

1 Variables

2 root

| | var | symbol | documentation | type | units | tokens | eqs |
|----|-----------|----------------|------------------------------------|----------|-------|--------|-----|
| 1 | $F_{N,A}$ | F | incidence matrix of directed graph | network | | [] | |
| 2 | t | t | time | frame | s | [] | |
| 3 | $\#$ | value | numerical value | constant | | [] | |
| 4 | 1 | one | numerical value 1 | constant | | [] | 1 |
| 5 | 0 | zero | numerical value 0 | constant | | [] | 2 |
| 6 | 1/2 | onehalf | numerical value 1/2 | constant | | [] | 3 |
| 58 | t^o | to | starting time | constant | s | [] | 41 |
| 59 | t^e | te | end time | constant | s | [] | 42 |

3 physical

| | var | symbol | documentation | type | units | tokens | eqs |
|----|----------|------------|------------------------------------|-------|---------------------------|--------|-----------|
| 15 | r_{xN} | r_x | x-coordinate | frame | m | [] | |
| 16 | r_{yN} | r_y | y-coordinate | frame | m | [] | |
| 17 | r_{zN} | r_z | z-coordinate | frame | m | [] | |
| 18 | n_{NS} | n | foundation state – species mass | state | mol | [] | 119 |
| 19 | U_N | U | foundation state – internal energy | state | $kg\,m^2\,s^{-2}$ | [] | |
| 20 | S_N | S | foundation state – entropy | state | $kg\,m^2\,K^{-1}\,s^{-2}$ | [] | |
| 21 | V_N | V | foundation state – volume | state | m^3 | [] | |
| 29 | H_N | H | enthalpy | state | $kg\,m^2\,s^{-2}$ | [] | 13 122 |
| 30 | A_N | A | Helmholtz energy | state | $kg\,m^2\,s^{-2}$ | [] | 14 |

Continued on next page

| | var | symbol | documentation | type | units | tokens | eqs |
|-----|------------|----------|-------------------------|----------------|-------------------------------------|--------|-----|
| 31 | G_N | G | Gibbs energy | state | $kg\,m^2\,s^{-2}$ | [] | 15 |
| 27 | B_N | B | Boltzmann constant | constant | $kg\,m^2\,K^{-1}\,s^{-2}$ | [] | 11 |
| 101 | A_N^v | Av | Avogadro number | constant | mol^{-1} | [] | |
| 102 | R_N | R | Gas constant | constant | $kg\,m^2\,mol^{-1}\,K^{-1}\,s^{-2}$ | [] | 82 |
| 22 | p_N | p | thermodynamic pressure | effort | $kg\,m^{-1}\,s^{-2}$ | [] | 7 |
| 23 | T_N | T | temperature | effort | K | [] | 8 |
| 24 | μ_{NS} | chem_pot | chemical potential | effort | $kg\,m^2\,mol^{-1}\,s^{-2}$ | [] | 9 |
| 36 | v_{xN} | v_x | velocity in x-direction | secondaryState | ms^{-1} | [] | 20 |
| 37 | v_{yN} | v_y | velocity in y-direction | secondaryState | ms^{-1} | [] | 21 |
| 38 | v_{zN} | v_z | velocity in z-direction | secondaryState | ms^{-1} | [] | 22 |
| 39 | v_N | v | velocity vector | secondaryState | ms^{-1} | [] | 23 |

4 control

| | var | symbol | documentation | type | units | tokens | eqs |
|-----|-------------|--------|---|-----------|----------|--------|-----|
| 141 | x_N | x | state | state | | [] | 131 |
| 142 | x_{oN} | xo | initial state | state | | [] | 123 |
| 139 | $A_{N,D}$ | A | dynamic matrix | constant | s^{-1} | [] | |
| 140 | $B_{A,D}$ | B | input gain matrix | constant | s^{-1} | [] | |
| 156 | $I_{N,D}$ | I_N_D | map D \rightarrow N – used in integration | constant | | [] | |
| 157 | u_{sA} | u_s | setpoint in terms of the measurement | constant | | [] | |
| 158 | T_{IN} | T_I | integrator time constant | constant | s | [] | |
| 155 | \dot{x}_D | dxdt | controller dynamics | diffState | s^{-1} | [] | 130 |
| 153 | u_A | u | controller input | input | | [] | 128 |

5 reactions

| | var | symbol | documentation | type | units | tokens | eqs |
|-----|-------------|--------|----------------------------------|----------------|-----------------------------|--------|-----|
| 98 | $N_{S,K}$ | N | stoichiometric matrix | constant | | [] | |
| 104 | $E_{a,NK}$ | Ea | Arrhenius's activation energy | constant | $kg\ m^2\ mol^{-1}\ s^{-2}$ | [] | 84 |
| 105 | K^o_K | Ko | Arrhenius's frequency factor | constant | $m^{-3}\ mol\ s^{-1}$ | [] | |
| 108 | c^o_{KS} | co_KS | standardisation of concentration | constant | $m^{-3}\ mol$ | [] | 87 |
| 106 | K_{NK} | K_NK | Arrhenius reaction constants | secondaryState | $m^{-3}\ mol\ s^{-1}$ | [] | 85 |
| 109 | ϕ_{KS} | phi_KS | propabilities to meet | secondaryState | | [] | 88 |

6 material

| | var | symbol | documentation | type | units | tokens | eqs |
|----|-------------|--------|---|----------------|------------------------------|--------|-----------|
| 40 | λ_S | Mm | species molecular masses | constant | $kg\ mol^{-1}$ | [] | |
| 41 | $C_{p,N}$ | Cp | total heat capacity at constant pressure | constant | $kg\ m^2\ K^{-1}\ s^{-2}$ | [] | 24 |
| 42 | $C_{v,N}$ | Cv | total heat capacity at constant volume | constant | $kg\ m^2\ K^{-1}\ s^{-2}$ | [] | 25 |
| 43 | $c_{p,S}$ | cp | specific heat capacity at constant pressure | constant | $m^2\ mol^2\ K^{-1}\ s^{-2}$ | [] | 26 133 |
| 44 | $c_{v,S}$ | cv | specific heat capacity at constant volume | constant | $m^2\ mol^2\ K^{-1}\ s^{-2}$ | [] | 27 134 |
| 45 | $k^q_{x,N}$ | kq_x | thermal conductivity in x-direction | secondaryState | $kg\ K^{-1}\ s^{-3}$ | [] | 28 |
| 46 | $k^q_{y,N}$ | kq_y | thermal conductivity in y-direction | secondaryState | $kg\ K^{-1}\ s^{-3}$ | [] | 29 |
| 47 | $k^q_{z,N}$ | kq_z | thermal conductivity in z-direction | secondaryState | $kg\ K^{-1}\ s^{-3}$ | [] | 30 |
| 48 | k^q_N | kq | Cartesian thermal conductivity vector | secondaryState | $kg\ K^{-1}\ s^{-3}$ | [] | 31 |
| 49 | $k^c_{x,N}$ | kc_x | convective mass convectivity in x-direction | secondaryState | $m^{-1}\ s$ | [] | 32 |
| 50 | $k^c_{y,N}$ | kc_y | convective mass convectivity in y-direction | secondaryState | $m^{-1}\ s$ | [] | 33 |
| 51 | $k^c_{z,N}$ | kc_z | convective mass convectivity in z-direction | secondaryState | $m^{-1}\ s$ | [] | 34 |

Continued on next page

| | var | symbol | documentation | type | units | tokens | eqs |
|----|-------------|--------|--|----------------|--------------------------|--------|-----|
| 52 | k_N^c | kc | Cartesian convective mass convectivity vector | secondaryState | $m^{-1} s$ | [] | 35 |
| 53 | k_{xNS}^d | kd_x | diffusional mass conductivity in x-direction | secondaryState | $kg^{-1} m^{-4} mol^2 s$ | [] | 36 |
| 54 | k_{yNS}^d | kd_y | diffusional mass conductivity in y-direction | secondaryState | $kg^{-1} m^{-4} mol^2 s$ | [] | 37 |
| 55 | k_{zNS}^d | kd_z | diffusional mass conductivity in z-direction | secondaryState | $kg^{-1} m^{-4} mol^2 s$ | [] | 38 |
| 56 | k_{NS}^d | kd | Cartesian diffusional mass conductivity vector | secondaryState | $kg^{-1} m^{-4} mol^2 s$ | [] | 39 |
| 60 | h_{NS} | h | partial molar enthalpies | secondaryState | $kg m^2 mol^{-1} s^{-2}$ | [] | 43 |

7 macroscopic

| | var | symbol | documentation | type | units | tokens | eqs |
|-----|------------------|--------|--|-----------|-----------------|--------|-----|
| 78 | d_A | d | direction of convective flow | transport | | [] | 61 |
| 80 | $A_{y,zN}$ | Ayz | cross sectional area in x-direction | transport | m^2 | [] | 63 |
| 83 | \hat{V}_A | fV | convective volumetric flow | transport | $m^3 s^{-1}$ | [] | 66 |
| 84 | c_{AS} | c_AS | molar species concentration in convective flow | transport | $m^{-3} mol$ | [] | 67 |
| 85 | \hat{n}_{AS}^c | fnc_AS | convective mass flow by stream | transport | $mol s^{-1}$ | [] | 68 |
| 86 | \hat{n}_{NS}^c | fnc | net convective mass flow | transport | $mol s^{-1}$ | [] | 69 |
| 115 | \hat{m}_A | fm_A | mass flow in arc | transport | $kg s^{-1}$ | [] | 94 |
| 125 | \hat{H}_A^c | fHc_A | enthalpy flow due to convection | transport | $kg m^2 s^{-3}$ | [] | 104 |
| 127 | \hat{H}_N^c | fHc | net enthalpy flow due to convection | transport | $kg m^2 s^{-3}$ | [] | 106 |
| 128 | \hat{n}_{AS}^d | fnd_AS | diffusional mass transfer in arc | transport | $mol s^{-1}$ | [] | 107 |
| 129 | \hat{n}_{NS}^d | fnd | net diffusional mass transfer | transport | $mol s^{-1}$ | [] | 108 |
| 130 | \hat{H}_A^d | fHd_A | enthalpy flow due to mass diffusion | transport | $kg m^2 s^{-3}$ | [] | 109 |
| 131 | \hat{H}_N^d | fHd | net enthalpy flow due to diffusion | transport | $kg m^2 s^{-3}$ | [] | 110 |
| 135 | \hat{w}_A | fw_A | example of work flow | transport | $kg m^2 s^{-3}$ | [] | 114 |
| 136 | \hat{w}_N | fw | net work flow | transport | $kg m^2 s^{-3}$ | [] | 115 |

Continued on next page

| | var | symbol | documentation | type | units | tokens | eqs |
|-----|------------------|---------|--|---------------|-----------------------|--------|-----|
| 176 | \hat{q}_{xA} | fq_A_x | conductive heat transfer in x-direction | transport | $kg\ m^2\ s^{-3}$ | [] | 162 |
| 177 | \hat{q}_{xN} | fq_x | net convective heat transfer in x-direction | transport | $kg\ m^2\ s^{-3}$ | [] | 163 |
| 10 | $F_{NS,AS}$ | F_NS_AS | click incidence matrix of directed species graph | network | | [] | 6 |
| 9 | $P_{NS,AS}$ | P_NS_AS | node species to arc species projection | projection | | [] | |
| 11 | $P_{K,NK}$ | P_K_NK | projection of conversion to node x conversion | projection | | [] | |
| 12 | $P_{S,NS}$ | P_S_NS | projection species to conversion x species | projection | | [] | |
| 13 | $P_{N,NK}$ | P_N_NK | projection node to node x conversion | projection | | [] | |
| 14 | $P_{NK,KS}$ | P_NK_KS | projection node x conversion to conversion x species | projection | | [] | |
| 95 | $P_{NS,KS}$ | P_NS_KS | projection node x species to conversion x species | projection | | [] | |
| 137 | n^o_{NS} | no | initial condition for species mass | state | mol | [] | 118 |
| 138 | H^o_N | Ho | initial condition for enthalpy | state | $kg\ m^2\ s^{-2}$ | [] | 120 |
| 159 | X | X | state for nodes with mass and energy | state | | [] | 132 |
| 92 | 1_{NK} | one_NK | one with energy | effort | | [] | 75 |
| 79 | c_{NS} | c | molar concentration | seconaryState | $m^{-3}\ mol$ | [] | 62 |
| 81 | m_N | m | mass in kg | seconaryState | kg | [] | 64 |
| 82 | ρ_N | density | density | seconaryState | $kg\ m^{-3}$ | [] | 65 |
| 91 | T_{NK} | T_NK | temperature in reactive systems | conversion | K | [] | 74 |
| 96 | c_{KS} | c_KS | concentration in the reactive systems | conversion | $m^{-3}\ mol$ | [] | 78 |
| 112 | ξ_{NK} | xi | extent of reaction | conversion | $m^{-3}\ mol\ s^{-1}$ | [] | 91 |
| 113 | $N_{NS,NK}$ | N_NS_NK | extended stoichiometry | conversion | | [] | 92 |
| 114 | \tilde{n}_{NS} | pn | production term | conversion | $mol\ s^{-1}$ | [] | 93 |
| 132 | \dot{n}_{NS} | dndt | species mass accumulation | diffState | $mol\ s^{-1}$ | [] | 111 |
| 133 | \dot{H}_N | dHdt | differential enthalpy balance | diffState | $kg\ m^2\ s^{-3}$ | [] | 164 |

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-reactions

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

13 reactions-control

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

14 control-material

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

15 material-control

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

16 control-macroscopic

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

17 macroscopic-control

| | var | symbol | documentation | type | units | tokens | eqs |
|-----|------------|--------|------------------------------------|-----------|----------------------|--------|-----|
| 143 | T_N^n | T_n | norming temperature | constant | K | [] | |
| 144 | p_N^n | p_n | norming pressure | constant | $kg\ m^{-1}\ s^{-2}$ | [] | |
| 145 | c_{NS}^n | c_n | norming concentration | constant | $m^{-3}\ mol$ | [] | |
| 146 | $F_{N,A}$ | F_N_A | projection N → A | constant | | [] | |
| 151 | $F_{A,NS}$ | F_A_NS | projection NS → A | constant | | [] | |
| 148 | s_{TA} | s_T | normed temperature signal | transform | | [] | 125 |
| 149 | s_{pA} | s_p | normed pressure signal | transform | | [] | 126 |
| 152 | s_{cA} | s_c | normed concentration signal vector | transform | | [] | 127 |

18 reactions-material

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

19 material–reactions

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

20 reactions–macroscopic

| | var | symbol | documentation | type | units | tokens | eqs |
|-----|-------------|--------|---------------|-----------|---------------------|--------|-----|
| 107 | K_{NK} | K_NK | link | transform | $m^{-3} mol s^{-1}$ | [] | 86 |
| 110 | ϕ_{KS} | phi_KS | link | transform | | [] | 89 |
| 111 | $N_{S,K}$ | N | link | transform | | [] | 90 |

21 macroscopic–reactions

| | var | symbol | documentation | type | units | tokens | eqs |
|-----|------------|--------|---------------------------------|-----------|--------------|--------|-----|
| 94 | T_{NK} | T_NK | temperature of reactive systems | transform | K | [] | 77 |
| 97 | c_{KS} | c_KS | link | transform | $m^{-3} mol$ | [] | 79 |
| 103 | $P_{N,NK}$ | P_N_NK | link | transform | | [] | 83 |

22 material–macroscopic

| | var | symbol | documentation | type | units | tokens | eqs |
|----|-------------|--------|----------------------|-----------|--------------------|--------|-----|
| 61 | λ_S | Mm | link to molar masses | transform | $kg mol^{-1}$ | [] | 44 |
| 62 | k_{xN}^q | kq_x | link | transform | $kg K^{-1} s^{-3}$ | [] | 45 |

Continued on next page

| | var | symbol | documentation | type | units | tokens | eqs |
|-----|-------------|--------|---------------|-----------|------------------------------|--------|-----|
| 63 | k_{yN}^q | kq_y | link | transform | $kg\ K^{-1}\ s^{-3}$ | [] | 46 |
| 64 | k_{zN}^q | kq_z | link | transform | $kg\ K^{-1}\ s^{-3}$ | [] | 47 |
| 65 | k_N^q | kq | link | transform | $kg\ K^{-1}\ s^{-3}$ | [] | 48 |
| 66 | k_{xN}^c | kc_x | link | transform | $m^{-1}\ s$ | [] | 49 |
| 67 | k_{yN}^c | kc_y | link | transform | $m^{-1}\ s$ | [] | 50 |
| 68 | k_{zN}^c | kc_z | link | transform | $m^{-1}\ s$ | [] | 51 |
| 69 | k_N^c | kc | link | transform | $m^{-1}\ s$ | [] | 52 |
| 70 | k_{xNS}^d | kd_x | link | transform | $kg^{-1}\ m^{-4}\ mol^2\ s$ | [] | 53 |
| 73 | k_{yNS}^d | kd_y | link | transform | $kg^{-1}\ m^{-4}\ mol^2\ s$ | [] | 56 |
| 74 | k_{zNS}^d | kd_z | link | transform | $kg^{-1}\ m^{-4}\ mol^2\ s$ | [] | 57 |
| 75 | k_{NS}^d | kd | link | transform | $kg^{-1}\ m^{-4}\ mol^2\ s$ | [] | 58 |
| 76 | c_{pS} | cp | link | transform | $m^2\ mol^2\ K^{-1}\ s^{-2}$ | [] | 59 |
| 77 | c_{vS} | cv | link | transform | $m^2\ mol^2\ K^{-1}\ s^{-2}$ | [] | 60 |
| 119 | h_{NS} | h | link | transform | $kg\ m^2\ mol^{-1}\ s^{-2}$ | [] | 98 |

23 macroscopic-material

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

24 gas-liquid

| | var | symbol | documentation | type | units | tokens | eqs |
|-----|-------------------|---------------|-------------------------|--------|-----------------------------|--------|------------|
| 160 | μ_{NS}^α | chem_pot_left | left chemical potential | effort | $kg\ m^2\ mol^{-1}\ s^{-2}$ | [] | 135 137 |

Continued on next page

| | var | symbol | documentation | type | units | tokens | eqs |
|-----|--------------------------------|----------------|-----------------------------|-----------|-----------------------------|--------|------------|
| 161 | μ^β_{NS} | chem_pot_right | right chemical potential | effort | $kg\,m^2\,mol^{-1}\,s^{-2}$ | [] | 136 138 |
| 164 | $T^{-\epsilon}_N$ | T_left | temparture left | effort | K | [] | 143 145 |
| 165 | $T^{+\epsilon}_N$ | T_right | right temperature | effort | K | [] | 144 146 |
| 166 | $p^{-\epsilon}_N$ | p_left | left pressure | effort | $kg\,m^{-1}\,s^{-2}$ | [] | 147 151 |
| 167 | $p^{+\epsilon}_N$ | p_right | right pressure | effort | $kg\,m^{-1}\,s^{-2}$ | [] | 148 150 |
| 162 | $(\hat{n}^d)^{-\epsilon}_{AS}$ | fnd_AS_left | left diffusional mass flow | transport | $mol\,s^{-1}$ | [] | 139 141 |
| 163 | $(\hat{n}^d)^{-\epsilon}_{AS}$ | fnd_AS_right | right diffusional mass flow | transport | $mol\,s^{-1}$ | [] | 140 142 |
| 168 | $(\hat{n}^c)^{-\epsilon}_{AS}$ | fnc_AS_left | left convective mass flow | transport | $mol\,s^{-1}$ | [] | 152 154 |
| 169 | $(\hat{n}^c)^{+\epsilon}_{AS}$ | fnc_AS_right | right convective mass flow | transport | $mol\,s^{-1}$ | [] | 153 155 |

25 gas–gas

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

26 liquid–liquid

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

27 gas–solid

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

28 solid–solid

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

29 liquid–solid

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

30 Equations

30.1 Model equations

| no | equation | documentation | layer |
|----|--|--|----------|
| 1 | $1 := Set(\#, \#)$ | numerical value 1 | root |
| 2 | $0 := Set(\#, \#)$ | numerical value 1 | root |
| 3 | $1/2 := Set(\#, \#)$ | numerical value 1/2 | root |
| 6 | $F_{NS,AS} := F_{N,A} \odot P_{NS,AS}$ | blick incidence matrix of directed species graph | physical |
| 7 | $p_N := \frac{\partial U_N}{\partial V_N}$ | thermodynamic pressure | physical |
| 8 | $T_N := \frac{\partial U_N}{\partial S_N}$ | temperature | physical |
| 9 | $\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$ | chemical potential | physical |
| 11 | $B_N := Set(S_N, \#)$ | Boltzmann constant | physical |
| 13 | $H_N := U_N + p_N \cdot V_N$ | enthalpy | physical |
| 14 | $A_N := U_N - T_N \cdot S_N$ | Helmholtz energy | physical |
| 15 | $G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$ | Gibbs energy | physical |
| 20 | $v_{xN} := \frac{\partial r_{xN}}{\partial t}$ | velocity in x-direction | physical |
| 21 | $v_{yN} := \frac{\partial r_{yN}}{\partial t}$ | velocity in y-direction | physical |
| 22 | $v_{zN} := \frac{\partial r_{zN}}{\partial t}$ | velocity in z-direction | physical |
| 23 | $v_N := Stack(v_{xN}, v_{yN}, v_{zN})$ | velocity vector | physical |

Continued on next page

| no | equation | documentation | layer |
|----|---|---|----------|
| 24 | $C_{pN} := \frac{\partial H_N}{\partial T_N}$ | total heat capacity at constant pressure | material |
| 25 | $C_{vN} := \frac{\partial U_N}{\partial T_N}$ | total heat capacity at constant volume | material |
| 26 | $c_{pS} := C_{pN} \cdot (\lambda_S)^{-1} \stackrel{N \in NS}{\star} n_{NS}$ | specific heat capacity at constant pressure | material |
| 27 | $c_{vS} := C_{vN} \cdot (\lambda_S)^{-1} \stackrel{N \in NS}{\star} n_{NS}$ | specific heat capacity at constant volume | material |
| 28 | $k_{xN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}$ | thermal conductivity in x-direction | material |
| 29 | $k_{yN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{yN}$ | thermal conductivity in y-direction | material |
| 30 | $k_{zN}^q := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{zN}$ | thermal conductivity in z-direction | material |
| 31 | $k_N^q := Stack(k_{xN}^q, k_{yN}^q, k_{zN}^q)$ | Cartesian thermal conductivity vector | material |
| 32 | $k_{xN}^c := \left(\lambda_S \stackrel{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$ | convective mass conductivity in x-direction | material |
| 33 | $k_{yN}^c := \left(\lambda_S \stackrel{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$ | convective mass conductivity in y-direction | material |
| 34 | $k_{zN}^c := \left(\lambda_S \stackrel{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$ | convective mass conductivity in z-direction | material |
| 35 | $k_N^c := Stack(k_{xN}^c, k_{yN}^c, k_{zN}^c)$ | Cartesian convective mass conductivity vector | material |
| 36 | $k_{xNS}^d := (\mu_{NS})^{-1} \cdot \left(v_{xN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$ | diffusional mass conductivity in x-direction | material |
| 37 | $k_{yNS}^d := (\mu_{NS})^{-1} \cdot \left(v_{yN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$ | diffusional mass conductivity in y-direction | material |

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| no | equation | documentation | layer |
|----|--|--|------------------------|
| 38 | $k_z^d_{NS} := (\mu_{NS})^{-1} \cdot \left(v_{zN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$ | diffusional mass conductivity in z-direction | material |
| 39 | $k^d_{NS} := Stack(k^d_{xNS}, k^d_{yNS}, k^d_{zNS})$ | Cartesian diffusional mass conductivity vector | material |
| 41 | $t^o := Set(t, t)$ | starting time | root |
| 42 | $t^e := Set(t, t)$ | end time | root |
| 43 | $h_{NS} := H_N \odot (n_{NS})^{-1}$ | partial molar enthalpies | material |
| 44 | $\lambda_S := \lambda_S$ | link to molar masses | material » macroscopic |
| 45 | $k^q_{xN} := k^q_{xN}$ | link | material » macroscopic |
| 46 | $k^q_{yN} := k^q_{yN}$ | link | material » macroscopic |
| 47 | $k^q_{zN} := k^q_{zN}$ | link | material » macroscopic |
| 48 | $k^q_N := k^q_N$ | link | material » macroscopic |
| 49 | $k^c_{xN} := k^c_{xN}$ | link | material » macroscopic |
| 50 | $k^c_{yN} := k^c_{yN}$ | link | material » macroscopic |
| 51 | $k^c_{zN} := k^c_{zN}$ | link | material » macroscopic |

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| 52 | $k_N^c := k_N^c$ | link | material » > macroscopic |
| 53 | $k_{xNS}^d := k_{xNS}^d$ | link | material » > macroscopic |
| 56 | $k_{yNS}^d := k_{yNS}^d$ | link | material » > macroscopic |
| 57 | $k_{zNS}^d := k_{zNS}^d$ | link | material » > macroscopic |
| 58 | $k_{NS}^d := k_{NS}^d$ | link | material » > macroscopic |
| 59 | $c_{pS} := c_{pS}$ | link | material » > macroscopic |
| 60 | $c_{vS} := c_{vS}$ | link | material » > macroscopic |
| 61 | $d_A := \text{sign} \left(F_{N,A} \overset{N}{\star} p_N \right)$ | direction of convective flow | macroscopic |
| 62 | $c_{NS} := (V_N)^{-1} \odot n_{NS}$ | molar concentration | macroscopic |
| 63 | $A_{y,zN} := r_{yN} \cdot r_{zN}$ | cross sectional area in x-direction | macroscopic |
| 64 | $m_N := \lambda_S \overset{S \in NS}{\star} n_{NS}$ | mass in kg | macroscopic |
| 65 | $\rho_N := (V_N)^{-1} \cdot m_N$ | density | macroscopic |
| 66 | $\hat{V}_A := (\rho_N)^{-1} \cdot k_{xN}^c \cdot A_{y,zN} \cdot F_{N,A} \overset{N}{\star} p_N$ | convective volumetric flow | macroscopic |
| 67 | $c_{AS} := (1/2 \cdot (F_{NS,AS} - d_A \odot F_{NS,AS})) \overset{NS}{\star} c_{NS}$ | molar species concentration in convective flow | macroscopic |

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| 68 | $\hat{n}_{AS}^c := \hat{V}_A \odot c_{AS}$ | convective mass flow by stream | macroscopic |
| 69 | $\hat{n}_{NS}^c := F_{NS,AS} \overset{AS}{\star} \hat{n}_{AS}^c$ | net convective mass flow | macroscopic |
| 74 | $T_{NK} := P_{N,NK} \overset{N}{\star} T_N$ | temperature in reactive systems | macroscopic |
| 75 | $1_{NK} := (T_{NK})^{-1} \cdot T_{NK}$ | one with energy | macroscopic |
| 77 | $T_{NK} := T_{NK}$ | temperature of reactive systems | macroscopic » > reactions |
| 78 | $c_{KS} := c_{NS} \overset{NS}{\star} P_{NS,KS}$ | concentration in the reactive systems | macroscopic |
| 79 | $c_{KS} := c_{KS}$ | link | macroscopic » > reactions |
| 82 | $R_N := A^v_N \cdot B_N$ | Gas constant | physical |
| 83 | $P_{N,NK} := P_{N,NK}$ | link | macroscopic » > reactions |
| 84 | $E_{aNK} := Set(P_{N,NK} \overset{N}{\star} R_N \cdot T_{NK}, \#)$ | Arrhenius's activation energy | reactions |
| 85 | $K_{NK} := K^o_K \odot exp((-E_{aNK}) \cdot (R_N \overset{N}{\star} P_{N,NK} \cdot T_{NK})^{-1})$ | Arrhenius reaction constants | reactions |
| 86 | $K_{NK} := K_{NK}$ | link | reactions » > macroscopic |
| 87 | $c^o_{KS} := Set(c_{KS}, \#)$ | standardisation of concentration | reactions |
| 88 | $\phi_{KS} := \prod (c_{KS} \cdot (c^o_{KS})^{-1})$ | propabilities to meet | reactions |
| 89 | $\phi_{KS} := \phi_{KS}$ | link | reactions » > macroscopic |

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| 90 | $N_{S,K} := N_{S,K}$ | link | reactions »> macroscopic |
| 91 | $\xi_{NK} := K_{NK} \cdot P_{NK,KS} \overset{KS}{\star} \phi_{KS}$ | extent of reaction | macroscopic |
| 92 | $N_{NS,NK} := P_{S,NS} \overset{S}{\star} \left(\left(P_{K,NK} \cdot T_{NK} \cdot (T_{NK})^{-1} \right) \overset{K}{\star} N_{S,K} \right)$ | extended stoichiometry | macroscopic |
| 93 | $\tilde{n}_{NS} := V_N \odot \left(N_{NS,NK} \overset{NK}{\star} \xi_{NK} \right)$ | production term | macroscopic |
| 94 | $\hat{m}_A := \lambda_S \overset{S \in AS}{\star} \hat{n}_{AS}^c$ | mass flow in arc | macroscopic |
| 98 | $h_{NS} := h_{NS}$ | link | material »> macroscopic |
| 104 | $\hat{H}_A^c := \left(F_{NS,AS} \overset{NS}{\star} h_{NS} \right) \overset{S \in AS}{\star} \hat{n}_{AS}^c$ | enthalpy flow due to convection | macroscopic |
| 106 | $\hat{H}_N^c := F_{N,A} \overset{A}{\star} \hat{H}_A^c$ | net enthalpy flow due to convection | macroscopic |
| 107 | $\hat{n}_{AS}^d := A_{y,zN} \odot \left(-k_{xNS}^d \right) \cdot F_{NS,AS} \overset{NS}{\star} \mu_{NS}$ | diffusional mass transfer in arc | macroscopic |
| 108 | $\hat{n}_{NS}^d := F_{NS,AS} \overset{AS}{\star} \hat{n}_{AS}^d$ | net diffusional mass transfer | macroscopic |
| 109 | $\hat{H}_A^d := \left(F_{NS,AS} \overset{NS}{\star} h_{NS} \right) \overset{S \in AS}{\star} \hat{n}_{AS}^d$ | enthalpy flow due to mass diffusion | macroscopic |
| 110 | $\hat{H}_N^d := F_{N,A} \overset{A}{\star} \hat{H}_A^d$ | net enthalpy flow due to diffusion | macroscopic |
| 111 | $\dot{n}_{NS} := \hat{n}_{NS}^c + \hat{n}_{NS}^d + \tilde{n}_{NS}$ | species mass accumulation | macroscopic |

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| 114 | $\hat{w}_A := Set(\hat{H}_A^c, \#)$ | example of work flow | macroscopic |
| 115 | $\hat{w}_N := F_{N,A} \overset{A}{\star} \hat{w}_A$ | net work flow | macroscopic |
| 118 | $n_{NS}^o := Set(n_{NS}, \#)$ | initial condition for species mass | macroscopic |
| 119 | $n_{NS} := \int_{t^o}^{t^e} \dot{n}_{NS} dt + n_{NS}^o$ | foundation state – species mass | macroscopic |
| 120 | $H_N^o := Set(H_N, \#)$ | initial condition for enthalpy | macroscopic |
| 122 | $H_N := \int_{t^o}^{t^e} \dot{H}_N dt + H_N^o$ | enthalpy | macroscopic |
| 123 | $xo_N := Set(x_N, \#)$ | initial state | control |
| 125 | $s_{TA} := F_{N,A} \overset{N}{\star} \left(T_N \cdot (T_N^n)^{-1} \right)$ | normed temperature signal | macroscopic control »> |
| 126 | $s_{pA} := F_{N,A} \overset{N}{\star} \left(p_N \cdot (p_N^n)^{-1} \right)$ | normed pressure signal | macroscopic control »> |
| 127 | $s_{cA} := F_{A,NS} \overset{NS}{\star} \left(c_{NS} \cdot (c_{NS}^n)^{-1} \right)$ | normed concentration signal vector | macroscopic control »> |
| 128 | $u_A := Stack(s_{TA}, s_{pA}, s_{cA})$ | controller input | control |
| 130 | $\dot{x}_D := A_{N,D} \overset{N}{\star} x_N + B_{A,D} \overset{A}{\star} u_A$ | controller dynamics | control |

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| 131 | $x_N := \int_{t^o}^{t^e} I_{N,D} \star \dot{x}_D dt$ | state | control |
| 132 | $X := MixedStack(n_{NS}, H_N)$ | state for nodes with mass and energy | macroscopic |
| 133 | $c_{pS} := Set(c_{pS}, \#)$ | specific heat capacity at constant pressure | material |
| 134 | $c_{vS} := Set(c_{vS}, \#)$ | specific heat capacity at constant volume | material |
| 135 | $\mu^\alpha_{NS} := (\mu_{NSaaaa})^{-\epsilon}$ | left chemical potential | gas » liquid |
| 136 | $\mu^\beta_{NS} := (\mu_{NSoooo})^{+\epsilon}$ | right chemical potential | gas » liquid |
| 137 | $\mu^\alpha_{NS} := Root(\mu^\alpha_{NS} - \mu^\beta_{NS}, \mu^\alpha_{NS})$ | left chemical potential | gas » liquid |
| 138 | $\mu^\beta_{NS} := Root(\mu^\beta_{NS} - \mu^\alpha_{NS}, \mu^\beta_{NS})$ | right chemical potential | gas » liquid |
| 139 | $(\hat{n}^d)^{-\epsilon}_{AS} := (\hat{n}^d_{ASaaaa})^{-\epsilon}$ | left diffusional mass flow | gas » liquid |
| 140 | $(\hat{n}^d)^{-\epsilon}_{AS} := (\hat{n}^d_{ASoooo})^{+\epsilon}$ | right diffusional mass flow | gas » liquid |
| 141 | $(\hat{n}^d)^{-\epsilon}_{AS} := Root\left((\hat{n}^d)^{-\epsilon}_{AS} - (\hat{n}^d)^{-\epsilon}_{AS}, (\hat{n}^d)^{-\epsilon}_{AS}\right)$ | left diffusional mass flow | gas » liquid |
| 142 | $(\hat{n}^d)^{-\epsilon}_{AS} := Root\left((\hat{n}^d)^{-\epsilon}_{AS} - (\hat{n}^d)^{-\epsilon}_{AS}, (\hat{n}^d)^{-\epsilon}_{AS}\right)$ | right diffusional mass flow | gas » liquid |

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|-----|--|----------------------------|---------------|
| 143 | $T^{-\epsilon}_N := (T_Naaaa)^{-\epsilon}$ | temparture left | gas »> liquid |
| 144 | $T^{+\epsilon}_N := (T_Noooo)^{+\epsilon}$ | right temperature | gas »> liquid |
| 145 | $T^{-\epsilon}_N := Root(T^{-\epsilon}_N - T^{+\epsilon}_N, T^{-\epsilon}_N)$ | temparture left | gas »> liquid |
| 146 | $T^{+\epsilon}_N := Root(T^{-\epsilon}_N - T^{+\epsilon}_N, T^{+\epsilon}_N)$ | right temperature | gas »> liquid |
| 147 | $p^{-\epsilon}_N := (p_Naaaa)^{-\epsilon}$ | left pressure | gas »> liquid |
| 148 | $p^{+\epsilon}_N := (p_Noooo)^{+\epsilon}$ | right pressure | gas »> liquid |
| 150 | $p^{+\epsilon}_N := Root(p^{-\epsilon}_N - p^{+\epsilon}_N, p^{+\epsilon}_N)$ | right pressure | gas »> liquid |
| 151 | $p^{-\epsilon}_N := Root(p^{-\epsilon}_N - p^{+\epsilon}_N, p^{-\epsilon}_N)$ | left pressure | gas »> liquid |
| 152 | $(\hat{n}^c)^{-\epsilon}_{AS} := (\hat{n}^c_{ASaaaa})^{-\epsilon}$ | left convective mass flow | gas »> liquid |
| 153 | $(\hat{n}^c)^{+\epsilon}_{AS} := (\hat{n}^c_{ASoooo})^{+\epsilon}$ | right convective mass flow | gas »> liquid |
| 154 | $(\hat{n}^c)^{-\epsilon}_{AS} := Root\left((\hat{n}^c)^{-\epsilon}_{AS} - (\hat{n}^c)^{+\epsilon}_{AS}, (\hat{n}^c)^{-\epsilon}_{AS}\right)$ | left convective mass flow | gas »> liquid |
| 155 | $(\hat{n}^c)^{+\epsilon}_{AS} := Root\left((\hat{n}^c)^{-\epsilon}_{AS} - (\hat{n}^c)^{+\epsilon}_{AS}, (\hat{n}^c)^{+\epsilon}_{AS}\right)$ | right convective mass flow | gas »> liquid |

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| 162 | $\hat{q}_{xA} := A_{y,zN} \cdot k_{xN}^q \cdot F_{N,A} \overset{N}{\star} T_N$ | conductive heat transfer in x-direction | macroscopic |
| 163 | $\hat{q}_{xN} := F_{N,A} \overset{A}{\star} \hat{q}_{xA}$ | net convective heat transfer in x-direction | macroscopic |
| 164 | $\dot{H}_N := \hat{H}_N^c + \hat{H}_N^d + \hat{q}_{xN} + \hat{w}_N$ | differential enthalpy balance | macroscopic |