

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_{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 | $kg\ m^2\ s^{-2}$ | [] | 9 122 123 |
| 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_{NS} | 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 | μ_{NS} | chem_pot | chemical potential | effort | $kg\ m^2\ mol^{-1}\ s^{-2}$ | [] | 32 114 |
| 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 |
|-----|-------------|----------|--|-----------|----------|--------|-----|
| 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_N^o | xo | controller initial condition | state | | [] | 103 |
| 133 | $C_{N,A}$ | Cx | measurement matrix | constant | | [] | |
| 134 | $D_{N,D}$ | Dx | event matrix (dimension issue) | constant | | [] | |
| 135 | y_A^o | setpoint | set point | constant | | [] | |
| 136 | D_A | D_A | event diagonal matrix (no dimension problem) | constant | | [] | |
| 142 | $A_{N,D}$ | Ax | dynamic control matrix | constant | s^{-1} | [] | |
| 143 | $B_{A,D}$ | Bx | input matrix | constant | s^{-1} | [] | |
| 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 | $E_{a,NK}$ | 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 | ϕ_{KS} | phi_KS | probability of species to meet | constant | | [] | 92 |

6 material

| | var | symbol | documentation | type | units | tokens | eqs |
|----|-------------|---------|--|----------|-----------------------------|--------|-----------|
| 29 | λ_S | Mm | species molecular masses | constant | $kg\ mol^{-1}$ | [] | 142 |
| 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 | $kg\ K^{-1}\ s^{-3}$ | [] | 22 131 |
| 35 | k_{yN}^q | kq_y | thermal conductivity in y-direction | property | $kg\ K^{-1}\ s^{-3}$ | [] | 23 132 |
| 36 | k_{zN}^q | kq_z | thermal conductivity in z-direction | property | $kg\ K^{-1}\ s^{-3}$ | [] | 24 133 |
| 37 | k_N^q | kq | Cartesian thermal conductivity vector | property | $kg\ K^{-1}\ s^{-3}$ | [] | 25 |
| 50 | k_{xN}^c | kc_x | convective mass conductivity in x-direction | property | $m^{-1}\ s$ | [] | 37 134 |
| 51 | k_{yN}^c | kc_y | convective mass conductivity in y-direction | property | $m^{-1}\ s$ | [] | 38 135 |
| 52 | k_{zN}^c | kc_z | convective mass conductivity in z-direction | property | $m^{-1}\ s$ | [] | 39 136 |
| 53 | k_N^c | kc | Cartesian convective mass conductivity vector | property | $m^{-1}\ s$ | [] | 40 |
| 54 | k_{xNS}^d | kd_x | diffusional mass conductivity in x-direction | property | $kg^{-1}\ m^{-4}\ mol^2\ s$ | [] | 41 137 |
| 55 | k_{yNS}^d | kd_y | diffusional mass conductivity in y-direction | property | $kg^{-1}\ m^{-4}\ mol^2\ s$ | [] | 42 138 |
| 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 diffusional mass conductivity vector | property | $kg^{-1}\ m^{-4}\ mol^2\ s$ | [] | 44 |
| 58 | h_{NS} | h | partial molar enthalpies | property | $kg\ m^2\ mol^{-1}\ s^{-2}$ | [] | 45 139 |
| 71 | ρ_N | density | mass density | property | $kg\ m^{-3}$ | [] | 49 |

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| | var | symbol | documentation | type | units | tokens | eqs |
|-----|--------|--------|---|----------|---------------------|--------|--|
| 148 | cp_N | cp | specific heat capacity at constant pressure | property | $m^2 K^{-1} s^{-2}$ | [] | 120 140 |
| 149 | cv_N | cv | specific heat capacity at constant volume | property | $m^2 K^{-1} s^{-2}$ | [] | 121 141 |

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}_{AS}^d | fnd_AS | diffusional mass transfer per arc | transport | $mol s^{-1}$ | [] | 80 |
| 105 | \hat{n}_{NS}^d | fnd | net diffusional mass transfer | transport | $mol s^{-1}$ | [] | 81 |
| 106 | \hat{H}_A^d | fHd_A | enthalpy flow due to mass diffusion per arc | transport | $kg m^2 s^{-3}$ | [] | 82 |
| 107 | \hat{H}_N^d | 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}_{AS}^c | fnc_AS | convective molar mass flow per arc | transport | $mol s^{-1}$ | [] | 86 |
| 111 | \hat{n}_{NS}^c | fnc | net convective molar mass flow | transport | $mol s^{-1}$ | [] | 87 |
| 120 | \hat{H}_A^c | fHc_A | enthalpy flow due to convective mass flow | transport | $kg m^2 s^{-3}$ | [] | 96 |
| 121 | \hat{H}_N^c | 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_{yzN} | Ayz | cross sectional area in x-direction | geometry | m^2 | [] | 71 |
| 96 | A_{xzN} | Axz | cross sectional area in y direction | geometry | m^2 | [] | 72 |
| 97 | A_{xyN} | 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 | ϕ | phi | state for mass and energy | state | | [] | 130 |
| 145 | $T_{ref,N}$ | T_ref | reference temperature | constant | K | [] | 117 |
| 150 | n_{NS}^o | no | initial condition for species mass in nodes | constant | mol | [] | 124 |
| 151 | H_N^o | 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 | [] | 84 127 |
| 152 | $\mathbf{intensities}$ | 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 | ξ_{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 | [] | 95 129 |
| 126 | \dot{H}_N | dHdt | differential enthalpy balance | diffState | kg m ² s ⁻³ | [] | 102 128 |

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 | $H_N := U_N - p_N \cdot V_N$ | 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 |

Continued on next page

| 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 |
| 37 | $k_{xN}^c := \left(\lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$ | convective mass conductivity in x-direction | material |
| 38 | $k_{yN}^c := \left(\lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{yN}$ | convective mass conductivity in y-direction | material |
| 39 | $k_{zN}^c := \left(\lambda_S^{S \in NS} \star (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{zN}$ | convective mass conductivity in z-direction | material |
| 40 | $k_N^c := \text{Stack}(k_{xN}^c, k_{yN}^c, k_{zN}^c)$ | Cartesian convective mass conductivity vector | material |
| 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 |

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| no | equation | documentation | layer |
|----|--|---|-------------|
| 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 |
| 46 | $d_A := \text{sign}\left(F_{N,A} \stackrel{N}{\star} p_N\right)$ | direction of convective ow | macroscopic |
| 47 | $m_N := \lambda_S \stackrel{S \in NS}{\star} n_{NS}$ | mass | macroscopic |
| 49 | $\rho_N := m_N \cdot (V_N)^{-1}$ | 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 | $T_{NK} := P_{N,NK} \stackrel{N}{\star} T_N$ | temperature in reactive systems | macroscopic |
| 64 | $E_{aNK} := \text{Instantiate}(P_{N,NK} \stackrel{N}{\star} R_N \cdot T_{NK}, \#)$ | Arrhenius's activation energy | reactions |
| 65 | $K_{NK} := K^o_K \odot \exp((-E_{aNK}) \cdot (R_N \stackrel{N}{\star} P_{N,NK} \cdot T_{NK})^{-1})$ | Arrhenius reaction constant | reactions |
| 69 | $N_{NS,NK} := P_{S,NS} \stackrel{S}{\star} \left((P_{K,NK} \cdot T_{NK} \cdot (T_{NK})^{-1}) \stackrel{K}{\star} N_{S,K} \right)$ | extended stoichiometric matrix | macroscopic |
| 71 | $A_{yzN} := r_{yN} \cdot r_{zN}$ | cross sectional area in x-direction | macroscopic |
| 72 | $A_{xzN} := r_{xN} \cdot r_{zN}$ | cross sectional area in y direction | macroscopic |
| 73 | $A_{xyN} := r_{xN} \cdot r_{yN}$ | cross sectional area in z-direction | macroscopic |
| 74 | $\hat{V}_A := (\rho_N)^{-1} \cdot k_{xN}^c \cdot A_{yzN} \cdot D_{N,A} \stackrel{N}{\star} p_N$ | volumetric flow in x-direction | macroscopic |
| 80 | $\hat{n}_{AS}^d := A_{yzN} \odot (-k_{xNS}^d) \cdot D_{NS,AS} \stackrel{NS}{\star} \mu_{NS}$ | diffusional mass transfer per arc | macroscopic |
| 81 | $\hat{n}_{NS}^d := F_{NS,AS} \stackrel{AS}{\star} \hat{n}_{AS}^d$ | net diffusional mass transfer | macroscopic |

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| 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 | $c_{AS} := (0.5 \cdot (F_{NS,AS} - d_A \odot F_{NS,AS})) \overset{NS}{\star} c_{NS}$ | molar 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 | $\phi_{KS} := \prod \left(c_{KS} \cdot (c^o_{KS})^{-1} \right)$ | probability of species to meet | reactions |
| 93 | $\xi_{NK} := K_{NK} \cdot P_{NK,KS} \overset{KS}{\star} \phi_{KS}$ | 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 |

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| no | equation | documentation | layer |
|-----|--|-------------------------------|-------------|
| 100 | $\hat{q}_A := A_{yzN} \cdot k_{xN}^q \cdot D_{N,A} \overset{N}{\star} T_N$ | heat flow in x-direction | macroscopic |
| 101 | $\hat{q}_N := F_{N,A} \overset{A}{\star} \hat{q}_A$ | net heat flow | macroscopic |
| 102 | $\dot{H}_N := \hat{H}_N^c + \hat{H}_N^d + \hat{q}_N + \hat{w}_N$ | differential enthalpy balance | macroscopic |
| 103 | $x_N^o := \text{Instantiate}(x_N, \#)$ | controller initial condition | control |
| 104 | $e_A := m_A - y_A^o$ | 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 | $n_{NS} := \int_{t_o}^{t_e} \dot{n}_{NS} \, dt + n_{NS}^o$ | species molar mass | macroscopic |
| 117 | $T_{refN} := \text{Instantiate}(T_N, \#)$ | reference temperature | macroscopic |

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| no | equation | documentation | layer |
|-----|--|---|-------------|
| 120 | $cp_N := C_{pN} \cdot (m_N)^{-1}$ | specific heat capacity at constant pressure | material |
| 121 | $cv_N := C_{vN} \cdot (m_N)^{-1}$ | specific heat capacity at constant volume | material |
| 122 | $H_N := m_N \cdot \int_{T_{ref_N}}^{T_N} cp_N \, dT_N$ | 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 | $k^q_{xN} := \text{Instantiate}(k^q_{xN}, \#)$ | thermal conductivity in x-direction | material |

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|-----|--|--|----------|
| 132 | $k_y^q := \text{Instantiate}(k_{yN}^q, \#)$ | thermal conductivity in y-direction | material |
| 133 | $k_z^q := \text{Instantiate}(k_{zN}^q, \#)$ | thermal conductivity in z-direction | material |
| 134 | $k_x^c := \text{Instantiate}(k_{xN}^c, \#)$ | convective mass convectivity in x-direction | material |
| 135 | $k_y^c := \text{Instantiate}(k_{yN}^c, \#)$ | convective mass convectivity in y-direction | material |
| 136 | $k_z^c := \text{Instantiate}(k_{zN}^c, \#, -)$ | convective mass convectivity in z-direction | material |
| 137 | $k_{xNS}^d := \text{Instantiate}(k_{xNS}^d, \#)$ | diffusional mass conductivity in x-direction | material |
| 138 | $k_{yNS}^d := \text{Instantiate}(k_{yNS}^d, \#)$ | 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 |