

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 | <i>s</i> | |
| 88 | to_N | to | initial time | frame | <i>s</i> | 63 |
| 89 | te_N | te | end time | frame | <i>s</i> | 64 |
| 5 | $\#$ | value | a value | constant | | |
| 6 | $1\backslash 2$ | half | one half | constant | | 1 |
| 7 | 0 | zero | zero | constant | | 2 |
| 120 | <i>one</i> | one | one | constant | | 94 |
| 8 | $\partial t_{N,dt}$ | dt | differential time | *diffFrame | <i>s</i> | 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_{xN} | rx | spatial coordinate x | frame | <i>m</i> | |
| 20 | r_{yN} | ry | spatial coordinate y | frame | <i>m</i> | |
| 21 | r_{zN} | rz | spatial coordinate z | frame | <i>m</i> | |
| 104 | r_N | r | radius | frame | <i>m</i> | |

Continued on next page

| | var | symbol | documentation | type | units | eqs |
|-----|------------|--------------|---|----------------|-------------------------------------|------------------------|
| 123 | $gugus$ | gugus | new | frame | | |
| 10 | n_{NS} | n | integral | state | mol | 98 |
| 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_{xN} | vx | definition of velocity in x direction | secondaryState | ms^{-1} | 8 |
| 22 | A_{xN} | 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 | μ_{NS} | 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 |

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| | var | symbol | documentation | type | units | eqs |
|----|---------------------|---------|--|------------|--------------------------|----------|
| 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 |
| 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 | $\hat{n}_{NS,dt}^v$ | fnv | convective species flow | transport | $mol s^{-1}$ | 60 |
| 86 | $\hat{n}_{NS,dt}^d$ | 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_{NS}^0 | n0 | initial condition | state | mol | 41 |
| 87 | $\dot{n}_{NS,dt}$ | dndt | zero accumulation | state | $mol s^{-1}$ | 62 97 |
| 62 | $N_{K,KS}$ | N_KS_K | stoichiometry for reaction k | constant | | |
| 64 | $K_{K,dt}^o$ | Ko | Arrhenius preexponential factor (matrix) | constant | $m^{-3} mol s^{-1}$ | |
| 65 | E_K^A | 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 stoichiometry 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_{KS}^o | 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 | ϕ_{NK} | phi | probability for the reactions to occur | conversion | | 52 |
| 76 | $\xi_{NK,dt}$ | xi | dynamic extent of reaction | conversion | $m^{-3} mol s^{-1}$ | 53 |

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| | var | symbol | documentation | type | units | eqs |
|----|---------------------|--------|---------------------|----------------|---------------|-----|
| 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 | λ_S | mm | molecular masses | constant | $kg\ mol^{-1}$ | |
| 106 | $k_{granulate\ dt}$ | k_granulate | kinetic constant for granulation dynamics | constant | s^{-1} | |
| 26 | c_{pN} | 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 | ρ_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 | s^{-1} | 96 |
| 122 | $dy_{N,dt}$ | dy | mixing differential equation | state | | |
| 114 | β | beta | mixing beta parameter | constant | | |
| 115 | γ | gamma | mixing gamma parameter | constant | | |
| 116 | f | f | stirrer frequency | constant | | |
| 117 | $a_{N,dt}$ | a | stirrer amplitude | constant | | |

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| | var | symbol | documentation | type | units | eqs |
|-----|-----------------|--------|----------------------------------|-----------|-------|-----|
| 121 | 1_N | y_one | a one of the same dimension as y | constant | | 95 |
| 118 | $\alpha_{N,dt}$ | 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 | $N_{tN,dt}$ | 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 gas-mixing

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

25 mixing–gas

| | var | symbol | documentation | type | units | eqs |
|--|-----|--------|---------------|------|-------|-----|
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26 liquid–materialDB

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

27 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 |

28 liquid–mixing

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

29 mixing–liquid

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

30 materialDB–mixing

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

31 mixing–materialDB

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

32 materialDB–solid

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

33 solid–materialDB

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

34 mixing–solid

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

35 solid–mixing

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

36 gas–liquid

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

37 gas–solid

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

38 liquid–solid

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

39 Equations

39.1 Model equations

| no | equation | documentation | layer |
|----|---|--|-----------------------|
| 1 | $1 \setminus 2 := Set(\#, -)$ | 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 | $H_N := U_N + p_N \cdot V_N$ | definition of enthalpy | physical |
| 8 | $v_{xN} := \frac{\partial r_{xN}}{\partial t_N}$ | definition of velocity in x direction | physical |
| 10 | $A_{xN} := r_{yN} \cdot r_{zN}$ | area at location x | physical |
| 14 | $c_{pN} := \frac{\partial H_N}{\partial T_N}$ | heat capacity at constant pressure | materialDB |
| 18 | $\mu_{NS} := \frac{\partial U_N}{\partial n_{NS}}$ | definition of chemical potential | physical |
| 31 | $k^{qx}_{A,dt} := (-P_{N,A,dt}) \stackrel{N}{\star} \left((V_N)^{-1} \cdot \frac{\partial U_N}{\partial T_N} \cdot v_{xN}\right)$ | heat transfer coefficient for an event-dynamic transfer system | materialDB |
| 32 | $k^{qx}_{A,dt} := k^{qx}_{A,dt}$ | link to get heat transfer coefficient | materialDB » > liquid |
| 39 | $\hat{q}_{N,dt} := F_{N,A} \stackrel{A}{\star} \left((-k^{qx}_{A,dt}) \cdot A_{xN} \cdot F_{N,A} \stackrel{N}{\star} T_N\right)$ | heat flow | macroscopic |
| 41 | $n^0_{NS} := Set(n_{NS}, -)$ | initial condition | macroscopic |
| 42 | $c_{NS} := (V_N)^{-1} \odot n_{NS}$ | 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 stoichiometry block matrix | macroscopic |
| 45 | $T_{NK} := P_{N,NK} \overset{N}{\star} T_N$ | temperature for reactions | macroscopic |
| 46 | $K_{NK,dt} := K^o_{K,dt} \odot \exp(E^A_K \odot (R \cdot T_{NK})^{-1})$ | reaction "constants" | macroscopic |
| 47 | $c^o_{KS} := Set(c_{KS}, -)$ | norming concentration – probability must have no units ! | macroscopic |
| 49 | $x_{KS} := (c^o_{KS})^{-1} \cdot c_{KS}$ | normed concentration little like more fractions | macroscopic |
| 52 | $\phi_{NK} := P_{NK,KS} \overset{KS}{\star} \left(\prod (x_{KS}^{N_{K,KS}}) \right)$ | probabiity for the reactions to occur | macroscopic |
| 53 | $\xi_{NK,dt} := K_{NK,dt} \cdot \phi_{NK}$ | dynamic 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 | $S_{NS,AS} := 1 \setminus 2 \cdot (F_{NS,AS} - d_A \odot F_{NS,AS})$ | selection of the flow sources | macroscopic |
| 59 | $c_{AS} := S_{NS,AS} \overset{NS}{\star} c_{NS}$ | concentration in the convective flows | macroscopic |
| 60 | $\hat{n}_{NS,dt}^v := F_{NS,AS} \overset{AS}{\star} \left(\hat{V}_{A,dt} \odot c_{AS} \right)$ | convective species flow | macroscopic |
| 62 | $\dot{n}_{NS,dt} := \hat{n}_{NS,dt}^v + \hat{n}_{NS,dt}^d + \tilde{n}_{NS,dt}$ | differential species balances | macroscopic |
| 63 | $to_N := Set(t_N, -)$ | initial time | root |
| 64 | $te_N := Set(t_N, -)$ | end time | root |

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| no | equation | documentation | layer |
|----|---|---|----------------------|
| 71 | $\rho_N := m_N \cdot (V_N)^{-1}$ | mass density | materialDB |
| 76 | $k^{c_x}_{N,A,dt} := (-P_{N,A,dt}) \overset{N}{\star} \left(\lambda_S \overset{S \in NS}{\star} (\mu_{NS})^{-1} \right) \cdot (V_N)^{-1} \cdot \frac{\partial U_N}{\partial p_N} \cdot v_{xN}$ | convective mass diffusivity per area | materialDB |
| 78 | $k^{v_x}_{N,A,dt} := (\rho_N)^{-1} \cdot k^{c_x}_{N,A,dt}$ | 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 | $k^{d_x}_{NS,AS,dt} := (-P_{NS,AS,dt}) \overset{NS}{\star} \left(v_{xN} \cdot (V_N)^{-1} \odot (\mu_{NS})^{-1} \right) \cdot \frac{\partial U_N}{\partial \mu_{NS}}$ | diffusional mass diffusivity per area. | materialDB |
| 82 | $\hat{n}_{NS,dt}^d := A_{xN} \odot F_{NS,AS} \overset{AS}{\star} \left((-k^{d_x}_{NS,AS,dt}) \cdot F_{NS,AS} \overset{NS}{\star} \mu_{NS} \right)$ | diffusional species flows | macroscopic |
| 83 | $\hat{V}_{A,dt} := F_{N,A} \overset{A}{\star} (-k^{v_x}_{N,A,dt}) \cdot A_{xN} \cdot F_{N,A} \overset{N}{\star} p_N$ | volumetric flow | macroscopic |
| 86 | $k_{granulate_{dt}} := k_{granulate_{dt}}$ | link to kinetic granulation constant | materialDB »> solid |
| 87 | $\tilde{N}_{N,dt} := k_{granulate_{dt}} \cdot r_N$ | granulation dynamics | solid |
| 89 | $N_{tN,dt} := \frac{\partial \tilde{N}_{N,dt}}{\partial r_N}$ | population balance PDE | solid |
| 90 | $A_N := U_N - T_N \cdot S_N$ | definition of Helmholtz energy | physical |
| 91 | $G_N := U_N + p_N \cdot V_N - T_N \cdot S_N$ | definition of Gibbs free energy | physical |
| 92 | $\mu_{NS} := \frac{\partial G_N}{\partial n_{NS}}$ | chemical potential from Gibbs free energy | physical |
| 93 | $\alpha_{N,dt} := a_{N,dt} \cdot \sin(t_N \cdot f)$ | stirrer function | mixing |
| 94 | $one := Set(\#, -)$ | one | root |
| 95 | $1_N := Set(y_N, -)$ | one of the same dimension as y | mixing |

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| no | equation | documentation | layer |
|----|---|------------------------------|-------------|
| 96 | $dy_{N,dt} := \alpha_{N,dt} \cdot (\gamma \cdot y_N - \beta \cdot (y_N - 1_N))$ | mixing differential equation | mixing |
| 97 | $\dot{n}_{NS,dt} := Set(\dot{n}_{NS,dt}, 0)$ | zero accumulation | macroscopic |
| 98 | $n_{NS} := \int_{t_{oN}}^{t_{eN}} \dot{n}_{NS,dt} dt$ | integral | macroscopic |

39.2 Instantiations

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