# 1 Variables

# 2 root

| | var | symbol | documentation | type | units | tokens | eqs |
|---|---|---|---|---|---|---|---|
| 5 | $F_{N,A}$ | `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 | $r_{x\,N}$ | `r_x` | x-coordinate | frame | $m$ | [] | |
| 10 | $r_{y\,N}$ | `r_y` | y-coordinate | frame | $m$ | [] | |
| 23 | $r_{z\,N}$ | `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 | $kg\,m^2\,s^{-2}$ | [] | 9 122 123 |
| 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 | $n_{N\,S}$ | `n` | species molar mass | state | $mol$ | [] | 116 |
| 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 | $kg\,m^{-1}\,s^{-2}$ | [] | 6 115 |
| 16 | $T_N$ | `T` | temperature | effort | $K$ | [] | 7 113 |
| 45 | $\mu_{N\,S}$ | `chem_pot` | chemical potential | effort | $kg\,m^2\,mol^{-1}\,s^{-2}$ | [] | 32 114 |
| 21 | $v_{x\,N}$ | `v_x` | velocity in x-direction | secondaryState | $ms^{-1}$ | [] | 12 |
| 22 | $v_{y\,N}$ | `v_y` | velocity in y direction | secondaryState | $ms^{-1}$ | [] | 13 |
| 24 | $v_{z\,N}$ | `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 |
|---|---|---|---|---|---|---|---|
| 139 | $m_A$ | `mc` | measurements | input | | [] | |
| 129 | $I_{N,D}$ | `I_N_D` | identity to shift from differential space integral space | network | | [] | |
| 130 | $I_{A,D}$ | `I_A_D` | identity to shift from differential space to arc | network | | [] | |
| 137 | $x_N$ | `x` | controller state | state | | [] | 112 |
| 138 | ${x^o}_N$ | `xo` | controller initial condition | state | | [] | 103 |
| 133 | $C_{N,A}$ | `Cx` | measurement matrix | constant | | [] | 144 |
| 134 | $D_{N,D}$ | `Dx` | event matrix (dimension issue) | constant | | [] | 145 |
| 135 | ${y^o}_A$ | `setpoint` | set point | constant | | [] | 146 |
| 136 | $D_A$ | `D_A` | event diagonal matrix (no dimension problem) | constant | | [] | 147 |
| 142 | $A_{N,D}$ | `Ax` | dynamic control matrix | constant | $s^{-1}$ | [] | 148 |
| 143 | $B_{A,D}$ | `Bx` | input matrix | constant | $s^{-1}$ | [] | 149 |
| 144 | $\dot{x}_D$ | `dxdt` | differential controller state | diffState | $s^{-1}$ | [] | 106 |
| 140 | $e_A$ | `e` | control error | algebraic | | [] | 104 |

## 5 reactions

| | var | symbol | documentation | type | units | tokens | eqs |
|---|---|---|---|---|---|---|---|
| 86 | $N_{S,K}$ | `N` | stoichiometric matrix | constant | | [] | |
| 87 | $E_{aNK}$ | `Ea` | Arrhenius's activation energy | constant | $kg\, m^2\, mol^{-1}\, s^{-2}$ | [] | 64 |
| 88 | ${K^o}_K$ | `Ko` | Arrhenius's frequency factor | constant | $m^{-3}\, mol\, s^{-1}$ | [] | |
| 89 | $K_{NK}$ | `K_NK` | Arrhenius reaction constant | constant | $m^{-3}\, mol\, s^{-1}$ | [] | 65 |
| 114 | $c_{KS}$ | `c_KS` | molar concentrations in reactive system | constant | $m^{-3}\, mol$ | [] | 90 |
| 115 | ${c^o}_{KS}$ | `co_KS` | norming molar concentrations | constant | $m^{-3}\, mol$ | [] | 91 |
| 116 | $\phi_{KS}$ | `phi_KS` | probability of species to meet | constant | | [] | 92 |

# 6 material

| | var | symbol | documentation | type | units | tokens | eqs |
|---|---|---|---|---|---|---|---|
| 29 | $\lambda_S$ | `Mm` | species molecular masses | constant | $kg\, mol^{-1}$ | [] | 142 |
| 30 | $C_{p\,N}$ | `Cp` | total heat capacity at constant pressure | property | $kg\, m^2\, K^{-1}\, s^{-2}$ | [] | 18 |
| 31 | $C_{v\,N}$ | `Cv` | total heat capacity at constant volume | property | $kg\, m^2\, K^{-1}\, s^{-2}$ | [] | 19 |
| 34 | $k^q_{x\,N}$ | `kq_x` | thermal conductivity in x-direction | property | $kg\, K^{-1}\, s^{-3}$ | [] | 22<br>131 |
| 35 | $k^q_{y\,N}$ | `kq_y` | thermal conductivity in y-direction | property | $kg\, K^{-1}\, s^{-3}$ | [] | 23<br>132 |
| 36 | $k^q_{z\,N}$ | `kq_z` | thermal conductivity in z-direction | property | $kg\, K^{-1}\, s^{-3}$ | [] | 24<br>133 |
| 37 | $k^q{}_N$ | `kq` | Carthesian thermal conductivity vector | property | $kg\, K^{-1}\, s^{-3}$ | [] | 25 |
| 50 | $k^c_{x\,N}$ | `kc_x` | convective mass convectivity in x-direction | property | $m^{-1}\, s$ | [] | 37<br>134 |
| 51 | $k^c_{y\,N}$ | `kc_y` | convective mass convectivity in y-direction | property | $m^{-1}\, s$ | [] | 38<br>135 |
| 52 | $k^c_{z\,N}$ | `kc_z` | convective mass convectivity in z-direction | property | $m^{-1}\, s$ | [] | 39<br>136 |
| 53 | $k^c{}_N$ | `kc` | Cartesian convective mass convectivity vector | property | $m^{-1}\, s$ | [] | 40 |
| 54 | $k^d_{x\,NS}$ | `kd_x` | diffusional mass conductivity in x-direction | property | $kg^{-1}\, m^{-4}\, mol^2\, s$ | [] | 41<br>137 |
| 55 | $k^d_{y\,NS}$ | `kd_y` | diffusional mass conductivity in y-direction | property | $kg^{-1}\, m^{-4}\, mol^2\, s$ | [] | 42<br>138 |
| 56 | $k^d_{z\,NS}$ | `kd_z` | diffusional mass conductivity in z-direction | property | $kg^{-1}\, m^{-4}\, mol^2\, s$ | [] | 43 |
| 57 | $k^d{}_{NS}$ | `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<br>139 |
| 71 | $\rho_N$ | `density` | mass density | property | $kg\, m^{-3}$ | [] | 49 |

*Continued on next page*

| | var | symbol | documentation | type | units | tokens | eqs |
|---|---|---|---|---|---|---|---|
| 148 | $cp_N$ | `cp` | specific heat capacity at constant pressure | property | $m^2\,K^{-1}\,s^{-2}$ | [] | 120<br>140 |
| 149 | $cv_N$ | `cv` | specific heat capacity at constant volume | property | $m^2\,K^{-1}\,s^{-2}$ | [] | 121<br>141 |
| 154 | $\theta$ | `data` | available data set | property | | [] | 143 |

# 7 macroscopic

| | var | symbol | documentation | type | units | tokens | eqs |
|---|---|---|---|---|---|---|---|
| 65 | $d_A$ | d | direction of convective flow | transport | | [] | 46 |
| 98 | $\hat{V}_A$ | fV | volumetric flow in x-direction | transport | $m^3\,s^{-1}$ | [] | 74 |
| 104 | $\hat{n}^d{}_{AS}$ | fnd_AS | diffusional mass transfer per arc | transport | $mol\,s^{-1}$ | [] | 80 |
| 105 | $\hat{n}^d{}_{NS}$ | fnd | net diffusional mass transfer | transport | $mol\,s^{-1}$ | [] | 81 |
| 106 | $\hat{H}^d{}_A$ | fHd_A | enthalpy flow due to mass diffusion per arc | transport | $kg\,m^2\,s^{-3}$ | [] | 82 |
| 107 | $\hat{H}^d{}_N$ | fHd | net enthalpy flow due to mass diffusion | transport | $kg\,m^2\,s^{-3}$ | [] | 83 |
| 109 | $c_{AS}$ | c_AS | moler concentration in convective arc | transport | $m^{-3}\,mol$ | [] | 85 |
| 110 | $\hat{n}^c{}_{AS}$ | fnc_AS | convective molar mass flow per arc | transport | $mol\,s^{-1}$ | [] | 86 |
| 111 | $\hat{n}^c{}_{NS}$ | fnc | net convective molar mass flow | transport | $mol\,s^{-1}$ | [] | 87 |
| 120 | $\hat{H}^c{}_A$ | fHc_A | enthalpy flow due to convective mass flow | transport | $kg\,m^2\,s^{-3}$ | [] | 96 |
| 121 | $\hat{H}^c{}_N$ | fHc | net enthalpy flow due to convective mass flow | transport | $kg\,m^2\,s^{-3}$ | [] | 97 |
| 122 | $\hat{w}_A$ | fw_A | example of work flow | transport | $kg\,m^2\,s^{-3}$ | [] | 98 |
| 123 | $\hat{w}_N$ | fw | net work flow | transport | $kg\,m^2\,s^{-3}$ | [] | 99 |
| 124 | $\hat{q}_A$ | fq_A_x | heat flow in x-direction | transport | $kg\,m^2\,s^{-3}$ | [] | 100 |
| 125 | $\hat{q}_N$ | fq | net heat flow | transport | $kg\,m^2\,s^{-3}$ | [] | 101 |
| 95 | $A_{yz\,N}$ | Ayz | cross sectional area in x-direction | geometry | $m^2$ | [] | 71 |
| 96 | $A_{xz\,N}$ | Axz | cross sectional area in y direction | geometry | $m^2$ | [] | 72 |
| 97 | $A_{xy\,N}$ | Axy | cross sectional area in z-direction | geometry | $m^2$ | [] | 73 |
| 73 | $F_{NS,AS}$ | F_NS_AS | incidence matrix of directed graphs for for species NS x AS | network | | [] | 51 |
| 59 | $P_{NS,AS}$ | P_NS_AS | node species to arc species projection | projection | | [] | |
| 60 | $P_{K,NK}$ | P_K_NK | projection of conversion to node x conversion | projection | | [] | |
| 61 | $P_{S,NS}$ | P_S_NS | projection species to conversion x species | projection | | [] | |

*Continued on next page*

| | var | symbol | documentation | type | units | tokens | eqs |
|---|---|---|---|---|---|---|---|
| 62 | $P_{N,NK}$ | P_N_NK | projection node to node x conversion | projection | | [] | |
| 63 | $P_{NK,KS}$ | P_NK_KS | projection node x conversion to conversion x species | projection | | [] | |
| 64 | $P_{NS,KS}$ | P_NS_KS | projection node x species to conversion x species | projection | | [] | |
| 127 | $D_{N,A}$ | D | difference operator | differenceOperator | | [] | |
| 128 | $D_{NS,AS}$ | D_NS_AS | block difference operator | differenceOperator | | [] | |
| 153 | $phi$ | phi | state for mass and energy | state | | [] | 130 |
| 145 | $T_ref_N$ | T_ref | refernce temperature | constant | $K$ | [] | 117 |
| 150 | $n^o{}_{NS}$ | no | initial condition for species mass in nodes | constant | $mol$ | [] | 124 |
| 151 | $H^o{}_N$ | Ho | initial condition for enthalpy in nodes | constant | $kg\, m^2\, s^{-2}$ | [] | 125 |
| 69 | $m_N$ | m | mass | secondaryState | $kg$ | [] | 47 |
| 108 | $c_{NS}$ | c | molar concentration | secondaryState | $m^{-3}\, mol$ | [] | 84<br>127 |
| 152 | $intensities$ | intensities | collected intensities | secondaryState | | [] | 126 |
| 77 | $T_{NK}$ | T_NK | temperature in reactive systems | conversion | $K$ | [] | 55 |
| 93 | $N_{NS,NK}$ | N_NS_NK | extended stoichiometric matrix | conversion | | [] | 69 |
| 117 | $\xi_{NK}$ | xi | extend of reaction per volume | conversion | $m^{-3}\, mol\, s^{-1}$ | [] | 93 |
| 118 | $\tilde{n}_{NS}$ | pn | production term | conversion | $mol\, s^{-1}$ | [] | 94 |
| 119 | $\dot{n}_{NS}$ | dndt | differential molar mass balance | diffState | $mol\, s^{-1}$ | [] | 95<br>129 |
| 126 | $\dot{H}_N$ | dHdt | differential enthalpy balance | diffState | $kg\, m^2\, s^{-3}$ | [] | 102<br>128 |

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

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| no | equation | documentation | layer |
|---|---|---|---|
| 18 | $C_{p\,N} := \frac{\partial H_N}{\partial T_N}$ | total heat capacity | material |
| 19 | $C_{v\,N} := \frac{\partial U_N}{\partial T_N}$ | total heat capacity at constant volume | material |
| 22 | $k^q_{x\,N} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{x\,N}$ | thermal conductivity in x-direction | material |
| 23 | $k^q_{y\,N} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{y\,N}$ | thermal conductivity in y-direction | material |
| 24 | $k^q_{z\,N} := (V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{z\,N}$ | thermal conductivity in z-direction | material |
| 25 | $k^q{}_N := \text{Stack}\left(k^q_{x\,N}, k^q_{y\,N}, k^q_{z\,N}\right)$ | Carthesian thermal conductivity vector | material |
| 32 | $\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$ | chemical potential | physical |
| 37 | $k^c_{x\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{x\,N}$ | convective mass convectivity in x-direction | material |
| 38 | $k^c_{y\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{y\,N}$ | convective mass convectivity in y-direction | material |
| 39 | $k^c_{z\,N} := \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{z\,N}$ | convective mass convectivity in z-direction | material |
| 40 | $k^c{}_N := \text{Stack}\left(k^c_{x\,N}, k^c_{y\,N}, k^c_{z\,N}\right)$ | Cartesian convective mass convectivity vector | material |
| 41 | $k^d_{x\,NS} := (\mu_{NS})^{-1} \cdot \left(v_{x\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$ | diffusional mass conductivity in x-direction | material |
| 42 | $k^d_{y\,NS} := (\mu_{NS})^{-1} \cdot \left(v_{y\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$ | diffusional mass conductivity in y-direction | material |
| 43 | $k^d_{z\,NS} := (\mu_{NS})^{-1} \cdot \left(v_{z\,N} \odot \left((V_N)^{-1} \odot \frac{\partial U_N}{\partial \mu_{NS}}\right)\right)$ | diffusional mass conductivity in z-direction | material |

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| no | equation | documentation | layer |
|---|---|---|---|
| 44 | ${k^d}_{NS} := \text{Stack}\left({k^d_x}_{NS}, {k^d_y}_{NS}, {k^d_z}_{NS}\right)$ | Cartesian dffusional mass conductivity vector | material |
| 45 | $h_{NS} := H_N \odot (n_{NS})^{-1}$ | partial molar enthalpies | material |
| 46 | $d_A := \text{sign}\left(F_{N,A} \overset{N}{\star} p_N\right)$ | direction of convective ow | macroscopic |
| 47 | $m_N := \lambda_S \overset{S \in NS}{\star} n_{NS}$ | mass | macroscopic |
| 49 | $\rho_N := m_N \, . \, (V_N)^{-1}$ | mass density | material |
| 51 | $F_{NS,AS} := F_{N,A} \odot P_{NS,AS}$ | incidence matrix of directed graphs for for species NS x AS | macroscopic |
| 55 | $T_{NK} := P_{N,NK} \overset{N}{\star} T_N$ | temperature in reactive systems | macroscopic |
| 64 | $E_{a\,NK} := \text{Instantiate}(P_{N,NK} \overset{N}{\star} R_N \, . \, T_{NK}, \#)$ | Arrhenius's activation energy | reactions |
| 65 | $K_{NK} := {K^o}_K \odot exp((-E_{a\,NK}) \, . \, \left(R_N \overset{N}{\star} P_{N,NK} \, . \, T_{NK}\right)^{-1})$ | Arrhenius reaction constant | reactions |
| 69 | $N_{NS,NK} := P_{S,NS} \overset{S}{\star} \left(\left(P_{K,NK} \, . \, T_{NK} \, . \, (T_{NK})^{-1}\right) \overset{K}{\star} N_{S,K}\right)$ | extended stoichiometric matrix | macroscopic |
| 71 | $A_{yz\,N} := r_{y\,N} \, . \, r_{z\,N}$ | cross sectional area in x-direction | macroscopic |
| 72 | $A_{xz\,N} := r_{x\,N} \, . \, r_{z\,N}$ | cross sectional area in y direction | macroscopic |
| 73 | $A_{xy\,N} := r_{x\,N} \, . \, r_{y\,N}$ | cross sectional area in z-direction | macroscopic |
| 74 | $\hat{V}_A := (\rho_N)^{-1} \, . \, {k^c_x}_N \, . \, A_{yz\,N} \, . \, D_{N,A} \overset{N}{\star} p_N$ | volumetric flow in x-direction | macroscopic |
| 80 | ${\hat{n}^d}_{AS} := A_{yz\,N} \odot \left(-{k^d_x}_{NS}\right) \, . \, D_{NS,AS} \overset{NS}{\star} \mu_{NS}$ | diffusional mass transfer per arc | macroscopic |
| 81 | ${\hat{n}^d}_{NS} := F_{NS,AS} \overset{AS}{\star} {\hat{n}^d}_{AS}$ | net diffusional mass transfer | macroscopic |

*Continued on next page*

| no | equation | documentation | layer |
|---|---|---|---|
| 82 | $\hat{H}^d{}_A := \left(F_{NS,AS} \overset{NS}{\star} h_{NS}\right) \overset{S\in AS}{\star} \hat{n}^d{}_{AS}$ | enthalpy flow due to mass diffusion per arc | macroscopic |
| 83 | $\hat{H}^d{}_N := F_{N,A} \overset{A}{\star} \hat{H}^d{}_A$ | net enthalpy flow due to mass diffusion | macroscopic |
| 84 | $c_{NS} := (V_N)^{-1} \odot n_{NS}$ | molar concentration | macroscopic |
| 85 | $c_{AS} := (0.5\,.\,(F_{NS,AS} - d_A \odot \lvert F_{NS,AS}\rvert)) \overset{NS}{\star} c_{NS}$ | moler concentration in convective arc | macroscopic |
| 86 | $\hat{n}^c{}_{AS} := \hat{V}_A \odot c_{AS}$ | convective molar mass flow per arc | macroscopic |
| 87 | $\hat{n}^c{}_{NS} := F_{NS,AS} \overset{AS}{\star} \hat{n}^c{}_{AS}$ | net convective molar mass flow | macroscopic |
| 90 | $c_{KS} := c_{NS} \overset{NS}{\star} P_{NS,KS}$ | molar concentrations in reactive system | reactions |
| 91 | $c^o{}_{KS} := \text{Instantiate}(c_{KS}, \#)$ | norming molar concentrations | reactions |
| 92 | $\phi_{KS} := \prod\left(c_{KS}\,.\,(c^o{}_{KS})^{-1}\right)$ | probability of species to meet | reactions |
| 93 | $\xi_{NK} := K_{NK}\,.\,P_{NK,KS} \overset{KS}{\star} \phi_{KS}$ | extend of reaction per volume | macroscopic |
| 94 | $\tilde{n}_{NS} := V_N \odot \left(N_{NS,NK} \overset{NK}{\star} \xi_{NK}\right)$ | production term | macroscopic |
| 95 | $\dot{n}_{NS} := \hat{n}^c{}_{NS} + \hat{n}^d{}_{NS} + \tilde{n}_{NS}$ | differential molar mass balance | macroscopic |
| 96 | $\hat{H}^c{}_A := \left(F_{NS,AS} \overset{NS}{\star} h_{NS}\right) \overset{S\in AS}{\star} \hat{n}^c{}_{AS}$ | enthalpy flow due to convective mass flow | macroscopic |
| 97 | $\hat{H}^c{}_N := F_{N,A} \overset{A}{\star} \hat{H}^c{}_A$ | net enthalpy flow due to convective mass flow | macroscopic |
| 98 | $\hat{w}_A := \text{Instantiate}(\hat{H}^c{}_A, \#)$ | example of work flow | macroscopic |
| 99 | $\hat{w}_N := F_{N,A} \overset{A}{\star} \hat{w}_A$ | net work flow | macroscopic |

*Continued on next page*

| no | equation | documentation | layer |
|---|---|---|---|
| 100 | $\hat{q}_A := A_{yz\,N} \, . \, k^q_{x\,N} \, . \, D_{N,A} \overset{N}{\star} T_N$ | heat flow in x-direction | macroscopic |
| 101 | $\hat{q}_N := F_{N,A} \overset{A}{\star} \hat{q}_A$ | net heat flow | macroscopic |
| 102 | $\dot{H}_N := \hat{H}^c{}_N + \hat{H}^d{}_N + \hat{q}_N + \hat{w}_N$ | differential enthalpy balance | macroscopic |
| 103 | $x^o{}_N := \text{Instantiate}(x_N, \#)$ | controller initial condition | control |
| 104 | $e_A := m_A - y^o{}_A$ | control error | control |
| 106 | $\dot{x}_D := A_{N,D} \overset{N}{\star} x_N + B_{A,D} \overset{A}{\star} e_A$ | differential controller state | control |
| 112 | $x_N := \int_{t_o}^{t_e} \; I_{N,D} \overset{D}{\star} \dot{x}_D \;\, dt$ | controller state | control |
| 113 | $T_N := \text{Instantiate}(T_N, \#)$ | temperature | physical |
| 114 | $\mu_{NS} := \text{Instantiate}(\mu_{NS}, \#)$ | chemical potential | physical |
| 115 | $p_N := \text{Instantiate}(p_N, \#)$ | thermodynamic pressure | physical |
| 116 | $n_{NS} := \int_{t_o}^{t_e} \; \dot{n}_{NS} \;\, dt + n^o{}_{NS}$ | species molar mass | macroscopic |
| 117 | $T_r ef_N := \text{Instantiate}(T_N, \#)$ | refernce temperature | macroscopic |

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| no | equation | documentation | layer |
|---|---|---|---|
| 120 | $cp_N := C_{pN} \,.\, (m_N)^{-1}$ | specific heat capacity at constant pressure | material |
| 121 | $cv_N := C_{vN} \,.\, (m_N)^{-1}$ | specific heat capacity at constant volume | material |
| 122 | $H_N := m_N \,.\, \int_{Tref_N}^{T_N} cp_N \;\, dT_N$ | enthalpy | macroscopic |
| 123 | $H_N := \int_{t_o}^{t_e} \dot{H}_N \;\, dt + H^o{}_N$ | enthalpy | macroscopic |
| 124 | $n^o{}_{NS} := \text{Instantiate}(n_{NS}, \#)$ | initial condition for species mass in nodes | macroscopic |
| 125 | $H^o{}_N := \text{Instantiate}(H_N, \#)$ | initial condition for enthalpy in nodes | macroscopic |
| 126 | $intensities := \text{MixedStack}\,(p_N, T_N, \mu_{NS}, c_{NS})$ | collected intensities | macroscopic |
| 127 | $c_{NS} := \text{Instantiate}(c_{NS}, \#)$ | molar concentration | macroscopic |
| 128 | $\dot{H}_N := \text{Instantiate}(\dot{H}_N, 0)$ | differential enthalpy balance | macroscopic |
| 129 | $\dot{n}_{NS} := \text{Instantiate}(\dot{n}_{NS}, 0)$ | differential molar mass balance | macroscopic |
| 130 | $phi := \text{MixedStack}\,(n_{NS}, H_N)$ | state for mass and energy | macroscopic |
| 131 | $k^q_{x}{}_N := \text{Instantiate}(k^q_{x}{}_N, \#)$ | thermal conductivity in x-direction | material |

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| no | equation | documentation | layer |
|---|---|---|---|
| 132 | $k^q_{y\,N} := \text{Instantiate}(k^q_{y\,N}, \#)$ | thermal conductivity in y-direction | material |
| 133 | $k^q_{z\,N} := \text{Instantiate}(k^q_{z\,N}, \#)$ | thermal conductivity in z-direction | material |
| 134 | $k^c_{x\,N} := \text{Instantiate}(k^c_{x\,N}, \#)$ | convective mass convectivity in x-direction | material |
| 135 | $k^c_{y\,N} := \text{Instantiate}(k^c_{y\,N}, \#)$ | convective mass convectivity in y-direction | material |
| 136 | $k^c_{z\,N} := \text{Instantiate}(k^c_{z\,N} . \#, -)$ | convective mass convectivity in z-direction | material |
| 137 | $k^d_{x\,NS} := \text{Instantiate}(k^d_{x\,NS}, \#)$ | diffusional mass conductivity in x-direction | material |
| 138 | $k^d_{y\,NS} := \text{Instantiate}(k^d_{y\,NS}, \#)$ | diffusional mass conductivity in y-direction | material |
| 139 | $h_{NS} := \text{Instantiate}(h_{NS}, \#)$ | partial molar enthalpies | material |
| 140 | $cp_N := \text{Instantiate}(cp_N, \#)$ | specific heat capacity at constant pressure | material |
| 141 | $cv_N := \text{Instantiate}(cv_N, \#)$ | specific heat capacity at constant volume | material |
| 142 | $\lambda_S := \text{Instantiate}(\lambda_S, \#)$ | species molecular masses | material |
| 143 | $\theta := \text{MixedStack}\left(k^q{}_N, k^c{}_N, k^d{}_{NS}, h_{NS}, cp_N, cv_N, \lambda_S, \rho_N\right)$ | available data set | material |

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| no | equation | documentation | layer |
|---|---|---|---|
| 144 | $C_{N,A} := \text{Instantiate}(C_{N,A}, \#)$ | measurement matrix | control |
| 145 | $D_{N,D} := \text{Instantiate}(D_{N,D}, \#)$ | event matrix (dimension issue) | control |
| 146 | $y^o{}_A := \text{Instantiate}(y^o{}_A, \#)$ | set point | control |
| 147 | $D_A := \text{Instantiate}(D_A, \#)$ | event diagonal matrix (no dimension problem) | control |
| 148 | $A_{N,D} := \text{Instantiate}(A_{N,D}, \#)$ | dynamic control matrix | control |
| 149 | $B_{A,D} := \text{Instantiate}(B_{A,D}, \#)$ | input matrix | control |