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# A new one-dimensional particle-in-cell model for multiphase vessel flow

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**Abstract** — A new one-dimensional particle-in-cell transport model for multiphase flow in a vessel is presented. The model aims at the consistent simulation of discontinuities as the top level of a multi-phase mixture. Thus it is possible to include models for the transient behaviour of a foam layer on top of a mixture, for example. The transport model, which is the basic component of a new computer code will be described. Flexible interfaces allow the implementation of models, constitutive laws or correlations for extra effects like phase transfer, generation and coalescence of bubbles or drops, foam behaviour, heat transfer, discharge from the vessel, etc. Due to these interfaces and a transparent code structure the code is a suitable basis for the development, testing and validation of models. It allows the completion or the replacement of such models according to the specific application.


**transient simulation / multiphase flow / particle method / numerical diffusion / chemical reactor / depressurisation / foam / discontinuity**

## Nomenclature

| | | |
|---|---|---|
| $A$ | vessel cross section | $m^2$ |
| $k_{out}$ | number of sink bricks | |
| $\dot{m}$ | mass source | $kg \cdot m^{-3} \cdot s^{-1}$ |
| $N_{bricks}$ | number of bricks per node | |
| $N_{nodes}$ | number of nodes | |
| $q$ | density of source for volume fraction | $s^{-1}$ |
| $t$ | time | s |
| $V$ | volume | $m^3$ |
| $w^i$ | velocity of the phase | $m \cdot s^{-1}$ |
| $w_0$ | superficial velocity of the mixture | $m \cdot s^{-1}$ |
| $z$ | axial vessel coordinate | m |
| $\varepsilon$ | phase volume fraction | |
| $\rho$ | density | $kg \cdot m^{-3}$ |

*Indices*

| | |
|---|---|
| $j$ | refers the phase |

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## 1. INTRODUCTION

Multiphase flow can be found in numerous technical facilities such as steam generators, cooling or heating devices or chemical reactors. The understanding of flow phenomena within such plants is important for design, process control, and to ensure safety. Besides experimental studies transient numerical simulations of processes within an apparatus will be required in the future to improve the efficiency and safety. In principle, modern commercial CFD codes enable two- or three-dimensional simulations of multiphase flow phenomena within a vessel, but there are limitations e.g. in the case of large volume fractions of the dispersed phases, or in the representation of the boundaries of the phases. For most cases the calculation times are very long. Available CFD codes often have limited capabilities to describe phenomena, which must be included into the simulation for special cases. This is why two- or three-dimensional simulations are mostly used only to investigate special phenomena, like the mixing of two fluids within a vessel, for example [1]. For more complex processes in practical applications often simpler models

are used, which neglect space effects or are based on one-dimensional approximations and include the relevant process phenomena [2].

In the case of multiphase flows in vessels, gravity driven separation effects are important. For this reason, at least the variation of important parameters such as phase fraction, temperature, velocity and concentration of components over the height of the apparatus should be considered. The scope of the phenomena to be included and the models applied depend on the actual problem to be solved. A foam layer e.g. on top of the mixture should be taken into account, when the fluid contains surface active substances. Existing finite-element and finite-difference methods are often not flexible enough and suffer from insufficient numerical stability in the case of certain constitutive laws being implemented. Another problem is numerical diffusion, which leads to a significant loss of accuracy when discontinuities are present.

For these reasons, the development of a new simulation method was started. The aim of this development was to have a flexible module, that allows us to simulate transport phenomena in a vessel and that, for simplicity, should be based on one-dimensional mass conservation equations. This module is equipped with flexible programming interfaces, which permit the convenient implementation of constitutive laws and models for additional effects. A particular goal of the development was the consistent simulation of discontinuities, especially the accurate simulation of the behaviour of the top level of the multiphase-mixture. This feature can be used for the implementation of foam models. Such an implementation makes the transient simulation of foam generation and decay possible. The consideration of foam is very important, e.g. when depressurisation processes are investigated, because the mass losses depend on the quality of the multiphase mixture at the relief line entrance.

## 2. BASIC IDEA OF THE BRICK MODEL

In the three-dimensional reality of multiphase flow there is only one phase at one point in space and time. Volume fractions of the single phases, which play an important role in numerical simulations, are produced by averaging over time or in space. Usually, the vessel volume is subdivided into vertical subvolumes (nodes) for the one-dimensional numerical representation [3–5]. For these nodes phase volume fractions and average values for other properties are calculated. The state of the phase distribution within the vessel is represented in the numerical model by the phase volume fractions for each vertical node. *Figure 1* shows a typical situation for the special case of two phases. The blue colour represents water. Air bubbles are marked white. The upper level of the water/air mixture is located within

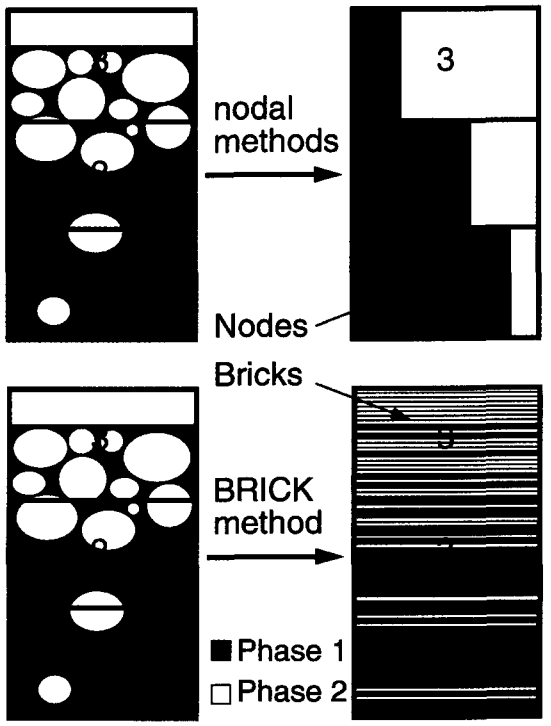


**Figure 1.** Methods of representation of volume phase fractions for discrete one-dimensional models.

the top node. As demonstrated at the upper row of the figure, the information on the height of this level is not contained in the numerical model. It should be mentioned that there are of course also special methods such as interface tracking methods [6, 7], which allow the calculation of the level position. However, they are in most cases complicated and are added as a supplementary procedure to the numerical solution algorithm. In real multiphase flow it is also possible that a number of levels exit over the vessel height. They may be generated or vanish during the transient process. In this case the handling of such additional methods is very complicated.

The new BRICK method, which belongs to the class of Particle-In-Cell (PIC) approaches [7, 8], also subdivides the whole vessel volume into a number of nodes ($N_{\text{nodes}}$). All nodes have equal volumes. These node volumes are subdivided again into a large number ($N_{\text{bricks}} \sim 1000$) of small elements of equal volume, subsequently called bricks. The bricks always represent a part of the volume of a phase in the node. Each brick belongs to a well defined phase. Because of the one-dimensional representation, these bricks are stacked on top of each other. The present state of the phase distribution within the vessel is represented by the arrangement of the bricks in the batch (see *figure 1*). As in the three-dimensional reality, only one phase

is at one point in space and time. Volume fractions are calculated by counting the number of bricks of each phase within the node volume. As demonstrated in *figure 1*, the complete information on phase distribution given by the usual nodal methods is also provided by the BRICK method. Additionally, there is an approximate information on the phase distribution within the nodes. In particular, the top level of the mixture is reflected by this method in an implicit way.

In addition to the information about which phase the brick belongs, further information like the specific enthalpy, the particle density (if the brick represents a dispersed phase) or the concentration of components may be assigned to all the bricks. Transport phenomena are modelled by means of displacement of the bricks as described below. As the result of one time step, a new arrangement of the bricks is generated, which describes the new state of the system.

The implemented model solves the balance of volume fractions of each phase. All volumes have to be related to the volume of one node. From the mass balance for each phase

$$\frac{\partial}{\partial t}(\varepsilon^j \rho^j) + \frac{\partial}{\partial z}(w^j \varepsilon^j \rho^j) = \dot{m}^\partial \qquad (1)$$

one can obtain an equation for the volume fraction of each phase:

$$\frac{\partial \varepsilon^j}{\partial t} + \frac{\partial}{\partial z}(w^j \varepsilon^j) = \frac{\dot{m}^j}{\rho^j} - \frac{\varepsilon^j}{\rho^j}\frac{\partial \rho^j}{\partial t} - \frac{w^j \varepsilon^j}{\rho^j}\frac{\partial \rho^j}{\partial z} \qquad (2)$$

These are the basic equations solved by the method presented here. Because of the particle representation, numerical diffusion is completely avoided. The conservation of momentum is considered through drift correlations.

## 3. CALCULATION OF A TIME STEP

The one-dimensional multiphase flow in a vessel can be characterized by two velocities:

– the motion of the mixture caused by volume sources (positive or negative); the corresponding velocity is the superficial velocity of the mixture; for the vertical position $z$, this velocity is calculated from the integral of the volume sources between the bottom of the vessel and the current position $z$:

$$w_0(z,t) = \frac{1}{A(z)} \int_0^z \dot{V}(z',t)\,\mathrm{d}z' \qquad (3)$$

– there is a relative motion of the single phases against each other; this may be considered as a relative drift velocity of the single phase, with respect to the superficial velocity of the mixture; correlations are available in literature for the drift velocity.

In BRICK the first stage of displacement is realised by the insertion of bricks into, or the removal of bricks from the batch according to the volume sources acting within that time step. All bricks above the source are lifted up or descent according to the number of inserted or removed bricks. The relative motion of the phases with respect to the superficial velocity is realised by an exchange of brick positions. The transport modelling within each time step will be discussed in detail below.

The transport model needs the drift velocities of $N_{\text{phases}} - 1$ phases and the densities of volume sources for each phase as a function of the vessel height as input parameters. These input parameters are calculated by the additional models for each node. The sum of the volume sources over the whole vessel has to be zero. In case of a closed vessel (pressurised vessels), this can be achieved via pressure dependent volume sources. These result from the compressibility of the phases and/or the phase transfer due to a variation of the pressure. A pressure iteration procedure is employed for that purpose. In case of an open vessel (vessel without a lid) an additional volume source at the top of the vessel compensates the sum of volume sources within the vessel.

Because of the discrete brick volumes, the model can only realise volume sources in discrete quantities. From the node values of the volume source density a number of source bricks is determined by rounding to these discrete values. In the pressure iteration the number of source bricks within every node is determined. The pressure is varied until the sum of all source bricks within the vessel is zero.

*Figure 2* shows on the left hand side an initial state as an example. For simplicity, the vessel is made from only one node. There are three phases present, which are marked by the colours of the bricks. The green colour marks the continuous phase (phase 1); red (phase 2) and blue (phase 3) represent two dispersed phases. The vessel volume is assumed to be 1 meter high and the time step width is 1 second. There are 20 bricks in the node. It is assumed that the additional models including the pressure iteration procedure supply the input given in the *table*.

In each time step 5 subtasks have to be solved. The procedure for the solution of each task is discussed subsequently. Each procedure is applied to all bricks before the next subtask is solved.

### Subtask 1

In the first subtask the negative volume sources are treated. They may be caused by the compressibility of the phases, by phase transfer or by external discharges. In the example, there is a sink for the phase 1 only. The number of bricks to be removed is calculated by:

$$k^1_{\text{out}} = \text{round}(-q^1 N_{\text{bricks}} \Delta t) = \text{round}(0.26 \times 20) = 5 \qquad (4)$$

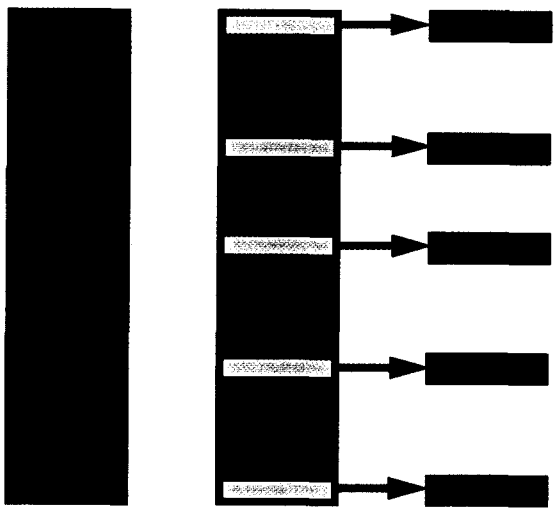

**Figure 2.** Removal of sink bricks from the initial stack (subtask 1).

| Input supplied to the transport model for the example case. | | |
|---|---|---|
| | Drift velocity | Volume source density |
| Phase 1 | - | $-0.26\ s^{-1}$ |
| Phase 2 | $0.21\ m{\cdot}s^{-1}$ | $-0.22\ s^{-1}$ |
| Phase 3 | $-0.16\ m{\cdot}s^{-1}$ | $0.04\ s^{-1}$ |

That means 5 bricks of phase 1 have to be removed. This corresponds to a volume source density of $-0.25\ s^{-1}$. The remainder of $-0.01\ s^{-1}$ is not realised. This residue might lead to an error which becomes non-negligible in time. Therefore, the remainders are stored for each node and each phase. They are taken into account in the calculation of the source values in the next time step. This procedure guarantees mass conservation. In the example, it is assumed that the sink is caused by the compressibility of the phases or phase transfer. In this case the bricks are removed as uniformly from the node as possible. This is shown in *figure 2* on the right side.

Another type of sinks are external discharges from the vessel. In this case, a compact stack of bricks is removed starting at the location of the discharge and going downwards. If this source type occurs in a node it is done as the first partial step. The remaining volume source densities are recalculated according to the number of bricks removed:

$$q^j_{\text{new}} = q^j_{\text{old}} + \frac{k^j_{\text{out}}}{N_{\text{bricks}}\,\Delta t} \tag{5}$$

Remaining sinks are realised in a second step as described above. In the case of top venting from a vessel a stack of the top bricks is removed. This guarantees that liquid is only discharged if the level of the mixture reaches the top of the vessel.

## Subtask 2

In the second subtask, the bricks of mobile phases are shifted over a distance according to the product of the drift velocity and the time step width. Mobile phases are the phases for which a drift correlation is available. Generally, the mobile phases are the dispersed phases except for foams. A foam model provides the velocity of drainage of the liquid, which is the continuous phase. In the example, the two dispersed phases have to be shifted. From the drift velocity given above and the time step width, distances of 0.21 m for phase 2 and $-0.16$ m for phase 3 result for the shift. Due to the assumed height of the vessel and the number of bricks this corresponds to a shift of +4 brick positions for phase 2 and $-3$ brick positions for phase 3. The bricks representing these phases are taken from the stack and put to the new positions as shown in *figure 3*.

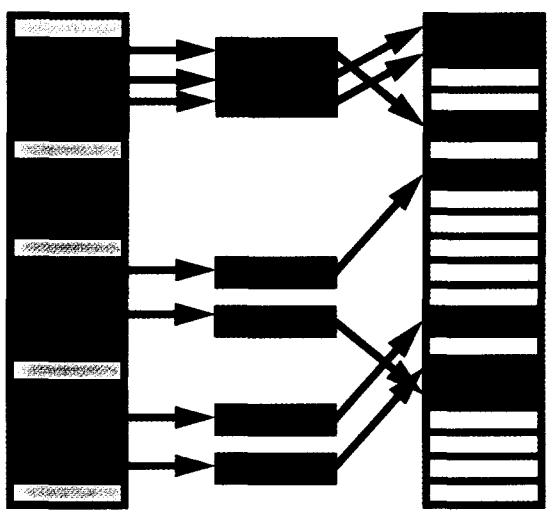

**Figure 3.** Displacement of the mobile phase (subtask 2).

Of course there is an error of discretisation because of the rounding of the distance of displacement. In practical calculations the number of bricks has to be chosen high enough so that the distance of the brick positions is very small. Typically the bricks are not shifted over 3 or 4 positions as in the example but usually over some hundred places. If the discretisation is chosen fine enough, the error is very small and far below that of the drift correlations. If the destination place for a brick is already occupied by another brick the next free place close to it is used. The error caused by this procedure is also negligible.

The destination location of a brick may lie outside the starting node. Drift velocities are supplied for every node. In the standard version of the code, the bricks move with a constant drift velocity within the node. If the brick reaches the node boundary, the velocity changes to the drift velocity valid for the next node. A version with a linear change of the brick velocity was also tested, but the results did not show any advantage over this method. A subroutine, which realises a displacement according to the drift velocity of the starting node all along the displacement of the brick is also available. If the destination lies outside the vessel or the considered region as discussed below, the lowest or the top places of the vessel or of the region are used.

## Subtask 3

In a further step, the displacement of the bricks representing the dependent phase is realised. Generally, the dependent phase is the continuous phase except in the case of foam. As shown in *figure 4*, the remaining bricks from the initial stack are transferred to the gaps of the new stack, which were generated earlier by subtask 2. This procedure starts at the bottom of the vessel and proceeds upwards. The gaps, which result from the bricks removed in the first subtask, are treated in this subtask like a dependent phase.

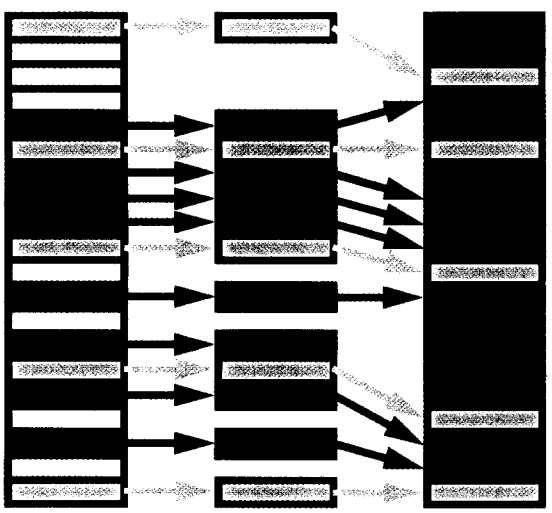

**Figure 4.** Displacement of the dependent phase (subtask 3).

## Subtask 4

The number of source bricks for each node and phase is calculated in analogy to equation 4. In the result 4 bricks of the phase 2 and 1 brick of the phase 3 are to be inserted. There are several options available for the arrangement of the source bricks within the node. In the example a uniform arrangement is assumed as shown in the centre of *figure 5*. Other options allow us to prefer the lower or the upper part of the node, the insertion as a compact stack at the lower or at the upper end of the node and the insertion beginning at the lower end of the node with a distance off-set for the inserted bricks according to the velocity of the phase. The last option is suitable e.g. for bubble columns where gas is injected at the bottom of the column. It ensures that the distances of the single gas bricks are uniform over the height of the column in case of a uniform gas velocity within the vessel. Other options produce an arrangement where bricks are accumulated in packages depending on the time step width. The results of the common nodal method would be best reproduced by a random distribution of the insertion places within the node.

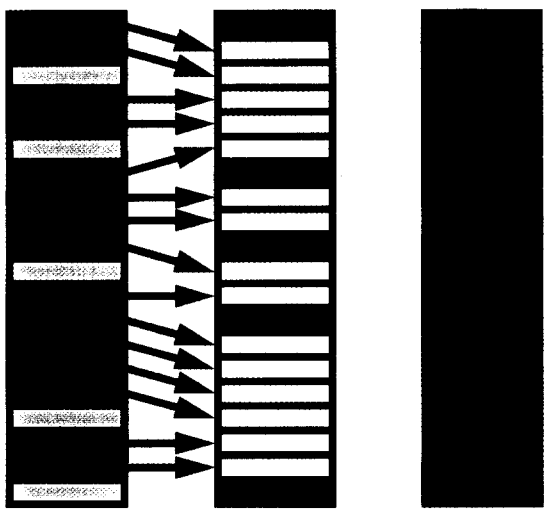

**Figure 5.** Insertion of source bricks (subtask 4) and final arrangement of the bricks (subtask 5).

In addition to the affiliation to a phase, the other properties have to be assigned to the source bricks (see below). The additional models supply such values for each node and phase, i.e. all inserted source bricks of a phase are assigned to the same values for the single properties within a node.

## Subtask 5

In the last subtask all the remaining gaps between the source bricks (batch in the centre of *figure 5*) are filled with the bricks from the stack generated by subtask 3 (right hand side of *figure 4* = left hand side of *figure 5*). The procedure again starts at the bottom of the vessel. All the gaps resulting from bricks removed within the

first subtask are skipped over now. The result of the transport calculation for the subtask is shown at the right hand side of *figure 5.*

It is an important advantage of the method, that besides the affiliation to a phase, marked in the example by different colours, the bricks may carry further properties. All properties that undergo transport, such as specific enthalpy, particle density or concentration of components may be attributed to the bricks. All these properties are then transported in a consistent manner.

After completion of the transport calculation, the node values for phase fractions are calculated by counting the number of bricks of each phase within the nodes. Node values for the other properties are calculated by averaging over the bricks. The node values serve as input data to the additional models in order to calculate new drift velocities and new volume density sources for the next time step. There is no iteration of the transport model and the additional models within the time step.

The code uses a pointer vector, which stores the brick positions. Each brick has a number. The number of a removed brick is assigned to a source brick. Only this pointer vector is recalculated within a single time step.

There is an additional option, which allows a relative motion of the phases to be calculated without the mobile and dependent phases having to be distinguished. For this option, consistent drift velocities for all phases have to be supplied to the transport model. The code calculates a destination vector for all bricks. Instead of the execution of the subtasks 2 and 3, the bricks are located according to this destination vector. This option may be useful if additional information on the motion of the continuous phase (e.g. a backflow) has to be considered.

Node values are calculated by averaging of the brick properties as mentioned above. In addition to the node values, properties assigned to the remainders from the sources are considered. This is important in particular if a new phase is generated. In case of non-equilibrium phase transfer, the mass transfer rate depends on the density of the surface area between the phases. Beginning evaporation first generates very small bubbles. Although the void fraction may be very small and consequently no brick will be generated, the density of the surface area, which may be calculated from the phase fraction and the bubble density, must not be neglected. If the properties of the remainder are taken into account the density of surface area may be calculated. This guarantees an exact handling of all properties and avoids violation of conservation laws.

## 4. DISCONTINUITIES AND REGIONS

The model allows us to introduce discontinuities (levels). One kind of discontinuity is the change of the continuous phase. This takes place at the top level of the mixture for example, where the continuous phase changes from liquid to gas. Other discontinuities can appear, when two or more immiscible liquid phases are present. The sections between two levels will be called regions. A foam layer is treated as a special region. At the lower boundary of this region a fictitious level marks the change of the drift laws. Below this level, the drift law for bubble flow must be applied. In the foam region, a special foam model has to supply the drainage velocity of liquid. Levels may be generated or vanish during the transient calculation.

The displacement of the mobile phases (subtask 2) is calculated separately for each region. That means, if a brick of a dispersed phase moves upwards and reaches a level, it does not cross this level. Instead it is placed at a free place directly below the level. This is done in order to avoid the displacement of the brick with a false drift velocity. If e.g. a gas bubble reaches the top level of the mixture, it should not further move in the gas volume with the drift velocity calculated for the gas bubble in the liquid. In this way the bricks representing gas bubbles accumulate below the level. After completion of the transport calculation the level is moved downwards to the next brick representing liquid. The former bubbles are now marked as continuous phase and added to the gas volume.

The shift of the levels after completion of the transport calculation is done simultaneously with the determination of the new node values. The procedure starts from the bottom of the vessel. The particle density is a property assigned to the bricks. The bricks representing the continuous phase are marked by a negative number. Starting at the bottom of the vessel, the first brick assigned to the continuous phase is searched. The phase of this brick determines the continuous phase of the lowest region. Going upwards, the procedure is seeking a brick marked as a continuous phase but assigned to a phase other than the present continuous phase. If such a brick is found, a level is introduced at the position of the last brick of the former continuous phase. Above the level, the new phase is defined as a continuous phase.

## 5. THE INTERFACE FOR THE IMPLEMENTATION OF A FOAM MODEL

The interface for the implementation of a foam model demonstrates the capabilities of the method. It is a particular option of the code to consider the generation and decay of a foam layer at the top level of the mixture. For this option, the number of phases is limited to a liquid and a gas phase. The top level of the mixture marks the upper boundary of the foam layer. A second level is introduced, which marks the lower boundary of the foam layer. At this boundary, the drift correlation

changes. If no foam exists, the top level of the mixture and the lower boundary of the foam layer are at the same location.

The two discontinuities subdivide the vessel volume into three regions: the region of bubble rise, the foam region and the gas volume above the foam. As discussed above, the relative motion of the phases is calculated separately. For the region of bubble rise, a drift correlation for rising gas bubbles in liquid is used, while for the gas volume a drift correlation for falling drops is used. For the foam layer a foam model is needed, which provides the velocity of the drainage of liquid within the foam structure.

The calculation of the relative motion within the individual regions results in layers of bubbles accumulated below the lower boundary of the foam region. At the top of the same boundary, a layer of drained liquid collects as shown in *figure 6.* A second layer of bubbles accumulates below the upper boundary of the foam layer.

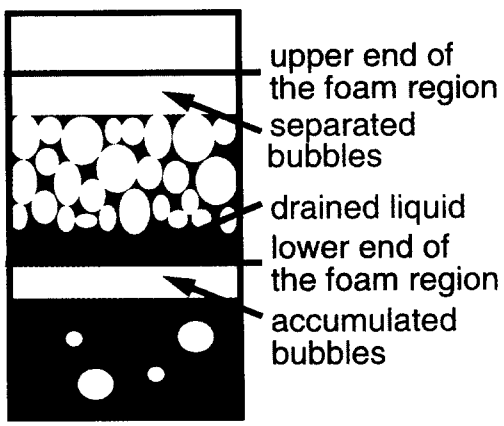


**Figure 6.** Result of a transport step in case of consideration of foam.

The bubbles accumulated at the top of the foam layer are added to the gas volume by shifting the top level of the mixture. This is realised by the standard level calculation procedure described above. Special measures are necessary at the boundary between the region of bubble rise and the foam region. At this location new foam is generated. For this reason, the accumulated bubbles have to be mixed with the drained liquid. The gas volume fraction of the resulting new foam is an input parameter. The corresponding bricks are stacked on top of each other to produce this value. If a gas volume fraction of 75 % is required for example, portions of three bricks representing accumulated bubbles and one brick representing drained liquid are stacked as shown in *figure 7.*

In general, the bricks representing accumulated bubbles and the bricks representing drained liquid do

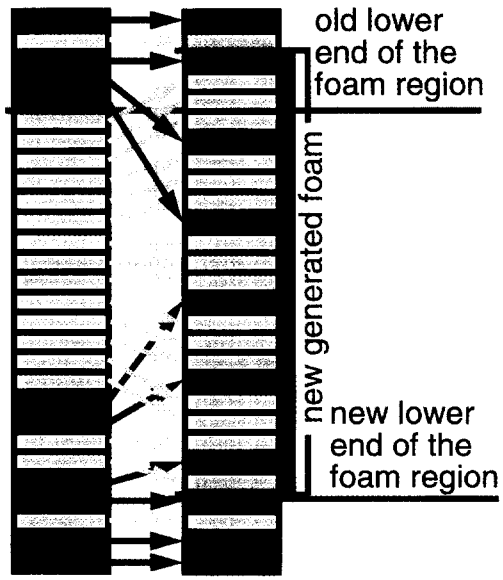


**Figure 7.** Displacement of the bricks at the lower end of the foam region.

not comply with the phase ratio given by the input parameter. The remainder has to be treated in a special way: If there is an excess of accumulated bubbles, they have to be mixed with liquid taken from the bubble rise region. This case is shown in *figure 7.* It causes a growth of the foam layer into the bubble rise region. The lower boundary of the foam region moves downwards. Any excess of drained liquid must be added to the region of bubble rise. In this case the foam decays.

The interface for a foam model was tested using simple correlations for the drain velocity of the liquid within the foam. The generation of foam, stable foam layers as well as the decay of the foam were simulated successfully. The brick model is suitable to perform tests of different foam models with a high efficiency.

## 6. LINKS BETWEEN THE TRANSPORT MODEL AND ADDITIONAL MODELS

There are different levels of links between the transport model and additional models. The exchange of data between the models is enabled by a common data field. It stores all the parameters of the system. On the one hand, some models use only these parameters and recalculate the related properties. An example is the model for homogeneous chemical reactions. Using the temperature, the phase fraction and the concentration of the components which the phase consists of, heat release and new concentrations for each node and phase are calculated. Other parts of the model are not affected

by this module except the data input, which has to supply the data for the kinetics of the reaction. No explicit interface is required for such models. They can be easily implemented or replaced. Such models are:

- heat exchange (vessel wall, heating devices or cooling devices);
- models for external sources except discharge model;
- models for the coalescence or decay of particles;
- models for homogeneous chemical reactions.

On the other hand, there is a very close link between the transport module and the pressure iteration module. As mentioned above this module has to guarantee that the sum of all source bricks within the vessel is zero. For this reason, the equations used by the transport model for the calculation of the source bricks for each node and each phase have to be taken into account by this module. The procedure for the pressure iteration itself has to call modules for the calculation of the phase transfer, because it depends sensitively on the system pressure. In a first step, an initial interval of the pressure is determined in a way that the sign of the sum of the sources changes within this interval. Then an interval nesting is carried out until the sum of all source bricks is zero. In the case of nodes with exactly the same properties it may happen that this iteration does not converge, because even for very small changes of pressure the number of source bricks changes by more than one. In this case, a random modification of the sources is carried out, which is set back at the next time step. This trick guarantees the convergence of the iteration.

For other phenomena like drift or phase transfer it should be possible to add new models easily, but they can not be programmed in only one independent routine in general. They also affect other models. For this reason, flexible interfaces were implemented for the following models:

- drift correlations,
- phase transfer models and connected with that different formulations of the equations for conservation of energy;
- discharge models;
- correlations for the heat transfer between the fluid and the vessel wall;
- the foam model as discussed above.

## 7. MOST IMPORTANT ADDITIONAL MODELS AND THEIR MAIN FEATURES

### 7.1. Drift flux correlations

The drift flux models provide drift velocities for a dispersed phase within a continuous phase. This means, that for several dispersed phases within one continuous phase, different drift correlations may be valid. For liquid droplets within the gas volume another drift correlation can be defined, other than that for gas bubbles within the liquid phase, for example. For the calculation of the properties of the continuous phase, such as density or viscosity, different options are available. Besides the option to use the properties of the pure continuous phase it is also possible to calculate averaged properties from all phases including or excluding the considered dispersed phase. The drift models included up to now are:

- constant drift velocity;
- single particle rise with consideration of the deformation of the particle [9];
- single particle rise with consideration of the deformation of the particle combined with a swarm correction;
- Labuntzov drift model [10];
- Ishii bubbly drift model [11];
- Ishii churn turbulent drift model [11];
- Kataoka-Ishii drift model [12].

### 7.2. Phase transfer and conservation of energy

For phase transfer the following models are available:

- thermodynamic equilibrium for one component;
- thermodynamic non-equilibrium for one component;
- dissolving gas without evaporation;
- phase transfer for multi-component mixtures with evaporating and dissolving components based on the ideal mixture approximation.

According to these different models of phase transfer, different formulations of the equations for energy conservation are used. All these are Lagrangian formulations, because the specific enthalpy (in case of multi-component mixtures the temperature) is treated as a brick property. Terms of the conservation equation for the energy describing transport phenomena have to be omitted. In case of the thermodynamic non-equilibrium model, an approximate analytical solution for the change of the enthalpy within the time step guarantees numerical stability even at relatively large time steps.

### 7.3. Heat transfer from the vessel wall

In order to simulate the heat release from the vessel wall, a model from the code BLDN [13–15] was used. It includes the heat release from the vessel jacket as well as the heat release from the bottom and the top of the vessel. The wall of the vessel is subdivided into axial nodes. In nodes where a level is present, the calculation

of the heat flux between wall and fluid is performed separately for the volume below and above the level. For different regions, different correlations for the heat transfer coefficient can be defined.

## 7.4. Discharge models

At present only one frozen flow model is implemented for the simulation of critical flow. It is valid for small orifices. The discharge model uses the microstructure of the arrangement of bricks at the entrance of the ventline (see § 2.2, subtask 1). This gives the possibility of using different averaging methods to determine phase fractions. One borderline case is an ideal plug flow. In this case, there is no mixing of the phases considered. The single phases are discharged sequentially. This is realized by discharge without ventline or a presentation of the ventline as a simple delay line. This means, that only the time for transport from the vessel to the location of discharge is taken into account. The brick structure is maintained in the ventline. The discharge is supplied with the individual phases in the same successive order, in which the bricks appear at the entrance of the ventline. Other options are based on averaging within the time step or within a given volume. A more detailed one- dimensional ventline model is also included [16].

## 7.5. Homogeneous chemical reactions

Homogeneous chemical reactions are described by kinetics. There is no limitation in the number of simultaneously running reactions.

## 8. VALIDATION

The complete model as well as parts of it were verified using numerous test cases, including comparisons with analytical solutions for special cases. The code was also validated with depressurisation experiments with water/steam.

*Figures 8* and *9* show a comparison of experimental and calculated values for the pressure and the local void volume fraction of a 175 L vessel [15]. The initial filling of the vessel was 72 %. A 15 mm diameter orifice was used for discharge. The measurement of the void fraction was located at 85 % of the vessel height.

At the same facility experiments were carried out in order to investigate oscillations of the discharge mass flow rate caused by the feedback of level motion and the critical discharge rate [17, 18]. *figure 10* shows

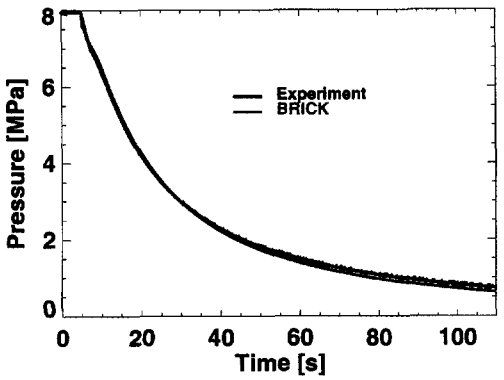


**Figure 8.** Experimental and calculated vessel pressure at the 175 L vessel. Initial filling: 72 %. Diameter of the orifice: 15 mm.

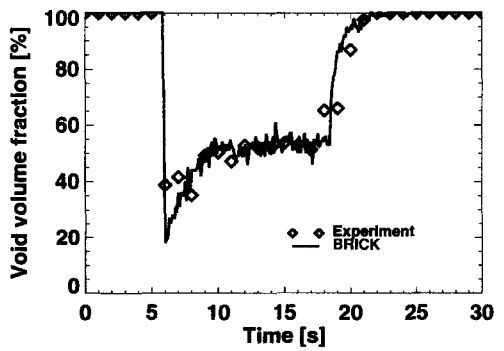


**Figure 9.** Experimental and calculated local volume void fraction at the 175 L vessel at 85 % of vessel height.

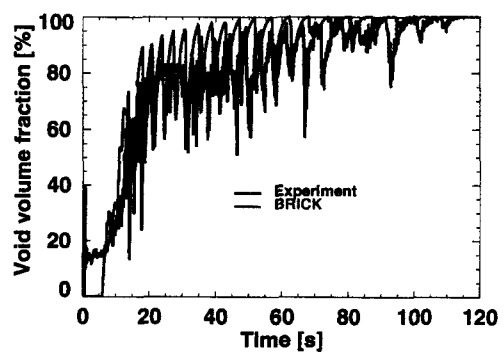


**Figure 10.** Experimental and calculated averaged void volume fraction within the ventline in case of pulsations of the discharge mass flow rate.

experimental and calculated volume void fractions averaged over the 1.8 m long ventline. The oscillations are a very sensitive measure for the quality of the model. As the figure shows, the observed frequency of the oscillations as well as the shape (sawtooth) and the decrease of the frequency with the time were reproduced by the calculations.

The last example of validation concerns the description of foam. Small scale experiments were carried out with water/steam and water/steam/isobutyl alcohol [19]. A 1.95 L vessel was vented through a 3 mm orifice. The addition of isobutyl alcohol increases the discharged mass because of a dynamic foam layer. The foam impedes the pressure relief in the initial period of discharge. Since more mass is discharged, the depressurisation accelerates after the end of liquid discharge. *Figures 11* and *12* compare experimental and calculated pressure and discharged mass. A simple correlation for the velocity of drainage of liquid within the foam layer was fitted to reproduce the experimental results. Note that the calculated pressure as well as the calculated discharged mass are in a good agreement with experimental results.

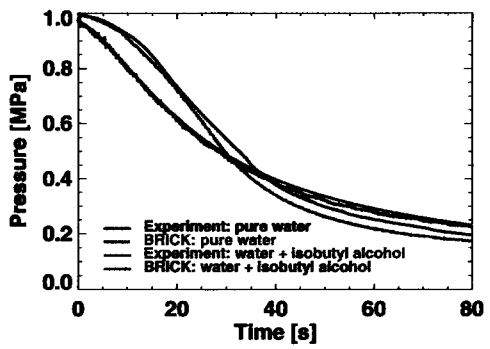


**Figure 11.** Experimental and calculated vessel pressure at the 1,95 L vessel. Initial filling: 90 %. Diameter of the orifice: 3 mm.

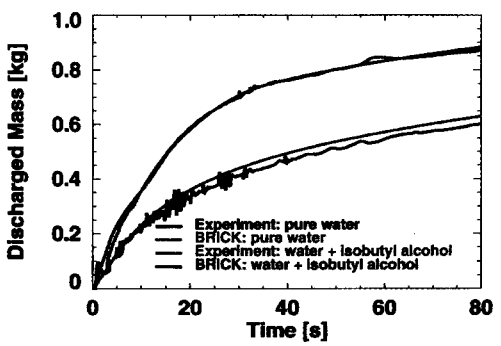


**Figure 12.** Measured and calculated discharged mass at the 1,95 L vessel.

## 9. CONCLUSIONS

The new transport model belongs to the class of Particle-In-Cell (PIC) methods [8]. A specific feature of the presented method is that the particles represent discrete volume elements, which displace each other. The model may be characterised by the following main features:

- the model is limited to one dimension;
- the cross section of the vessel may change with the height;
- the model considers any number of phases;
- the model distinguishes between continuous and dispersed phases;
- the heights of discontinuities (locations where the continuous phase changes) are calculated;
- the transport problem is solved without any numerical diffusion;
- the pressure is only a function of time; the axial pressure distribution is neglected, i.e. the momentum equations are not solved; the interaction between the phases is considered by drift models;
- external volume sources may be defined for any location;
- internal volume sources are caused by the change of the phase density with pressure and temperature and by phase transfer;
- the model works for closed vessels (pressure iteration) or open vessels (pressure remains unchanged);
- flexible interfaces enable the coupling of constitutive laws and of models for extra effects;
- the transport is consistent for all transported properties. New quantities for transport can be introduced easily; this does not affect the solution algorithm;
- models for extra effects may use averaged node values or the microstructure of the arrangement of the bricks within the stack.

These features make the BRICK code a flexible simulation tool for multiphase flow in a vessel. It is suitable for case studies and testing of the influence of models for extra effects taking into account the interaction of all simultaneously running processes. The code gives the possibility to simulate density distributions of parameters, e.g. the particle diameter. Special effects such as the generation of foam can be considered by special manipulations of the arrangement of the bricks.

The algorithm works in a very stable manner. Relatively large time steps may be chosen. Through the variation of the time step width, number of nodes and number of bricks per node the accuracy of the integration and calculation time can be adapted to the actual needs. Very fast estimations with large time steps and a low number of nodes and bricks are possible; however, even more detailed calculations run speedily. Calculation times for the results presented in section 8 are in the range of 1 to 4 times of the process. In all cases a representation with 20 nodes and 1000 bricks per node was used. The time step width varied between 0.01 s to 1 s.

### *Acknowlegements*

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