# 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 | $A^v{}_N$ | 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 | $\mu_{NS}$ | chem_pot | chemical potential | effort | $kg\,m^2\,mol^{-1}\,s^{-2}$ | [] | 9 |
| 36 | $v_{xN}$ | v_x | velocity in x-direction | seconaryState | $ms^{-1}$ | [] | 20 |
| 37 | $v_{yN}$ | v_y | velocity in y-direction | seconaryState | $ms^{-1}$ | [] | 21 |
| 38 | $v_{zN}$ | v_z | velocity in z-direction | seconaryState | $ms^{-1}$ | [] | 22 |
| 39 | $v_N$ | v | velocity vector | seconaryState | $ms^{-1}$ | [] | 23 |

# 4    control

| | var | symbol | documentation | type | units | tokens | eqs |
|---|---|---|---|---|---|---|---|
| 141 | $x_N$ | x | state | state | | [] | 131 |
| 142 | $xo_N$ | 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 $->$ 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 | $E_{aNK}$ | 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 | seconaryState | $m^{-3}\,mol\,s^{-1}$ | [] | 85 |
| 109 | $\phi_{KS}$ | phi_KS | propabilities to meet | seconaryState | | [] | 88 |

# 6 material

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

*Continued on next page*

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

# 7 macroscopic

| | var | symbol | documentation | type | units | tokens | eqs |
|---|---|---|---|---|---|---|---|
| 78 | $d_A$ | d | direction of convective flow | transport | | [] | 61 |
| 80 | $A_{y,z\,N}$ | 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 | $\hat{n}^c_{AS}$ | fnc_AS | convective mass flow by stream | transport | $mol\,s^{-1}$ | [] | 68 |
| 86 | $\hat{n}^c_{NS}$ | 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 | $\hat{H}^c_A$ | fHc_A | enthalpy flow due to convection | transport | $kg\,m^2\,s^{-3}$ | [] | 104 |
| 127 | $\hat{H}^c_N$ | fHc | net enthalpy flow due to convection | transport | $kg\,m^2\,s^{-3}$ | [] | 106 |
| 128 | $\hat{n}^d_{AS}$ | fnd_AS | diffusional mass transfer in arc | transport | $mol\,s^{-1}$ | [] | 107 |
| 129 | $\hat{n}^d_{NS}$ | fnd | net diffusional mass transfer | transport | $mol\,s^{-1}$ | [] | 108 |
| 130 | $\hat{H}^d_A$ | fHd_A | enthalpy flow due to mass diffusion | transport | $kg\,m^2\,s^{-3}$ | [] | 109 |
| 131 | $\hat{H}^d_N$ | 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 |

| | var | symbol | documentation | type | units | tokens | eqs |
|---|---|---|---|---|---|---|---|
| 10 | $F_{NS,AS}$ | F_NS_AS | blick 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 | $\rho_N$ | 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 | $\xi_{NK}$ | 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 | $kg\,m^2\,s^{-3}$ | [] | 116 |

# 8 solid

5

| | 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 | $c^n{}_{NS}$ | 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 | $s_{T\,A}$ | s_T | normed temperature signal | transform | | [] | 125 |
| 149 | $s_{p\,A}$ | s_p | normed pressure signal | transform | | [] | 126 |
| 152 | $s_{c\,A}$ | s_c | noremed 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 | $\phi_{KS}$ | 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 reacive 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 | $\lambda_S$ | 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 | | $k^q_{y\,N}$ | kq_y | link | transform | $kg\,K^{-1}\,s^{-3}$ | [] | 46 |
| 64 | | $k^q_{z\,N}$ | kq_z | link | transform | $kg\,K^{-1}\,s^{-3}$ | [] | 47 |
| 65 | | $k^q_{\,N}$ | kq | link | transform | $kg\,K^{-1}\,s^{-3}$ | [] | 48 |
| 66 | | $k^c_{x\,N}$ | kc_x | link | transform | $m^{-1}\,s$ | [] | 49 |
| 67 | | $k^c_{y\,N}$ | kc_y | link | transform | $m^{-1}\,s$ | [] | 50 |
| 68 | | $k^c_{z\,N}$ | kc_z | link | transform | $m^{-1}\,s$ | [] | 51 |
| 69 | | $k^c_{\,N}$ | kc | link | transform | $m^{-1}\,s$ | [] | 52 |
| 70 | | $k^d_{x\,NS}$ | kd_x | link | transform | $kg^{-1}\,m^{-4}\,mol^2\,s$ | [] | 53 |
| 73 | | $k^d_{y\,NS}$ | kd_y | link | transform | $kg^{-1}\,m^{-4}\,mol^2\,s$ | [] | 56 |
| 74 | | $k^d_{z\,NS}$ | kd_z | link | transform | $kg^{-1}\,m^{-4}\,mol^2\,s$ | [] | 57 |
| 75 | | $k^d_{\,NS}$ | kd | link | transform | $kg^{-1}\,m^{-4}\,mol^2\,s$ | [] | 58 |
| 76 | | $c_{p\,S}$ | cp | link | transform | $m^2\,mol^2\,K^{-1}\,s^{-2}$ | [] | 59 |
| 77 | | $c_{v\,S}$ | 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 | | $\mu^\alpha_{\,NS}$ | chem_pot_left | left chemical potential | effort | $kg\,m^2\,mol^{-1}\,s^{-2}$ | [] | 135 137 |

| | var | symbol | documentation | type | units | tokens | eqs |
|---|---|---|---|---|---|---|---|
| 161 | $\mu^{\beta}{}_{NS}$ | chem_pot_right | right chemical potential | effort | $kg\,m^2\,mol^{-1}\,s^{-2}$ | [] | 136<br>138 |

## 25   gas–solid

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

## 26   liquid–solid

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

# 27 Equations

## 27.1 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 | $v_N := Stack\left(v_{xN}, v_{yN}, v_{zN}\right)$ | velocity vector | physical |

| 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 | $c_{pS} := C_{pN} \cdot (\lambda_S)^{-1} \overset{N \in NS}{\underset{\star}{}} n_{NS}$ | specific heat capacity at constant pressure | material |
| 27 | $c_{vS} := C_{vN} \cdot (\lambda_S)^{-1} \overset{N \in NS}{\underset{\star}{}} n_{NS}$ | specific heat capacity at constant volume | material |
| 28 | $k^q_{xN} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}$ | thermal conductivity in x-direction | material |
| 29 | $k^q_{yN} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{yN}$ | thermal conductivity in y-direction | material |
| 30 | $k^q_{zN} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{zN}$ | thermal conductivity in z-direction | material |
| 31 | $k^q_N := Stack\left(k^q_{xN}, k^q_{yN}, k^q_{zN}\right)$ | Carthesian thermal conductivity vector | material |
| 32 | $k^c_{xN} := \left(\lambda_S \overset{S \in NS}{\underset{\star}{}} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$ | convective mass convectivity in x-direction | material |
| 33 | $k^c_{yN} := \left(\lambda_S \overset{S \in NS}{\underset{\star}{}} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$ | convective mass convectivity in y-direction | material |
| 34 | $k^c_{zN} := \left(\lambda_S \overset{S \in NS}{\underset{\star}{}} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$ | convective mass convectivity in z-direction | material |
| 35 | $k^c_N := Stack\left(k^c_{xN}, k^c_{yN}, k^c_{zN}\right)$ | Cartesian convective mass convectivity vector | material |
| 36 | $k^d_{xNS} := (\mu_{NS})^{-1} \cdot \left(v_{xN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$ | diffusional mass conductivity in x-direction | material |
| 37 | $k^d_{yNS} := (\mu_{NS})^{-1} \cdot \left(v_{yN} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$ | diffusional mass conductivity in y-direction | material |

| no | equation | documentation | layer |
|---|---|---|---|
| 38 | $k^d_{zNS} := (\mu_{NS})^{-1} . \left( v_{zN} \odot \left( (V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}} \right) \right)$ | diffusional mass conductivity in z-direction | material |
| 39 | $k^d_{NS} := Stack \left( k^d_{xNS}, k^d_{yNS}, k^d_{zNS} \right)$ | 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 |

| no | equation | documentation | layer |
|---|---|---|---|
| 52 | $k^c{}_N := k^c{}_N$ | link | material »> macroscopic |
| 53 | $k^d_{x\,NS} := k^d_{x\,NS}$ | link | material »> macroscopic |
| 56 | $k^d_{y\,NS} := k^d_{y\,NS}$ | link | material »> macroscopic |
| 57 | $k^d_{z\,NS} := k^d_{z\,NS}$ | link | material »> macroscopic |
| 58 | $k^d{}_{NS} := k^d{}_{NS}$ | link | material »> macroscopic |
| 59 | $c_{p\,S} := c_{p\,S}$ | link | material »> macroscopic |
| 60 | $c_{v\,S} := c_{v\,S}$ | link | material »> macroscopic |
| 61 | $d_A := \mathrm{sign}\left(F_{N,A} \overset{N}{\star} p_N\right)$ | direction of convective flow | macroscopic |
| 62 | $c_{NS} := (V_N)^{-1} \odot n_{NS}$ | molar concentration | macroscopic |
| 63 | $A_{y,z\,N} := r_{y\,N} \cdot r_{z\,N}$ | 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 | $\hat{V}_A := (\rho_N)^{-1} \cdot k^c_{x\,N} \cdot A_{y,z\,N} \cdot F_{N,A} \overset{N}{\star} p_N$ | 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 |

*Continued on next page*

| no | equation | documentation | layer |
|---|---|---|---|
| 68 | $\hat{n}^c_{AS} := \hat{V}_A \odot c_{AS}$ | convective mass flow by stream | macroscopic |
| 69 | $\hat{n}^c_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^c_{AS}$ | net convective mass flow | macroscopic |
| 74 | $T_{NK} := P_{N,NK} \overset{N}{\star} T_N$ | temperature in reactive systems | macroscopic |
| 75 | $1_{NK} := (T_{NK})^{-1} . T_{NK}$ | one with energy | macroscopic |
| 77 | $T_{NK} := T_{NK}$ | temperature of reacive 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 | $R_N := A^v{}_N . B_N$ | Gas constant | physical |
| 83 | $P_{N,NK} := P_{N,NK}$ | link | macroscopic »> reactions |
| 84 | $E_{aNK} := Set(P_{N,NK} \overset{N}{\star} R_N . T_{NK}, \#)$ | Arrhenius's activation energy | reactions |
| 85 | $K_{NK} := K^o{}_K \odot exp((-E_{aNK}) . \left( R_N \overset{N}{\star} P_{N,NK} . T_{NK} \right)^{-1})$ | Arrhenius reaction constants | reactions |
| 86 | $K_{NK} := K_{NK}$ | link | reactions »> macroscopic |
| 87 | $c^o{}_{KS} := Set(c_{KS}, \#)$ | standardisation of concentration | reactions |
| 88 | $\phi_{KS} := \prod \left( c_{KS} . (c^o{}_{KS})^{-1} \right)$ | propabilities to meet | reactions |
| 89 | $\phi_{KS} := \phi_{KS}$ | link | reactions »> macroscopic |

*Continued on next page*

| no | equation | documentation | layer |
|---|---|---|---|
| 90 | $N_{S,K} := N_{S,K}$ | link | reactions »> macroscopic |
| 91 | $\xi_{NK} := K_{NK} \,.\, P_{NK,KS} \overset{KS}{\star} \phi_{KS}$ | extent of reaction | macroscopic |
| 92 | $N_{NS,NK} := P_{S,NS} \overset{S}{\star} \left( \left( P_{K,NK} \,.\, T_{NK} \,.\, (T_{NK})^{-1} \right) \overset{K}{\star} N_{S,K} \right)$ | extended stoichiometry | macroscopic |
| 93 | $\tilde{n}_{NS} := V_N \odot \left( N_{NS,NK} \overset{NK}{\star} \xi_{NK} \right)$ | production term | macroscopic |
| 94 | $\hat{m}_A := \lambda_S \overset{S \in AS}{\star} \hat{n}^c_{AS}$ | mass flow in arc | macroscopic |
| 98 | $h_{NS} := h_{NS}$ | link | material »> macroscopic |
| 104 | $\hat{H}^c_A := \left( F_{NS,AS} \overset{NS}{\star} h_{NS} \right) \overset{S \in AS}{\star} \hat{n}^c_{AS}$ | enthalpy flow due to convection | macroscopic |
| 106 | $\hat{H}^c_N := F_{N,A} \overset{A}{\star} \hat{H}^c_A$ | net enthalpy flow due to convection | macroscopic |
| 107 | $\hat{n}^d_{AS} := A_{y,z\,N} \odot \left( -k^d_{x\,NS} \right) .\, F_{NS,AS} \overset{NS}{\star} \mu_{NS}$ | diffusional mass transfer in arc | macroscopic |
| 108 | $\hat{n}^d_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^d_{AS}$ | net diffusional mass transfer | macroscopic |
| 109 | $\hat{H}^d_A := \left( F_{NS,AS} \overset{NS}{\star} h_{NS} \right) \overset{S \in AS}{\star} \hat{n}^d_{AS}$ | enthalpy flow due to mass diffusion | macroscopic |
| 110 | $\hat{H}^d_N := F_{N,A} \overset{A}{\star} \hat{H}^d_A$ | net enthalpy flow due to diffusion | macroscopic |
| 111 | $\dot{n}_{NS} := \hat{n}^c_{NS} + \hat{n}^d_{NS} + \tilde{n}_{NS}$ | species mass accumulation | macroscopic |

*Continued on next page*

| no | equation | documentation | layer | |
|----|----------|---------------|-------|--|
| 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 | |
| 116 | $\dot{H}_N := \hat{H}_N^c + \hat{H}_N^d + \hat{w}_N$ | differential enthalpy balance | macroscopic | |
| 118 | $n^o{}_{NS} := Set(n_{NS}, \#)$ | initial condition for species mass | macroscopic | |
| 119 | $n_{NS} := \int_{t^o}^{t^e} \dot{n}_{NS} \; dt + n^o{}_{NS}$ | foundation state – species mass | macroscopic | |
| 120 | $H^o{}_N := Set(H_N, \#)$ | initial condition for enthalpy | macroscopic | |
| 122 | $H_N := \int_{t^o}^{t^e} \dot{H}_N \; dt + H^o{}_N$ | enthalpy | macroscopic | |
| 123 | $xo_N := Set(x_N, \#)$ | initial state | control | |
| 125 | $s_{TA} := F_{N,A} \overset{N}{\star} \left( T_N \, . \, (T^n{}_N)^{-1} \right)$ | normed temperature signal | macroscopic control | »> |
| 126 | $s_{pA} := F_{N,A} \overset{N}{\star} \left( p_N \, . \, (p^n{}_N)^{-1} \right)$ | normed pressure signal | macroscopic control | »> |
| 127 | $s_{cA} := F_{A,NS} \overset{NS}{\star} \left( c_{NS} \, . \, (c^n{}_{NS})^{-1} \right)$ | noremed concentration signal vector | macroscopic control | »> |
| 128 | $u_A := Stack \left( s_{TA}, s_{pA}, s_{cA} \right)$ | controller input | control | |

*Continued on next page*

| no | equation | documentation | layer |
|---|---|---|---|
| 130 | $\dot{x}_D := A_{N,D} \overset{N}{\star} x_N + B_{A,D} \overset{A}{\star} u_A$ | controller dynamics | control |
| 131 | $x_N := \int_{t^o}^{t^e} I_{N,D} \overset{D}{\star} \dot{x}_D \ dt$ | 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 | $\mu^{\alpha}{}_{NS} := \mu_{NS}^{-\epsilon}$ | left chemical potential | gas »> liquid |
| 136 | $\mu^{\beta}{}_{NS} := \mu_{NS}^{+\epsilon}$ | right chemical potential | gas »> liquid |
| 137 | $\mu^{\alpha}{}_{NS} := Root\left(\mu^{\alpha}{}_{NS} - \mu^{\beta}{}_{NS}, \mu^{\alpha}{}_{NS}\right)$ | left chemical potential | gas »> liquid |
| 138 | $\mu^{\beta}{}_{NS} := Root\left(\mu^{\beta}{}_{NS} - \mu^{\alpha}{}_{NS}, \mu^{\beta}{}_{NS}\right)$ | right chemical potential | gas »> liquid |