BFB Model v7.0.0

Noted Errors:

* Gas and solids energy balances: fix reaction transfer term (rg)
* B11: hvap should come from sol\_prop\_c
* Check solids balances for dl terms (notably Ksbulk)
* B8: add other boundary conditions
* H6: use vg,0 instead of calculating from feed, move division by Dt
* I2: Try moving db term again
* Combine J6 into J7?

Semantic changes:

* Rename B7, B8 – sorbent to solid
* Rename energy balances as enthalpy balances (and F2, F4)
* Swap C1 Else with C4
* Rename C6 & C7 – enthalpy should be component
* Renumber hydrodynamic constraints (H3 missing)
* Is H12 needed?
* Use aliases rather than equality constraints to link properties
* Rename reaction equation constraints

# Nomenclature

Indexes:

i – finite element (integers between 0 and nfe)

j – gas component list

k – solid component list

# Geometric Constraints

A1: Finite element locations

A2: Finite element size

A3: Cross-sectional area

A4: Distributor design

HX Tube Dependent Geomerty

A5: Relating bed cross-section to total reactor cross-section

A6: Hydraulic diameter of bed

A7: HX tube pitch

A8: HX tube spacing

A9: Surface area of HX tubes

# Mass and Energy Balances

B1: Bubble region gas component balances (i > 0)

B2: Cloud-wake region gas component balances (i > 0)

B3: Emulsion region gas component balances (i > 0)

B4: Bubble region gas energy balances (i > 0)

B5: Cloud-wake region gas energy balances (i > 0)

B6: Emulsion region gas energy balances (i > 0)

B7: Cloud-wake region sorbentlids balances

If i = 1:

If i > 1:

B8: Emulsion region solids balances (i > 1)

If solids inlet and outlet at same location:

If Top feed and Underflow outlet:

If Bottom feed and Overflow outlet:

B9: Cloud-wake region adsorbed species balances

If i = 1:

If i > 1:

B10: Emulsion region adsorbed species balances

If 1 < i < nfe:

B11: Cloud-wake region solids enthalpy balances

If i = 1:

If i > 1:

B12: Emulsion region adsorbed specisolids enthalpy balances

If 1 < i < nfe:

Reactor Configuration Dependent Mass and Energy Balances (Boundary Conditions)

Bottom Feed, Underflow Outlet

B13: Emulsion region adsorber species balance lower boundary (i = 1)

B14: Emulsion region adsorbed species balance upper boundary (i = nfe)

B15: Emulsion region solids enthalpy balance lower boundary (i = 1)

B16: Emulsion region solids enthalpy balance upper boundary (i = nfe)

Top Feed, Underflow Outlet

B13: Emulsion region adsorber species balance lower boundary (i = 1)

B14: Emulsion region adsorbed species balance upper boundary (i = nfe)

B15: Emulsion region solids enthalpy balance lower boundary (i = 1)

B16: Emulsion region solids enthalpy balance upper boundary (i = nfe)

Bottom Feed, Overflow Outlet

B13: Emulsion region adsorber species balance lower boundary (i = 1)

B14: Emulsion region adsorbed species balance upper boundary (i = nfe)

B15: Emulsion region solids enthalpy balance lower boundary (i = 1)

B16: Emulsion region solids enthalpy balance upper boundary (i = nfe)

Top Feed, Overflow Outlet

B13: Emulsion region adsorber species balance lower boundary (i = 1)

B14: Emulsion region adsorbed species balance upper boundary (i = nfe)

B15: Emulsion region solids enthalpy balance lower boundary (i = 1)

B16: Emulsion region solids enthalpy balance upper boundary (i = nfe)

# Flowrate and Flux Relationships

C1: Superficial gas velocity

If i = 0:

Else:

C2: Initial emulsion region gas flow rate

C3: Initial bubble region gas flowrate

C4: Bubble volume fraction (i > 0)

C5: Emulsion gas flowrate (i > 0)

C6: Bubble region gas component flowrate

C7: Emulsion region gas component flowrate

C8: Bubble region gas enthalpy flowrate

C9: Emulsion region gas enthalpy flowrate

C10: Cloud-wake region solids flux (i > 0)

C11: Emulsion region solids velocity (i > 1)

C12: Cloud-wake region adsorbed species flux (i > 0)

C13: Emulsion region adsorbed species flux (i > 1):

C14: Cloud-wake region solids enthalpy flux (i > 0)

C15: Emulsion region solids enthalpy flux (i > 1)

# Inlet and Outlet Conditions

D1: Initial bubble region gas mole fractions

D2: Initial emulsion region gas mole fractions

D3: Initial bubble region gas temperature

D4: Initial emulsion region gas temperature

D5: Outlet gas flowrate

D6: Outlet gas enthalpy (not working yet)

D7: Outlet gas pressure

D8: Outlet gas mole fractions

Reactor Configuration Dependent Outlets

Overflow Outlet

D9: Outlet solids flowrate

D10: Outlet solids temperature

D11: Outlet solids loadings

Underflow Outlet

D9: Outlet solids flowrate

D10: Outlet solids temperature

D11: Outlet solids loadings

# Mole Fraction Relationships

E1: Bubble region gas component concentrations (i > 0)

E2: Cloud-wake region gas component concentrations (i > 0)

E3: Emulsion region gas component concentrations (i > 0)

E4: Bubble region total gas concentration (i > 0)

E5: Cloud-wake region total gas concentration (i > 0)

E6: Emulsion region total gas concnetraion (i > 0)

# Bulk Flow and Mixing Relationships

F1: Bulk gas mass transfer (i > 0)

F2: Bulk gas enthalpy transfer (i > 0)

F3: Bulk solids mass transfer (i > 0)

F4: Bulk solids enthalpy transfer (i > 0)

F5: Bulk solids component mixing (i > 0)

# Other General Constraints

G1: Pressure drop

If i = 0:

Else:

H1: Archimedes Number (i > 0)

# Hydrodynamic Constraints

H2: Emulsion region gas velocity (i > 0)

H4: Bubble size coefficient (i > 0)

H5: Maximum bubble diameter (i > 0)

H6: Constrained bubble diameter

If i = 0:

Else:

H7: Bubble rise velocity (i > 0)

H8: Bubble velocity (i > 0)

H9: Cloud to bubble volume ratio (i > 0) (known singularity, fix in comments)

H10: Cloud-wake to bubble volume ratio (i > 0)

H11: Emulsion region voidage (i > 0)

H12: Average voidage (i > 0)

# Heat and Mass Transfer Coefficient Constraints

I1: Bubble to cloud-wake gas mass transfer coefficient (i > 0)

I2: Cloud-wake to emulsion gas mass transfer coefficient (i > 0)

I3: Cloud-wake to emulsion solid mass transfer coefficient (i > 0)

I4: Bubble to cloud wake gas heat transfer coefficient (i > 0)

I5: Cloud-wake to emulsion gas heat transfer coefficient (i > 0)

I6: Convective heat transfer coefficient (i > 0)

# HX Tube Transfer Model Constraints

J1: Thermal conductivity of bed at minimum fluidization (i > 0)

J2: Fluidisation number (i > 0)

J3: Residence time of emulsion packets at HX surface (i > 0)

J4: Fraction of time HX surface is exposed to mulsion packets (i > 0)

J5: Dense region heat transfer coefficient (i > 0)

J6: Bubble region heat transfer coefficient – Prandlt number (i > 0)

J7: Bubble region heat transfer coefficient (i > 0)

J8: Total HX heat transfer coefficient (i > 0)

# HX Fluid Heat and Mass Balances

K1: Total heat duty

K2: HX tube heat transfer (i > 0)

K3: HX fluid pressure drop (i > 0)

If i = nfe:

Else:

K4: HX fluid energy balance (i > 0)

If I = nfe:

Else:

K5: Temperature difference between tubes and bed (i > 0)

K6: HX tube wall energy balance (i > 0)

# Reaction Rate Constraints

L1 (spropc\_rg): Cloud-wake region gas reaction rate (i > 0)

L2 (spropc\_rs): Cloud-wake region adsorbed species reaction rate (i > 0)

L3 (sprope\_rg): Emulsion region gas reaction rate (i > 0)

L4 (sprope\_rs): Emulsion region gas reaction rate (i > 0)