

Kunii-Levenspiel Bubbling Fluidised Bed Model

Version and Change Log 10/6/2015

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Version History

Version	Release Date	Author	Comments
6.3	30 Oct 2015	A Lee	Improvements to model performance
6.2.1	24 Jun 2015	A Lee	Error corrections
6.2	May 2014	Y Chen, B Omell	
6.0	Unknown	J Morinelly	UQ added
5.2.2	Unknown	J Morinelly	
5.1.1	6 Dec 2011	A Lee	1 st Full release of model
5.2	21 Mar 2012	A Lee	
5.1	6 Oct 2011	A Lee	Initial internal release of model
5.0	4 Aug 2011	A Lee	Corrected errors in mass balance
4.0	6 Jul 2011	A Lee	Error in mass balance
3.0	22 Jun 2011	A Lee	
2.2.4	13 Mar 2011	A Lee	EN Kinetic model
2.2.2	1 Mar 2011	A Lee	
2.1	15 Sep 2010	A Lee	First build of current model with hydrodynamics
1.0	6 May 2010	A Lee	0 dimensional model

Issues of Note in Current Model

- Note that point 0 in the discretisation domain is a non-physical point (with volume 0), used to calculate conditions in the system immediately above the distributor plate
- Dynamic terms in mass and energy balances consider only one temporal derivative, whilst there are a number of other terms that can potentially vary with time. This has been examined and it has been determined that the error introduced is small, whilst correcting this significantly increases the computational complexity.
- Dynamic terms in energy balances for cloud-wake and emulsion regions use `cpg_mol`, which is calculated based on bubble region conditions. In most cases, the error introduced by this should be negligible, unless there are significant changes in conditions between the different regions (i.e. very rapid reactions).
- The liquid density of the heat exchanger fluid is currently calculated using a correlation of liquid water as a function of temperature. It has been determined that the Peng-Robinson equation of state with Boston-Matthias alpha function currently used by the ACM implementation of the model gives an incorrect value for the density of liquid water. To maintain backwards compatibility of results, a correlation for this property has been coded into model in place of the property call, thus users with different heat exchange fluids will need to change this. This only affects the ACM implementation, and not the gProms version.

Detailed Change Log

V1

Initial model based on Kunii-Levenspiel model.

V1.0 – 6th May 2010

- Simple reactor model based on model developed by Kunii and Levenspiel.
- 0-Dimensional, well mixed isothermal model
- Simple first order reaction kinetics for CO₂ with equilibrium.
- Assumed no adsorption of water.

V2

First functioning 1-D model of bubbling bed. Extends on the work of Kunii and Levenspiel to allow for non-isothermal conditions, non-first order reaction kinetics and includes additional correlations based on subsequent research.

V2.1 – 15th September 2010

- New version of model developed as a 1-Dimension steady state model.
- Horio and Nonaka bubble growth model added.
- Hilligardt and Werther bubble velocity model added.
- Sit and Grace heat and mass transfer improvement factor added.
- Navier-Stokes equation for pressure drop.
- Includes model of freeboard behaviour.
- First order reaction kinetics with equilibrium for CO₂.
- Adsorption of water assumed to be equal to that of CO₂.
- Physical properties of gas calculated using Aspen Properties.
- Correlations for regime transitions included.

V2.2.2 – 1st March 2011

- Added correlations for internal heat exchangers.

V2.2.4 – 13th May 2011

- Added simple kinetic model for EN sorbent.
- Removed freeboard model.

V3

Minor update of v2 to address issues with integrating model with Excel and modeFRONTIER, plus minor improvements to equations.

V3.0 – 22nd June 2011

- Separated axial distribution domain from bed depth to allow homotopy to change bed depth.
- Introduced derivative scale factor to convert between partial derivative in axial domain and bed depth.
- Added calculations for varying solids heat capacity with loading.

V4

Update of previous versions to improve performance and simplify model. Released to CMU to develop surrogate models.

V4.0 – 6th July 2011

Known to have an error in mass balances.

- Split axial domain into two – one for positive axial flow and one for reverse flow (emulsion region).
- Added different boundary conditions for solids overflow and underflow exits and the ability to select which to use.
- Changed from using multiports for solid sorbent flows to custom port specification.
- Solids loadings expressed in terms of molar concentrations (mol/m^3) rather than kmol/kg sorbent.
- Simplified pressure drop calculation (solids mass term only).
- Added solids residence time calculation.
- Improved distributor plate pressure drop estimation.

V5

Rebuild of v4 to address critical errors in mass balances and to include dynamic terms for use by CCSI Task Set 4. Released to CMU for development of surrogate models for regenerator.

V5.0 – 4th August 2011

Version 5.X released early to CMU due to issues with v4.

- Mass and energy balances now include time variant (dynamic) terms.
- Axial derivative terms are now expressed explicitly, rather than using partial differential terms. This significantly reduces the error in the mass and energy balance equations.

V5.1 – 6th October 2011

First general release of model, provided to TS4 for dynamic study and CMU for next round of surrogate models. Incorporated improvements based on 2nd Edition of Kunii and Levenspiel.

- Corrected unit conversion issue in mass transfer correlations and updated based on 2nd edition.
- Changed gas velocity calculation (vg) to use Aspen Properties call instead of ideal gas law.
- Fixed minor error in heat transfer equations between bed and immersed heat exchanger tubes.
- Improved calculation for heat exchanger tube pitch.
- Added variable to describe Geldart group classifications and corrected equation used to determine Geldart classification.
- Added correlations for emulsion region voidage and gas velocity for Geldart group A materials.
- Changed mass and energy balances and other correlations to use new correlations for emulsion region voidage.
- Added total heat duty calculation for internal heat exchanger.
- Added correlation for cloud to bubble volume ratio.
- Updated distributor plate pressure drop correlation based on 2nd Edition.

V5.1.1 – 6th December 2011

First full release of model as part of CCSI V1 toolset, used for A650.1 study. Updated version of V5.1 based on feedback from other groups. Version implemented in both ACM and gPROMS with minor variations.

- Corrected energy balances to address dependence on reference temperature. This required assuming constant heat capacities for gas and solids.
- Add bulk gas flow term between emulsion and bubble regions to address significant pressure variation in highly reactive systems.
- Corrected minor error in implementation of lumped parameter kinetic model.
- Minor error corrections.

V5.2a – 28th March 2012

Updated version of V5.1.1 based on results of CFD simulations by Task Set 2 and other feedback.

- Further revision of energy balances based on paper by Walton and LeVan. A specific enthalpy is now calculated for all solid flows which includes the adsorbed species and heat of reaction.
- Modified solids circulation calculations to better reflect Kunii and Levenspiel's analysis.
- Added correlation for emulsion phase gas velocity for Group B particles.
- Added calculation of hydraulic diameter to model to account for effects of internal heat exchangers on hydrodynamics, and integrated this with existing correlations.
- Added bubble velocity calculation for slug flow conditions arising due bubbles being limited by hydraulic diameter.
- Modified solid boundary conditions to allow for top and bottom solid inlets.

- Switched to using U-tube heat exchangers rather than single pass exchangers. Added terms to account for pressure drop and heat transfer resistance in heat exchanger tubes.
- Replaced total gas balance with sum of mole fractions relationship for the bubble phase to address singularity issue in dynamic simulations.
- Minor error correction in calculating solids residence time.
- Corrected unit conversion error in heat exchanger tube energy balance in ACM version of model.

V5.2.2 – (Date Unknown) Juan Morinelly

- Organized code
- Correction in solid mass balances boundary conditions
- Corrected unit conversion error in heat exchanger tube energy balance
- Minor error correction in calculating solids residence time.
- Modified solid ports type
- Added initialization procedure (script, variables, and simplified equations)
- Added distributed variables for adsorbed species solids loading
- Modified heat exchanger model to single pass counter-current to gas flow
- Added pre-defined distributed variable plots and input/output tables
- Added variable for inlet heat exchange fluid velocity, v_{hx}
- Added variables for heat exchanger tube spacing and tube wall thickness, l_{hx} and w_{thx}
- Added variable for gas superficial velocity at inlet, v_{gi}
- Added flash call for heat exchanger inlet

V6

Update of V5.2.2 to include Uncertainty Quantification variables.

V6.0 – (Date Unknown) J Morinelly

- Added specific component lists for the heat exchange medium and the gas phase to allow different property sets
- Added specific variable for water removal and eliminated regeneration variable
- Eliminated intermediate variables for adsorbents solids loading and updated equations accordingly
- Added UQ coefficients
- Simplified kinetic model code
- Separated kinetic model variables declaration in order to enable users to modify those sections
- Included scaling factor for kinetic model equations to allow an user to achieve convergence for a wider range of orders of magnitude

V6.2 – May 2014, Y Chen and B Omell

- Modified cloud-wake and emulsion region gas and solids balances to be calculated between 1 and ND-1 to be consistent with bubble region
- Modified calculation of bulk transfer terms to be between 2 and ND-1 to agree with new mass and energy balances
- Modified heat exchanger calculations to suit new system boundaries
- Added boundary value calculations at point 0 for necessary variables

V6.2.1 – 22 May 2015, A Lee

- Corrected significant error in solids enthalpy calculation
- Corrected error in calculation of discretisation length
- Corrected error in hydrodynamics model relating to height above distributor
- Corrected minor error in calculation of average bed voidage (eavg)

V6.3 – 6 Oct 2015, A Lee

- Added Run Mode selectors to allow user to modify specific model behaviours to suit their needs
- Redefined discretisation domain to allow non-uniform discretisation and implemented options for 2-stage and adaptive discretisation schemes with selector
- Incorporated simplified correlations for physical properties and the ability to choose between these and calls to a physical properties package using selector
- Reworked heat exchanger fluid physical properties calculations to simplify system and improve robustness with selector
- Added option to use Smoothed Maximum operations in place of some IF statements to improve robustness with selector
- Added run mode selector to allow steady-state users to use a simpler summation of concentrations in place of a full mass balance for gas phase components. This is not suitable for dynamic simulations as it results in a singularity issue
- Modified bubble and emulsion region correlations to fit new discretisation definition
- Corrected error in calculation of initial bubble diameter
- Updated scaling of equations and variables
- Updated variable definitions to improve initial values, upper and lower bounds and units
- Added a component list for adsorbed species and redefined sorbent port to be consistent with other port definitions. This will make it easier to substitute new sorbents in future
- Rewrote some equations to remove potential divisions by zero
- Renamed m1 to m3 for consistency, as it is used in calculating the rate of reaction 3
- Cleaned up code and removed some excess variables and equations (such as unit conversions)

- Replaced incorrect property call for the density of liquid water in ACM implementation with a correlation
- Added initialisation script for regeneration conditions and improved script for adsorption conditions
- Corrected a number of variable bounds which were limiting model flexibility and robustness
- Corrected an error in the hydrostatic pressure drop term in HX Fluid pressure drop correlations