{xN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$ | diffusional mass conductivity in x-direction | material |
| 42 | $k_{yNS}^d := (\mu_{NS})^{-1} \cdot \left(v_{yN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$ | diffusional mass conductivity in y-direction | material |
| 43 | $k_{zNS}^d := (\mu_{NS})^{-1} \cdot \left(v_{zN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$ | diffusional mass conductivity in z-direction | material |
| 44 | $k_{NS}^d := \text{Stack}(k_{xNS}^d, k_{yNS}^d, k_{zNS}^d)$ | Cartesian diffusional mass conductivity vector | material |
| 45 | $h_{NS} := H_N \odot (n_{NS})^{-1}$ | partial molar enthalpies | material |