# 1 Variables

# 2 root

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 2 | $F_{N,A}$ | `F` | incidence matrix of directed graph | network | | |
| 1 | $t_N$ | `t` | time | frame | $s$ | |
| 88 | $to_N$ | `to` | initial time | frame | $s$ | 63 |
| 89 | $te_N$ | `te` | end time | frame | $s$ | 64 |
| 5 | $\#$ | `value` | a value | constant | | |
| 6 | $1\backslash 2$ | `half` | one half | constant | | 1 |
| 7 | $0$ | `zero` | zero | constant | | 2 |
| 8 | $\partial t_{N,dt}$ | `dt` | differential time | *diffFrame | $s$ | 3 |

# 3 physical

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 30 | $F_{NS,AS}$ | `F_NS_AS` | incidence matrix for species network | network | | |
| 41 | $P_{N,A,dt}$ | `P_N_A_dt` | projection of node to arc (used for mapping transport system material to application arc) | projection | | |
| 49 | $P_{NS,AS,dt}$ | `P_NS_AS_dt` | projection of node to arc (used for mapping transport system material to application arc) | projection | | |
| 9 | $r_{x\,N}$ | `rx` | spatial coordinate x | frame | $m$ | |
| 20 | $r_{y\,N}$ | `ry` | spatial coordinate y | frame | $m$ | |
| 21 | $r_{z\,N}$ | `rz` | spatial coordinate z | frame | $m$ | |
| 104 | $r_N$ | `r` | radius | frame | $m$ | |
| 10 | $n_{NS}$ | `n` | species mass in moles | state | $mol$ | 65 |

*Continued on next page*

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 11 | $U_N$ | `U` | internal energy | state | $kg\,m^2\,s^{-2}$ | |
| 12 | $S_N$ | `S` | entropy | state | $kg\,m^2\,K^{-1}\,s^{-2}$ | |
| 13 | $V_N$ | `V` | volume | state | $m^3$ | |
| 92 | $m_N$ | `m` | mass | state | $kg$ | |
| 66 | $R$ | `R` | gas constant | constant | $kg^{-1}\,m^{-2}\,mol\,K^{-1}\,s^2$ | |
| 17 | $H_N$ | `H` | definition of enthalpy | secondaryState | $kg\,m^2\,s^{-2}$ | 7 |
| 18 | $v_{x\,N}$ | `vx` | definition of velocity in x direction | secondaryState | $ms^{-1}$ | 8 |
| 22 | $A_{x\,N}$ | `Ax` | area at location x | secondaryState | $m^2$ | 10 |
| 111 | $A_N$ | `A` | definition of Helmholtz energy | secondaryState | $kg\,m^2\,s^{-2}$ | 90 |
| 112 | $G_N$ | `G` | definition of Gibbs free energy | secondaryState | $kg\,m^2\,s^{-2}$ | 91 |
| 14 | $T_N$ | `T` | definition of temperature | effort | $K$ | 4 |
| 15 | $p_N$ | `p` | definition of pressure | effort | $kg\,m^{-1}\,s^{-2}$ | 5 |
| 31 | $\mu_{N\,S}$ | `mu` | chemical potential from Gibbs free energy | effort | $kg\,m^2\,mol^{-1}\,s^{-2}$ | 18 92 |

# 4 control

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

# 5 macroscopic

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 54 | $\hat{q}_{N,dt}$ | `fq` | heat flow | transport | $kg\,m^2\,s^{-3}$ | 39 |
| 81 | $\hat{V}_{A,dt}$ | `fV` | volumetric flow | transport | $m^3\,s^{-1}$ | 83 |
| 82 | $d_A$ | `dir` | direction of flow relative to reference coordinate | transport | | 57 |

*Continued on next page*

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 83 | $S_{NS,AS}$ | S_NS_AS | selection of the flow sources | transport | | 58 |
| 84 | $c_{AS}$ | c_AS | concentration in the convective flows | transport | $m^{-3}\,mol$ | 59 |
| 85 | $\hat{n}^{v}_{NS,dt}$ | fnv | convective species flow | transport | $mol\,s^{-1}$ | 60 |
| 86 | $\hat{n}^{d}_{NS,dt}$ | fnd | diffusional species flows | transport | $mol\,s^{-1}$ | 82 |
| 57 | $P_{NS,KS}$ | P_NS_KS | projection of node species onto reaction species | projection | | |
| 58 | $P_{K,NK}$ | P_K_NK | projection reaction on node x reactions | projection | | |
| 59 | $P_{N,NK}$ | P_N_NK | projection node to node x reactions | projection | | |
| 74 | $P_{NK,KS}$ | P_NK_KS | projection node x conversion to conversion x species | projection | | |
| 56 | ${n^0}_{NS}$ | n0 | initial condition | state | $mol$ | 41 |
| 87 | $\dot{n}_{NS,dt}$ | dn | | state | $mol\,s^{-1}$ | 62 |
| 62 | $N_{K,KS}$ | N_KS_K | stoichiometry for reaction k | constant | | |
| 64 | ${K^o}_{K,dt}$ | Ko | Arrhenius prexponential factor (matrix) | constant | $m^{-3}\,mol\,s^{-1}$ | |
| 65 | ${E^A}_{K}$ | ka | Arrhenius activation energy | constant | $kg^{-1}\,m^{-2}\,mol\,s^{2}$ | |
| 61 | $c_{KS}$ | c_KS | molar concentrations assigned to reaction K | conversion | $m^{-3}\,mol$ | 43 |
| 63 | $N_{NS,NK}$ | N_NS_NK | global stoichiomety block matrix | conversion | | 44 |
| 67 | $T_{NK}$ | T_NK | temperature for reactions | conversion | $K$ | 45 |
| 68 | $K_{NK,dt}$ | K | reaction "constants" | conversion | $m^{-3}\,mol\,s^{-1}$ | 46 |
| 69 | ${c^o}_{KS}$ | c_KS_o | norming concentration – probability must have no units ! | conversion | $m^{-3}\,mol$ | 47 |
| 71 | $x_{KS}$ | x_KS | normed concentration little like more fractions | conversion | | 49 |
| 75 | $\phi_{NK}$ | phi | probabiity for the reactions to occur | conversion | | 52 |
| 76 | $\xi_{NK,dt}$ | xi | dyamic extend of reaction | conversion | $m^{-3}\,mol\,s^{-1}$ | 53 |
| 77 | $\tilde{n}_{NS,dt}$ | pn | production term | conversion | $mol\,s^{-1}$ | 54 |
| 60 | $c_{NS}$ | c | molar concentration | secondaryState | $m^{-3}\,mol$ | 42 |

# 6 materialDB

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 94 | $\lambda_S$ | `mm` | molecular masses | constant | $kg\,mol^{-1}$ | |
| 106 | $k_{granulate}{}_{dt}$ | `k_granulate` | kinetic constant for granulation dynamics | constant | $s^{-1}$ | |
| 26 | $c_p{}_N$ | `cp` | heat capacity at constant pressure | property | $kg\,m^2\,K^{-1}\,s^{-2}$ | 14 |
| 45 | $k^{q_x}{}_{A,dt}$ | `kq_x` | heat transfer coefficient for an event-dynamic transfer system | property | $kg\,K^{-1}\,s^{-3}$ | 31 |
| 93 | $k^{d_x}{}_{NS,AS,dt}$ | `kd_x` | diffusional mass diffusivity per area. | property | $kg^{-1}\,m^{-4}\,mol^2\,s$ | 81 |
| 95 | $k^{c_x}{}_{N,A,dt}$ | `kc_x` | convective mass diffusivity per area | property | $m^{-1}\,s$ | 76 |
| 96 | $\rho_N$ | `rho` | mass density | property | $kg\,m^{-3}$ | 71 |
| 98 | $k^{v_x}{}_{N,A,dt}$ | `kv_x` | convective volume flow per area | property | $kg^{-1}\,m^2\,s$ | 78 |

# 7 mixing

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 113 | $y_N$ | `y` | mixing index | state | | |
| 114 | $\beta$ | `beta` | mixing beta parameter | constant | | |
| 115 | $\gamma$ | `gamma` | mixing gamma parameter | constant | | |
| 116 | $f$ | `f` | stirrer frequency | constant | $s^{-1}$ | |
| 117 | $a_{N,dt}$ | `a` | stirrer amplitude | constant | | |
| 118 | $\alpha$ | `alpha` | stirrer function | parameter | | 93 |

# 8 fluid

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

## 9 solid

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 101 | $N_N$ | `N` | number of particles | state | | |
| 110 | $N_{t\,N,dt}$ | `dN` | population balance PDE | state | $s^{-1}$ | 89 |
| 108 | $\tilde{N}_{N,dt}$ | `pN` | granulation dynamics | conversion | $ms^{-1}$ | 87 |

## 10 liquid

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

## 11 gas

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

## 12 control–gas

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

## 13 gas–control

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

## 14 control–liquid

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

## 15 liquid–control

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

## 16 control–materialDB

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

## 17 materialDB–control

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

## 18 control–mixing

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

## 19 mixing–control

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

## 20 control–solid

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

## 21 solid–control

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

## 22 gas–materialDB

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

## 23 materialDB–gas

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

## 24 liquid–materialDB

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

## 25 materialDB–liquid

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 46 | ${k^{q_x}}_{A,dt}$ | `kq_x` | link to get heat transfer coefficient | transform | $kg\,K^{-1}\,s^{-3}$ | 32 |
| 99 | ${k^{v_x}}_{N,A,dt}$ | `kv_x` | link to get volumetric flow coefficient | transform | $kg^{-1}\,m^{2}\,s$ | 79 |
| 100 | ${k^{d_x}}_{NS,AS,dt}$ | `kd_x` | link to get diffusional mass flow coefficient | transform | $kg^{-1}\,m^{-4}\,mol^{2}\,s$ | 80 |

## 26 materialDB–mixing

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

## 27 mixing–materialDB

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

## 28 materialDB–solid

| | var | symbol | documentation | type | units | eqs |
|---|---|---|---|---|---|---|
| 107 | $k_{granulate}{}_{dt}$ | `k_granulate` | link to kinetic granulation constant | transform | $s^{-1}$ | 86 |

## 29 solid–materialDB

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

## 30 gas–liquid

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

## 31 gas–mixing

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

## 32 gas–solid

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

## 33 liquid–mixing

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

## 34 liquid–solid

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

## 35 mixing–solid

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

# 36 Equations

## 36.1 Model equations

| no | equation | documentation | layer |
|---|---|---|---|
| 1 | $1\backslash 2 := Set(\#, -)$ | one half | root |
| 2 | $0 := Set(\#, -)$ | zero | root |
| 3 | $\partial t_{N,dt} := diffSpace(t_N)$ | differential time | root |
| 4 | $T_N := \frac{\partial U_N}{\partial S_N}$ | definition of temperature | physical |
| 5 | $p_N := \left(-\frac{\partial U_N}{\partial V_N}\right)$ | definition of pressure | physical |
| 7 | $H_N := U_N + p_N \,.\, V_N$ | definition of enthalpy | physical |
| 8 | $v_{x\,N} := \frac{\partial r_{x\,N}}{\partial t_N}$ | definition of velocity in x direction | physical |
| 10 | $A_{x\,N} := r_{y\,N} \,.\, r_{z\,N}$ | area at location x | physical |
| 14 | $c_{p\,N} := \frac{\partial H_N}{\partial T_N}$ | heat capacity at constant pressure | materialDB |
| 18 | $\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$ | definition of chemical potential | physical |
| 31 | $k^{q_x}{}_{A,dt} := \left(-P_{N,A,dt}\right) \overset{N}{\star} \left(\left(V_N\right)^{-1} \,.\, \frac{\partial U_N}{\partial T_N} \,.\, v_{x\,N}\right)$ | heat transfer coefficient for an event-dynamic transfer system | materialDB |
| 32 | $k^{q_x}{}_{A,dt} := k^{q_x}{}_{A,dt}$ | link to get heat transfer coefficient | materialDB »> liquid |
| 39 | $\hat{q}_{N,dt} := F_{N,A} \overset{A}{\star} \left(\left(-k^{q_x}{}_{A,dt}\right) \,.\, A_{x\,N} \,.\, F_{N,A} \overset{N}{\star} T_N\right)$ | heat flow | macroscopic |
| 41 | $n^0{}_{NS} := Set(n_{NS}, -)$ | initial condition | macroscopic |
| 42 | $c_{NS} := \left(V_N\right)^{-1} \odot n_{NS}$ | molar concentration | macroscopic |

*Continued on next page*

| no | equation | documentation | layer |
|---|---|---|---|
| 43 | $c_{KS} := P_{NS,KS} \overset{NS}{\star} c_{NS}$ | molar concentrations assigned to reaction K | macroscopic |
| 44 | $N_{NS,NK} := P_{NS,KS} \overset{KS}{\star} N_{K,KS} \overset{K}{\star} P_{K,NK}$ | global stoichiomety block matrix | macroscopic |
| 45 | $T_{NK} := P_{N,NK} \overset{N}{\star} T_N$ | temperature for reactions | macroscopic |
| 46 | $K_{NK,dt} := {K^o}_{K,dt} \odot exp({E^A}_K \odot (R \,.\, T_{NK})^{-1})$ | reaction "constants" | macroscopic |
| 47 | ${c^o}_{KS} := Set(c_{KS}, -)$ | norming concentration – probability must have no units ! | macroscopic |
| 49 | $x_{KS} := ({c^o}_{KS})^{-1} \,.\, c_{KS}$ | normed concentration little like more fractions | macroscopic |
| 52 | $\phi_{NK} := P_{NK,KS} \overset{KS}{\star} \left(\prod \left(x_{KS}^{N_{K,KS}}\right)\right)$ | probabiity for the reactions to occur | macroscopic |
| 53 | $\xi_{NK,dt} := K_{NK,dt} \,.\, \phi_{NK}$ | dyamic extend of reaction | macroscopic |
| 54 | $\tilde{n}_{NS,dt} := V_N \odot \left(N_{NS,NK} \overset{NK}{\star} \xi_{NK,dt}\right)$ | production term | macroscopic |
| 57 | $d_A := \text{sign}\left(F_{N,A} \overset{N}{\star} p_N\right)$ | direction of flow relative to reference coordinate | macroscopic |
| 58 | $S_{NS,AS} := 1\backslash 2 \,.\, (F_{NS,AS} - d_A \odot \lvert F_{NS,AS} \rvert)$ | selection of the flow sources | macroscopic |
| 59 | $c_{AS} := S_{NS,AS} \overset{NS}{\star} c_{NS}$ | concentration in the convective flows | macroscopic |
| 60 | $\hat{n}^v_{NS,dt} := F_{NS,AS} \overset{AS}{\star} \left(\hat{V}_{A,dt} \odot c_{AS}\right)$ | convective species flow | macroscopic |
| 62 | $\dot{n}_{NS,dt} := \hat{n}^v_{NS,dt} + \hat{n}^d_{NS,dt} + \tilde{n}_{NS,dt}$ | differential species balances | macroscopic |
| 63 | $to_N := Set(t_N, -)$ | initial time | root |
| 64 | $te_N := Set(t_N, -)$ | end time | root |

*Continued on next page*

| no | equation | documentation | layer |
|---|---|---|---|
| 65 | $n_{NS} := \int_{to_N}^{te_N} \dot{n}_{NS,dt} \ d\,t_N + n^0{}_{NS}$ | integration of differential species balances | macroscopic |
| 71 | $\rho_N := m_N \,.\, (V_N)^{-1}$ | mass density | materialDB |
| 76 | $k^{c_x}{}_{N,A,dt} := (-P_{N,A,dt}) \overset{N}{\star} \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1}\right) \,.\, (V_N)^{-1} \,.\, \frac{\partial U_N}{\partial p_N} \,.\, v_{x\,N}$ | convective mass diffusivity per area | materialDB |
| 78 | $k^{v_x}{}_{N,A,dt} := (\rho_N)^{-1} \,.\, k^{c_x}{}_{N,A,dt}$ | convective volume flow per area | materialDB |
| 79 | $k^{v_x}{}_{N,A,dt} := k^{v_x}{}_{N,A,dt}$ | link to get volumetric flow coefficient | materialDB »> liquid |
| 80 | $k^{d_x}{}_{NS,AS,dt} := k^{d_x}{}_{NS,AS,dt}$ | link to get diffusional mass flow coefficient | materialDB »> liquid |
| 81 | $k^{d_x}{}_{NS,AS,dt} := (-P_{NS,AS,dt}) \overset{NS}{\star} \left(v_{x\,N} \,.\, (V_N)^{-1} \odot (\mu_{NS})^{-1}\right) \,.\, \frac{\partial U_N}{\partial \mu_{NS}}$ | diffusional mass diffusivity per area. | materialDB |
| 82 | $\hat{n}^d_{NS,dt} := A_{x\,N} \odot F_{NS,AS} \overset{AS}{\star} \left(\left(-k^{d_x}{}_{NS,AS,dt}\right) \,.\, F_{NS,AS} \overset{NS}{\star} \mu_{NS}\right)$ | diffusional species flows | macroscopic |
| 83 | $\hat{V}_{A,dt} := F_{N,A} \overset{A}{\star} (-k^{v_x}{}_{N,A,dt}) \,.\, A_{x\,N} \,.\, F_{N,A} \overset{N}{\star} p_N$ | volumetric flow | macroscopic |
| 86 | $k_{granulate}{}_{dt} := k_{granulate}{}_{dt}$ | link to kinetic granulation constant | materialDB »> solid |
| 87 | $\tilde{N}_{N,dt} := k_{granulate}{}_{dt} \,.\, r_N$ | granulation dynamics | solid |
| 89 | $N_{t\,N,dt} := \frac{\partial \tilde{N}_{N,dt}}{\partial r_N}$ | population balance PDE | solid |
| 90 | $A_N := U_N - T_N \,.\, S_N$ | definition of Helmholtz energy | physical |
| 91 | $G_N := U_N + p_N \,.\, V_N - T_N \,.\, S_N$ | definition of Gibbs free energy | physical |
| 92 | $\mu_{NS} := \frac{\partial G_N}{\partial n_{NS}}$ | chemical potential from Gibbs free energy | physical |
| 93 | $\alpha := a_{N,dt} \,.\, sin(t_N \,.\, f)$ | stirrer function | mixing |

## 36.2 Instantiations

| | no | equation | documentation | layer |
|---|---|---|---|---|