

EVALUATION OF ALTERNATIVE SWELL MODELS FOR REACTOR RELIEF

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The accurate estimation of reactor level swell is critical for realistic sizing of emergency relief systems. The bubble slip models developed by Kataoka & Ishii and by Boesmans, on the basis of bubble columns experiments, linked with the droplet slip model by Wallis, have been implemented as DLLs in the JRC RELIEF simulation code for reactor venting. This paper presents the results of the comparison of the simulations with experimental data from water blowdown experiments by Sozzi, DIERS and also with the experimental results obtained by HSL in a 2.3 m^3 reactor as part of the EU AWARD project. The results show that the inclusion of a separate droplet flow model for high void fractions is important. The best correlation of both the level swell in the vessel and the vented mass was obtained with the Kataoka & Ishii bubble slip model, which was further modified to allow for the continuous variation of the gas flux.

INTRODUCTION

When a runaway chemical reaction generates gas or vapour during the emergency relief, bubbles are formed throughout the bulk of the liquid. Because the bubbles are buoyant, they will tend to rise through the liquid in order to disengage at the surface. However, whilst they remain in the liquid, they occupy volume and so cause the liquid level to rise or swell. If the level rises to the inlet of the pressure relief system during the relief process, then two-phase venting will occur (Figure 1).

The vapour and liquid motion inside a reactor or storage vessel during emergency relief venting is an extremely complex hydrodynamic problem. The question of vapour or gas versus two-phase relief depends primarily on the prevailing disengagement regime. The disengagement regime is strongly dependent on the foaminess behaviour of the system, as foamy systems behave really different to non-foamy systems. It is possible to differentiate between a foamy or non-foamy system using experiments(1), but an assumption of non-foamy behaviour should be made with care because only trace of impurities (such as might be formed during a runaway reaction) may cause the system to become inherently foamy. Thus it is recommended that the laboratory experiments used to characterise the system, are designed to simulate as near as possible runaway reaction under plant-scale conditions(2).

Many reacting systems are inherently foamy(1), and current theory suggests that they always vent a two-phase mixture which is homogeneous, i.e. the fluid entering the vent has the same ratio of gas or vapour to liquid as the average in the vessel. Such systems would in

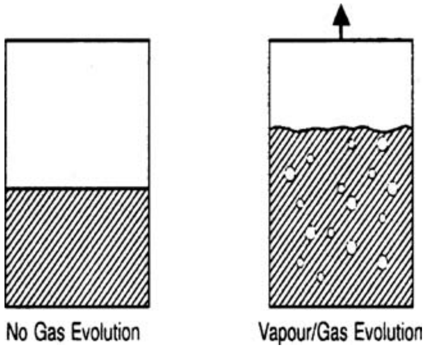

Figure 1. Illustration of the level swell

theory continue to vent a two-phase mixture until the vessel was empty. On the other hand, 3 flow regimes can occur in non-foamy systems: bubbly, churn-turbulent or droplet flow regime (Figure 2). Which flow regime occurs will depend on the system's components and their properties[1] including the rate of vapour or gas generation, viscosity, surface tension, etc. The flow regime markedly affects two-phase relief venting. In bubbly flow, the bubbles are small and discrete and rise through the liquid relatively slowly, this is similar to homogeneous flow when the swelled fluid fills the vessel i.e. when the gas or vapour phase present is completely dispersed through the liquid. In churn-turbulent flow, many of the bubbles have coalesced to form larger bubbles which rise faster. In droplet flow the liquid exists as a fluidised bed of droplets in a continuous gas phase.

All the tests used in this work to check the slip models have been carried out using water, which is expected to develop a churn-turbulent regime during the relief process[1].

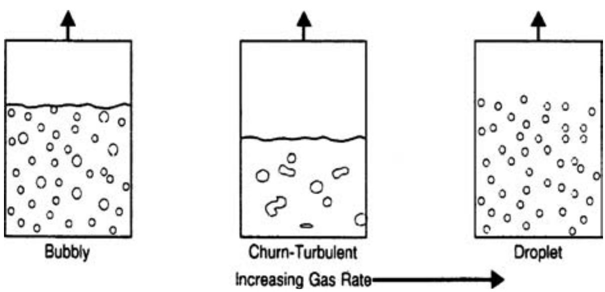

Figure 2. Illustration of non-foamy flow regimes

THE DRIFT FLUX THEORY

A Drift Flux model[3] can be used to describe the flows occurring in a two-phase mixture and it is used to determine the level swell in both the hand calculations[1] as well as in the computer simulation of reactor relief. It is a separated flow model with a focus on the relative motion between the phases. Its major advantage arises because this relative motion is determined by a few key parameters and is independent of the flow rate of each phase. For bubbles in a vertical vessel the velocity is determined by a balance between the buoyancy and the drag forces, and is therefore a function of the void fraction or number of bubbles and not of the flow rate.

The drift flux model evaluates the slip between the phases using the following expression (Eq. 1):

$$J_{21} = V_{gas} - V_{liquid} = U_\infty \cdot f(\alpha) \tag{1}$$

where J_{21} is the drift flux, U_∞ is the maximum value of the drift velocity, i.e. the bubble rise velocity for the bubbles. (In a droplet model, described below, this is also the droplet fall velocity for the droplets.) $f(\alpha)$ is a function of the void fraction, which takes into account the size of the bubbles and their interaction. The models of Zuber & Findlay[4], Kataoka & Ishii[5] and Boesmans[6] all use the drift flux theory to evaluate the slip between the phases, and thus, these models show the same form of this expression.

The 3 models also use the same void fraction function to evaluate the slip (Eq. 2), where α is the void fraction and C_0 is a correlating parameter that takes into account the channelling of the bubbles in the vessel, and has values between $1 < C_0 < 1.5$

$$f(\alpha) = \frac{\alpha(1-\alpha)}{1 - C_0\alpha} \tag{2}$$

BUBBLE RISE VELOCITY

Different correlations for the maximum slip velocity, have been developed in the three models. These are based on the different bubble column experiments which were carried by the different researchers. The main differences between the experiments were the different liquid substances (water, glycerine, organic solvents), different gases (Air, steam) and different column diameters which were used.

Zuber & Findlay describes the maximum drift velocity, U_∞^B as:

$$U_\infty^B = 1.53\left(\frac{\sigma \cdot g \cdot \Delta\rho}{\rho_l^2}\right)^{1/4} \tag{3}$$

where, $\Delta\rho = \rho_l - \rho_g$ is the difference between the liquid and gas densities. Correlations for the surface tension, density, etc can be found for example in Perry[7].

Kataoka & Ishii point out that for larger column diameters combined with higher velocities none of the drift flux correlations for the bubbly or churn-turbulent regimes developed by Zuber and Findlay[4], give an adequate description of the flow. This can be attributed to the formation of large bubbles which are deformed and called cap bubbles. Kataoka & Ishii[5] developed a drift flux correlation for this regime taking into account the influence of the pressure, the mixture viscosity as well as the gas superficial velocity. For this purpose they use the following dimensionless quantities,

$$j^{+} = \frac{j_{\mathrm{g}}}{\left(\frac{\sigma \cdot g \cdot \Delta\rho}{\rho_l^2}\right)^{0.25}} \tag{4}$$

$$D_{\mathrm{H}}^{*} = \frac{D_H}{\sqrt{\frac{\sigma}{g \cdot \Delta\rho}}} \tag{5}$$

$$N_{\mu l} = \frac{\mu_l}{\sqrt{\rho_l \cdot \sigma \sqrt{\frac{\sigma}{g \cdot \Delta\rho}}}} \tag{6}$$

where, j^{+} is the Froude Number, also called dimensionless superficial gas velocity, D_{H}^{*} is the dimensionless diameter and $N_{\mu\mathrm{l}}$ is the dimensionless mixture viscosity. Kataoka & Ishii proposed the following expressions for the maximum drift velocity:

For $j^{+} > 0.5$ and $\mathrm{N}_{\mu\mathrm{l}} < = 2.2 * 10^{-3}$ with $D_{\mathrm{H}}^{*} < = 30$

$$U_{\infty}^{B} = 00019 D_{\mathrm{H}}^{0.809} \cdot \left(\frac{\rho_g}{\rho_l}\right)^{-0.157} \left(N_{\mu l}\right)^{-0.562} \left(\frac{\sigma \cdot g \cdot \Delta\rho}{\rho_l^2}\right)^{1/4} \tag{7}$$

with $D_{\mathrm{H}}^{*} > 30$

$$U_{\infty}^{B} = 0.030 \cdot \left(\frac{\rho_g}{\rho_l}\right)^{-0.157} (N_{\mu l})^{-0.562} \left(\frac{\sigma \cdot g \cdot \Delta\rho}{\rho_l^2}\right)^{1/4} \tag{8}$$

For $j^{+} > 0.5$ and $N_{\mu\mathrm{l}} > 2.2 * 10^{-3}$ and $D_{\mathrm{H}}^{*} > 30$

$$U_{\infty}^{B} = 0.92 \cdot \left(\frac{\rho_g}{\rho_l}\right)^{-0.157} \left(\frac{\sigma \cdot g \cdot \Delta\rho}{\rho_l^2}\right)^{1/4} \tag{9}$$

For $j^{+} < 0.5$

$$U_{\infty}^{B} = \sqrt{2}\left(\frac{\sigma \cdot g \cdot \Delta\rho}{\rho_l^2}\right)^{1/4} \tag{10}$$

Boesmans[6] proposes an alternative expression for the maximum drift velocity to take into account the big bubbles which are formed in the churn-turbulent regime as well as the recirculation that is induced by density differences:

$$U_{\infty}^{B} = F_{ci} \cdot C_1 \cdot \left(\frac{\sigma \cdot g \cdot \Delta\rho}{\rho_l^2}\right)^{1/4} \tag{11}$$

where F_{ci} is a multiplication factor arising from the liquid circulation that is always equal to 2. Boesmans uses the same parameter as Kataoka & Ishii, the Froude number (Eq. 4), to differentiate between the big and faster bubbles and the small and slower rising bubbles. Then using a value of 1.2 for C_0 in equation 2 for the channelling of bubbles, he proposes the following values for C_1 depending on the Froude number:

For $j^{+} < 0.5$

$$C_1 = 1.373$$

For $j^{+} > 0.5$

$$C_1 = 1.373 + 0.177\left(\frac{\rho_g}{\rho_l}\right)^{-0.25}$$

BUBBLE RISE VELOCITY CONTINUOUS WITH THE GAS VELOCITY

Using the definition of the bubble rise velocity given by Kataoka & Ishii and Boesmans, the bubble growth is modelled in a discontinuous way, and thus, the bubble rise velocity only has values for small bubbles and big bubbles. However bubbles are expected to grow in a continuous way depending on the gas flux that is vented, and hence, the slip between the phases. Here a simple modification of the models is presented to allow the continuous growth of the bubbles,

For $j^{+} < 0.5$

$$U_{\infty}^{B} = U_{\infty}^{B\,\min} + \left(U_{\infty}^{B\,\max} - U_{\infty}^{B\,\min}\right)\frac{j^{+}}{0.5} \tag{12}$$

For $j^+ > 0.5$

$$U_\infty^B = U_\infty^{B\max}$$

where, $U_\infty^{B\min}$ is the bubble rise velocity for small bubbles, $U_\infty^{B\max}$ is the bubble rise velocity for the big bubbles. Equation 12 allows the linear interpolation of the maximum drift velocity for a given superficial gas velocity and has been used in the computer implementation of the two models–see below.

COMPARISON BETWEEN THE BUBBLE SLIP MODELS

When the model of Zuber & Findlay[(4)] is compared with the models of Kataoka & Ishii[(5)] and Boesmans[(6)], it is possible to see that new parameters have been introduced into the bubble rise velocity correlation in order to produce a more accurate description of the system behaviour. Both Kataoka & Ishii and Boesmans relate the drift flux to the density, and they both take the influence of pressure into account by using the density ratio. In contrast there is no agreement on the influence of viscosity on the drift flux. The model of Kataoka & Ishii includes a factor whereby increasing viscosity causes a decrease in bubble rise velocity, while Boesmans model has no influence of the velocity if it is enough small.

ONE-DIMENSIONAL SIMULATION OF LEVEL SWELL

The models of Zuber & Findlay, Kataoka & Ishii or Boesmans were developed using the results from bubble columns, and are thus really only valid for the bubble regime (up to void fraction of ca. 0.6–0.8). In an emergency relief, regions of high void fraction will also occur when droplets are present in the system instead of bubbles. In addition droplets can coexist with the bubbles at the same time in different parts of the reactor (swelled liquid with droplet entrainment above the liquid surface). Hand calculation methods[(1)] only allow one flow regime, whether bubbles (Bubbly or Churn-Turbulent) or droplets to be chosen. A more realistic representation of the physical processes which occur is possible by computer simulation particularly if a one-dimensional model over the height of the reactor is used. The RELIEF computer code[(8)], developed by JRC, is a complete "stand alone" package that comprises the physical models that describe chemical conversion, heat and mass transfer between the multi-component liquid and vapour phases, two-phase fluid dynamics and the interaction between these processes during an emergency relief. The RELIEF code allows the vessel height to be divided into control volume elements giving a one-dimensional description of the fluid dynamic behaviour and thus the use of different flow regime models at different positions in the reactor[(9)].

A major problem appears when the drift flux model[(3)] is used in a one-dimensional representation of a vessel as it does not provide a continuous function of the drift flux with void fraction This was solved in the original RELIEF code as follows:

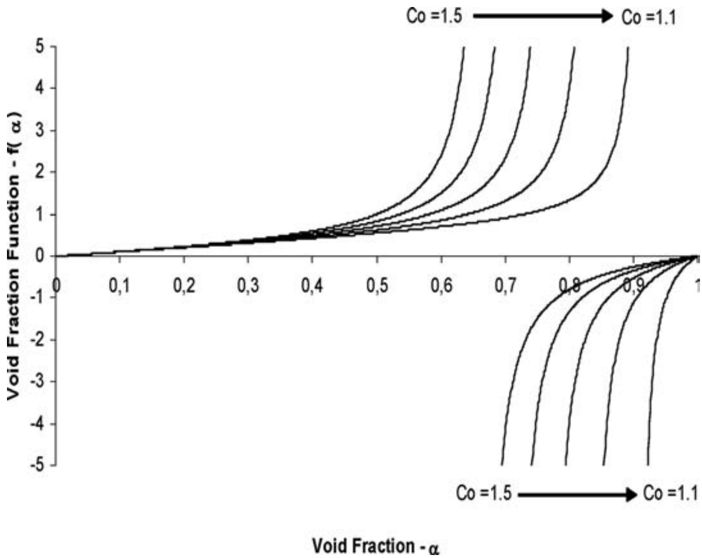

Figure 3. Original void fraction function (Eq. 2)

THE VOID FRACTION FUNCTION

For computer simulations the void fraction function must be continuous over the whole range of void fractions(9). 2 void fraction zones can be considered to occur: a bubble zone where the vapour bubbles rise in a continuous liquid phase; and a droplet zone (at high void fractions) where the liquid droplets fall in continuous vapour phase.

The drift flux models of Zuber & Findlay, Kataoka & Ishii and Boesmans were developed for the bubble zone using bubble column experiments. Unfortunately the void fraction function which is used in all the models to calculate the slip between the phases (Eq. 2) is not continuous for the whole range of void fraction (Figure 3), a discontinuity occurs at void fractions greater than 0.6 depending on the value of C_0 that is used. Hence a problem occurs when it is intended to use this model for all the range of void fraction, because the drift flux won't be continuous and it will take negative values for high void fractions, which are not physically realistic.

To achieve a simulation for the whole range of void fractions this functionality (Eq. 2) has to be changed, to one which is continuous for the whole range. In the original RELIEF(8) code this new functionality is given by,

$$f(\alpha) = \frac{\alpha^m (1-\alpha)^n}{\alpha_{\max}^{m-1}(1-\alpha_{\max})^{n-1}} \tag{13}$$

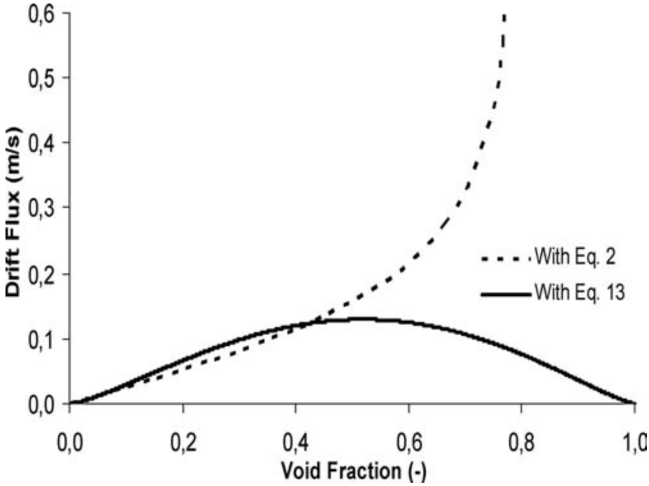

Figure 4. Drift Flux vs. Void Fraction showing original (Eq. 2) functionality and that used in RELIEF (Eq. 13)

where "*m*" and "*n*" are correlating parameters which control the form of the function and the void fraction where the slip is maximum, α_{max}. Their optimal values for, systems with a behaviour close to water, are 1.4 and 1.3 respectively, and α_{max} is given by,

$$\alpha_{max} = \frac{m}{m+n} \tag{14}$$

It can be seen (Figure 4) that the new functionality is continuous over the whole range of void fractions.

With both functions, the drift flux increases as the void fraction increases since the drag between the phases is less when the bubble size becomes bigger, due to lower area to volume. There is then a situation where the liquid begins to break up into droplets and the vapour becomes the continuous phase. This droplet zone is represented in the new function as a regime of decreasing drift flux for further increases of void fraction. This is a reasonable assumption in that it can be expected that the droplet size will decrease with increasing void fraction. The drag between the droplets and the vapour will increase as the droplet size decreases and so the slip decreases. At the extremes of all liquid and all vapour the slip must be 0, and at some intermediate void fraction, determined by the constants *m* and *n* in the new function, the slip will be maximum.

NEW SLIP MODELLING PROCEDURE

The original RELIEF code used the Zuber & Findlay drift flux model with the continuous void fraction function with default constants of $m = 1.4$ and $n = 1.3$. This gave a reasonable correlation with experimental results[(9)], though it under predicted the drift flux at high void fractions.

In order to solve the problem of the simultaneous existence of bubbles and droplets a new slip modelling procedure has been proposed by the JRC[(10)]. The new procedure allows the bubble to be described independently of the droplet flow with an intermediate break-up zone where liquid starts to break up and droplets are formed.

DROPLET FALL VELOCITY

For high void fractions droplets are present in the system instead of bubbles. This difference is taken into account by the maximum drift velocity. In the bubble zone this velocity is given by the terminal bubble rise velocity (given by the models of Zuber & Findlay[(4)], Kataoka & Ishii[(5)] or Boesmans[(6)]). In the droplet zone the maximum drift velocity is given by the terminal droplet fall velocity, given by Wallis[(3)] as,

$$U_\infty^D = \left(\frac{\sigma \cdot g \cdot \Delta\rho}{\rho_l^2}\right)^{1/4} \left(\frac{\rho_l}{\rho_g}\right)^{0.5} \tag{15}$$

The bubble model is related to the terminal rise velocity of a bubble in the churn-turbulent regime, U_∞^B, and the droplet model is related to the terminal droplet fall velocity, U_∞^D. The separate models are linked with a mathematical expression which results in a continuous function over the whole void fraction range. Then, the new slip model follows the following schema:

$$\begin{array}{lll} \alpha \le \alpha_{\max Jbubble} & \rightarrow & J_{21} = U_\infty^B \cdot \left[f(\alpha)_{Bubble}\right] \\ \alpha_{\max jbubble} < \alpha < \alpha_{\max Jdroplet} & \rightarrow & J_{21} = interpolation \\ \alpha \ge \alpha_{\max Jdroplet} & \rightarrow & J_{21} = U_\infty^D \cdot \left[f(\alpha)_{Droplet}\right] \end{array}$$

Then for the bubble zone

$$\alpha \le \alpha_{\max Jbubble} = \frac{m_{bubble}}{m_{bubble} + n_{bubble}} \tag{16}$$

$$\alpha \le \alpha_{\max Vbubble} = \frac{m_{bubble} - 1}{m_{bubble} + n_{bubble} - 2} \tag{17}$$

The drift flux for this region,

$$J_{21} = EF_{bubble} \cdot U_\infty^B \cdot \frac{\alpha^{m_{bubble}}(1-\alpha)^{n_{bubble}}}{\alpha_{\max Vbubble}^{m_{bubble}-1}(1-\alpha_{\max Vbubble})^{n_{bubble}-1}} \tag{18}$$

For the Droplet zone,

$$\alpha \geq \alpha_{\max Jdroplet} = \frac{m_{droplet}}{m_{droplet} + n_{droplet}} \tag{19}$$

$$\alpha \geq \alpha_{\max Vdroplet} = \frac{m_{droplet} - 1}{m_{droplet} + n_{droplet} - 2} \tag{20}$$

The drift flux for this region,

$$J_{21} = EF_{droplet} \cdot U_{\infty}^{D} \cdot \frac{\alpha^{m_{droplet}}(1-\alpha)^{n_{droplet}}}{\alpha_{\max Vdroplet}^{m_{droplet}-1}\left(1-\alpha_{\max Vdroplet}\right)^{n_{droplet}-1}} \tag{21}$$

For the intermediate zone where,

$$\alpha_{\max jbubble} < \alpha < \alpha_{\max Jdroplet}$$

The drift flux is given by (Eq. 22),

$$J_{21} = J_{21mb} + (J_{21md} - J_{21\mathrm{mb}}) \cdot \left(\sin\left(\left(\frac{\alpha - \alpha_{\max Jbubble}}{\alpha_{\max Jdroplet} - \alpha_{\max Jbubble}}\right)\pi - \frac{\pi}{2}\right) + 1\right)$$

where, $J_{21\mathrm{mb}}$ is equation 18 using $\alpha = \alpha_{\max Jbubble}$ (Eq. 16) and $J_{21\mathrm{md}}$ is Eq. 21 using $\alpha = \alpha_{\max Jdroplet}$ (Eq. 19).

The advantage of this new procedure is that different bubble slip and droplet models can be used to represent the two regimes.

In this work 10 different combinations of slip models have been compared. For this purpose the different bubble rise velocities given by Zuber & Findlay (Eq. 3), Kataoka & Ishii (Eq. 7 to Eq. 10) and Boesmans (Eq. 11) have been used. In addition for the bubble rise velocities given by Kataoka & Ishii and Boesmans, the modification that allows the continuous growth of the bubbles (Eq. 12) has been incorporated. The droplet fall velocity given by Wallis (Eq. 15) has been used in all cases to model the droplet zone.

The following table (table 1) shows the names of the different models that have been compared in this work,

The models are controlled by 6 empirical parameters. These parameters control the form of the curves as well as the void fractions where the interpolation starts and finishes. The values[11] for the 6 empirical parameters for the "Z&F + D" model, are presented in Table 2,

Figure 4 shows the drift flux vs. void fraction for the "Z&F" model. Two models are plotted, with the original void fraction function, Eq. 2, and with Eq. 13, which is continuous for the whole range of void fraction and is the default model in the RELIEF code. It is

Table 1. Names of the new slip models

Bubble Model	ZONE			
	Bubble		Bubble + Droplet	
	Bubble Growth		Bubble Growth	
	Discont.	Cont.	Discont.	Cont.
Zuber	Z&F	—	Z&F + D	—
Kataoka	K&I(d)	K&I(c)	K&I(d) + D	K&I(c) + D
Boesmans	B(d)	B(c)	B(d) + D	B(c) + D

possible to see that the two models are similar until void fraction around 0.5, then the original model takes higher values of the drift flux.

Figure 5 shows the combination "Z&F + D", which links the Zuber & Findlay bubble model with the Wallis droplet model. Now when the two models plotted are compared, they show better agreement than in Figure 5. It can be seen that the addition of the droplet model with its larger terminal droplet velocity provides a better fit to the original Zuber and Findley model than previously (Figure 4).

A similar observation can be made when the Kataoka & Ishii or Boesmans slip model is used. Figure 6 shows the combination of the Kataoka & Ishii slip model, which takes into account the gas superficial velocity, with the Wallis droplet model. The model is plotted using Eq. 2 and Eq. 13, where the "K&I(d) + D" is the original definition (Black lines) and "K&I(c) + D" uses the modification we are proposing to allow for continuous bubble growth definition, interpolation with Eq. 12 (Grey lines).

Figure 7 shows the same graph using the Boesmans slip model, "B(d) + D", also with modification for continuous growth in bubble size, "B(c) + D".

Table 2. Parameters for the new slip model

Parameter	Value	
	Bubble Zone	Droplet Zone
EF	2	2
m	1.4	3.3
n	1.3	1.1

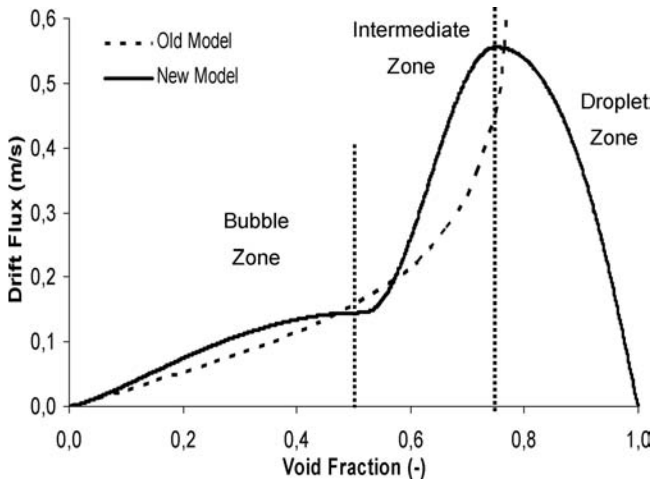

Figure 5. Drift Flux vs. Void Fraction for Z&F + D

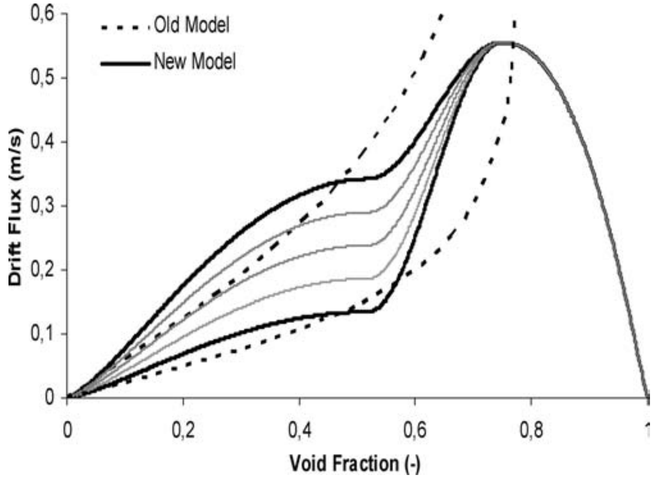

Figure 6. Drift Flux vs. Void Fraction for K&I(c)+D and K&I(d) + D

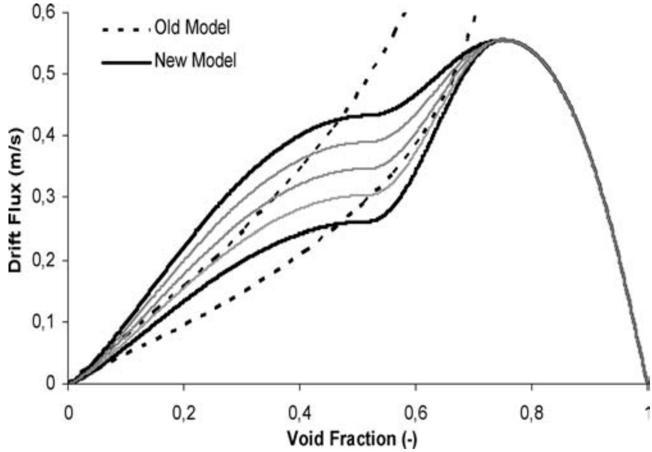

Figure 7. Drift Flux vs. Void Fraction for B(c)+D and B(d) + D

Figures 4 to Figure 7 have been produced using data for water at 400 K and vapour pressure conditions. The default parameters of the new slip model have been used as well as the values for the empirical parameters given in the Table 2, with the exception that a value of 1 has been used for the factor EF for the bubble zone to allow the comparison between the bubble slip models. The value of C_0 in Eq. 2 has been taken as 1.2.

CHECKING THE NEW SLIP MODELS

All of the model combinations (Table 1) have been coded as DLLs (Dynamic Link Library) for use with the RELIEF simulation program. In order to evaluate the models and identify which of the new combinations provides the best representation of the venting process they have been compared to void fraction data produced by water blow down tests. Initially the data produced by Sozzi[(12)] has been used.

Sozzi measured in his water blowdown experiments the local void fractions at different axial positions in the vessel by readings of differential pressure measurements. Using these local average void fractions one is able to check a specific void fraction range of the drift flux model. The Sozzi data have more information of how an emergency relief process happens and better describes the behaviour of the system, than experiments with only information on the average void fraction, such as the DIERS experiments[(1)].

Two Sozzi experiments[(12)] have been chosen: 5801–15 and 5702–16. They are quite similar, as the only difference is that the nozzle diameter of experiment 5702–16 is bigger (0.092 m) than the nozzle of 5801–15 (0.063 m). Then, with these two experiments it is possible to see the influence of a bigger nozzle, and thus, bigger mass flow released.

Figure 14 and 15 show the experimental void fractions measured at the 7 nodes in the reactor for the blow-down experiment 5702-15. Figure 14 shows the predictions using the original RELIEF slip model ("Z&F") and figure 15 the predicted void fractions using the Kataoka & Ishii bubble model with the droplet model ("K&I(c) + D"). It can be seen that the new slip model provides a better agreement with the experiment.

To enable a comparison of all the models, the simulation results have been plotted as graphs showing the simulated void fraction vs. the experimental void fraction for each model shown in Figures 10–15. From these data the relative deviation for each model has been calculated (Eq. 23) and the results shown in Table 3.

$$\delta = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\frac{\overline{\alpha}_{\mathrm{exp}} - \overline{\alpha}_{calc}}{\overline{\alpha}_{\mathrm{exp}}}\right)^2} \times 100 \tag{23}$$

In Figure 8 is possible to see the results for "Z&F" (Zuber & Findlay applied to the whole void fraction range), which is the RELIEF's default swell model. This model has the biggest deviation of all the models, 3.2. In Figure 10 the results of "K&I(c)" and "K&I(d)" (Kataoka & Ishii, continuous and discontinuous, applied to the whole void fraction range).

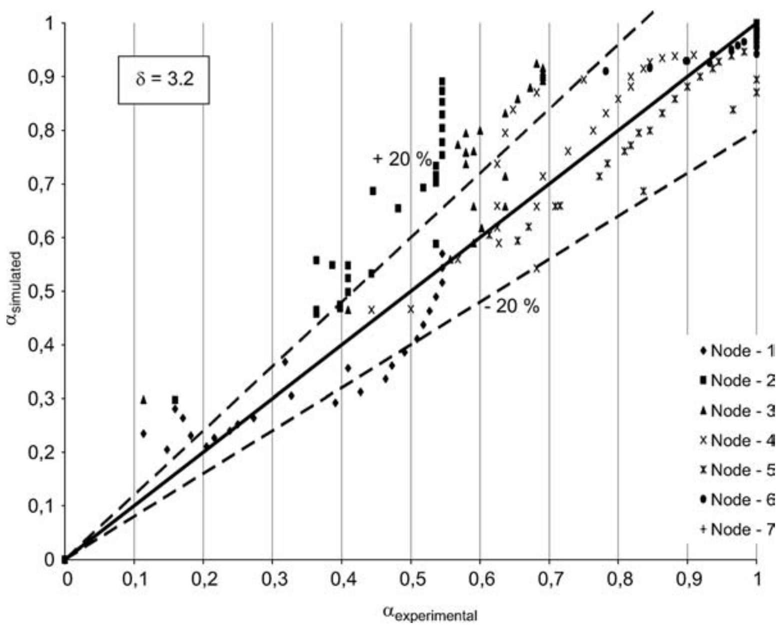

Figure 8. Results for Z&F

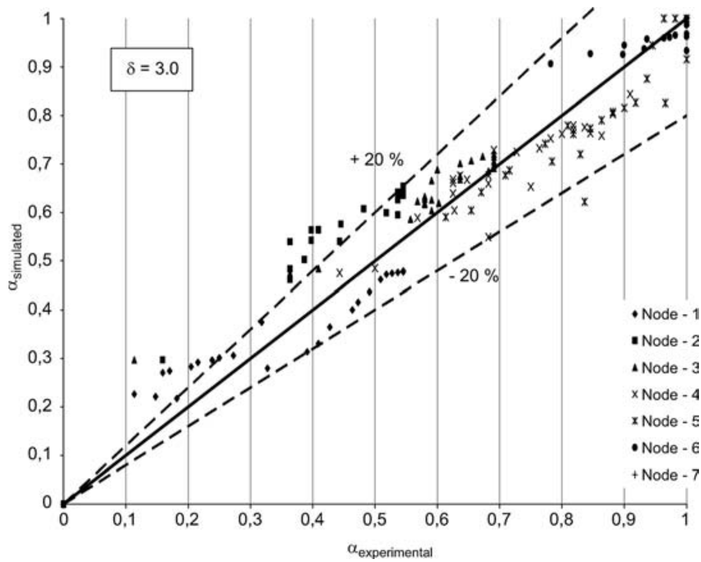

Figure 9. Results for Z&F + D

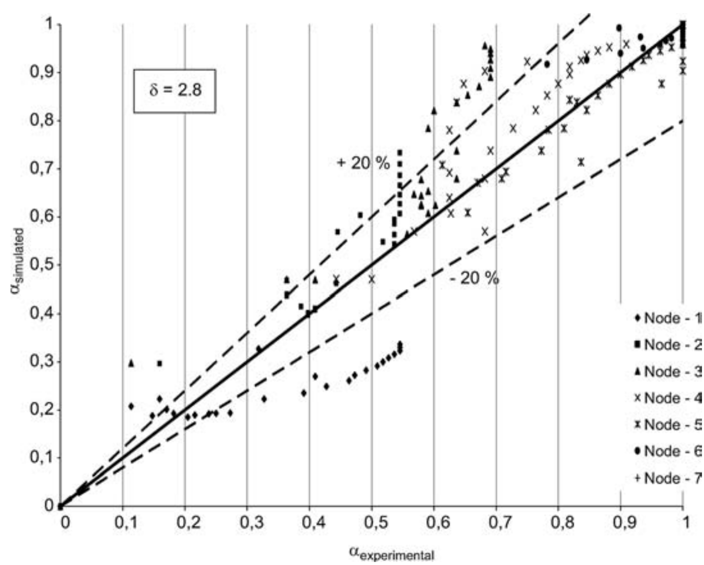

Figure 10. Results for K&I(c) and K&I(d)

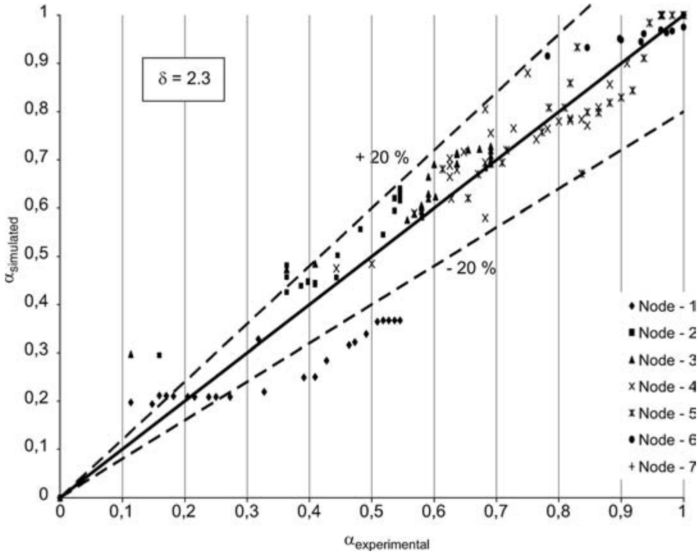

Figure 11. Results for K&I(c)+D and K&I(d) + D

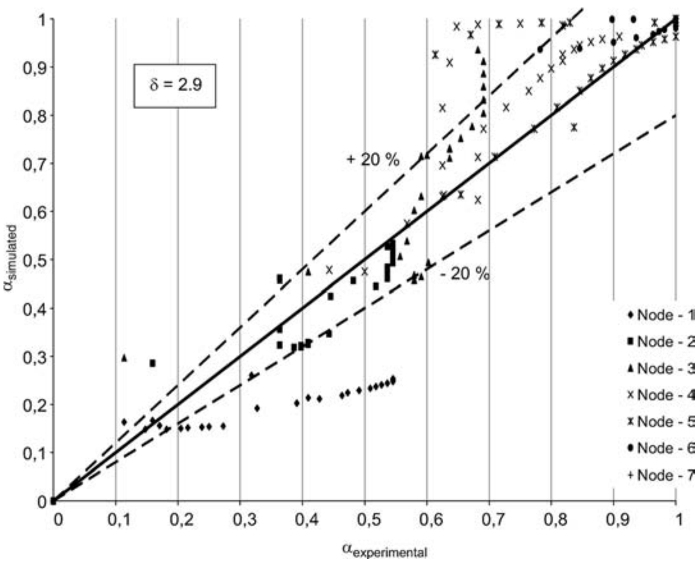

Figure 12. Results for B(c) and B(d)

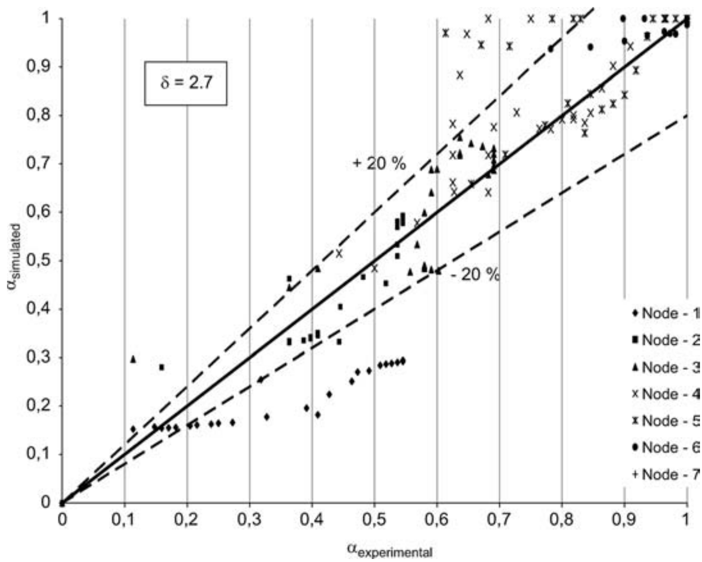

Figure 13. Results for B(c)+D and B(d) + D

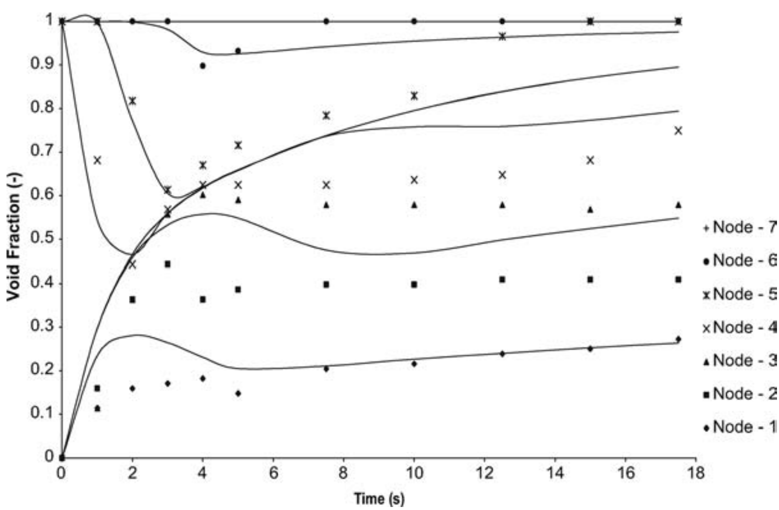

Figure 14. Local void fraction for experiment 5702-15 (Using the RELIEF default swell model "Z&F")

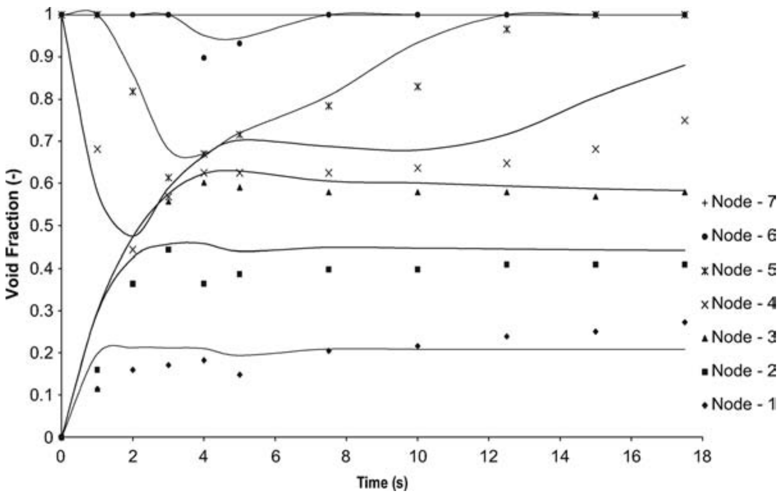

Figure 15. Local void fraction for experiment 5702-15 (Using the best swell model "K&I(c) + D")

This model has a deviation of 2.8. In figure 12 the results of "B(c)" and "B(d)" (Boesmans, continuous and discontinuous, applied to the whole void fraction range). This model has a deviation of 2.9.

It is possible to see that for the 3 models which don't take into account the droplet zone, the void fractions above 0.5 are over predicted, which means that the models are under predicting the drift flux in this regime.

The results shown in Figures 9, 11 and 13 show better agreement with the experimental data because the droplet zone has been taken into account in these models. The

Table 3. Relative deviation of the new slip models

	ZONE			
	Bubble Bubble Growth		Bubble + Droplet Bubble Growth	
Bubble Model	Discont.	Cont.	Discont.	Cont.
Zuber	3.2	—	3.0	—
Kataoka	2.8	2.8	2.3	2.3
Boesmans	2.9	2.9	2.7	2.7

best slip model is the “K&I(c) + D”, Figure 13, which has the lowest deviation, 2.3, and shows the best fitting with the experimental data.

Looking at Figures 10 to 13 it is possible to see that there is no difference in the simulation results using the original models of Kataoka & Ishii and Boesmans; and the modified models, allowing the continuous bubble growth (Eq. 12). This indicates that during the experiments the superficial gas velocity, j^+, has been bigger than 0.5, and thus, the Eq. 12 is not used. Hence the results for the models both with and without the continuous bubble growth modification are the same.

COMPARISON WITH HSL BLOWDOWN TESTS

As part of the EU AWARD project, a new facility has been constructed at the Health and Safety Laboratory (HSL) to investigate the void fraction distribution during pressure relief. The facility consists in a stainless steel reactor (2.3 m^3) connected to a catch tank (13 m^3) with a ventline of 200 mm diameter, where different orifice plates could be installed to allow the variation of the depressurisation rate. The reactor uses a jet mixing; the contents of the bottom of the reactor are re-pumped into the reactor after passing through a heat exchanger, which can use hot / cold water as well as steam. The reactor was insulated so it can be assumed as adiabatic.

In addition to tests with runaway chemical reactions(13) water blowdown were also carried out. In these tests water is heated up till the initial conditions are achieved (temperatures higher than 145 °C) and then a valve opened allowing the release of the reactor contents to the atmosphere or the catch tank. The advantage of the blowdown test is that since there are no chemical reactions involved, these tests provide a good opportunity to test the hydrodynamics part of the code (level swell) without uncertainties which may arise from modelling the chemical reaction, e.g. mixture composition, temperature etc.

Two of the tests are analysed, Blow 4 and Blow 5. The only difference between them is that in Blow4 the pipeline used is bigger than in Blow5.

In order to determine which flow regime (i.e. bubble churn-turbulent or droplet) is actually present during the course of the tests and thus better understand whether the assumptions in the new overall slip models are appropriate, the liquid and gas stability factors K_f (Eq. 24) and K_g (Eq. 25), have been calculated and plotted together with the measured vent quality for the course of the blowdown tests (Figures 17, 18).

$$K_\mathrm{f} = X(\rho_f)^{1/2} \tag{24}$$

$$K_\mathrm{g} = X(\rho_g)^{1/2} \tag{25}$$

where

$$X = \frac{j_g}{(\sigma g(\rho_f - \rho_g))^{0.25})} \tag{26}$$

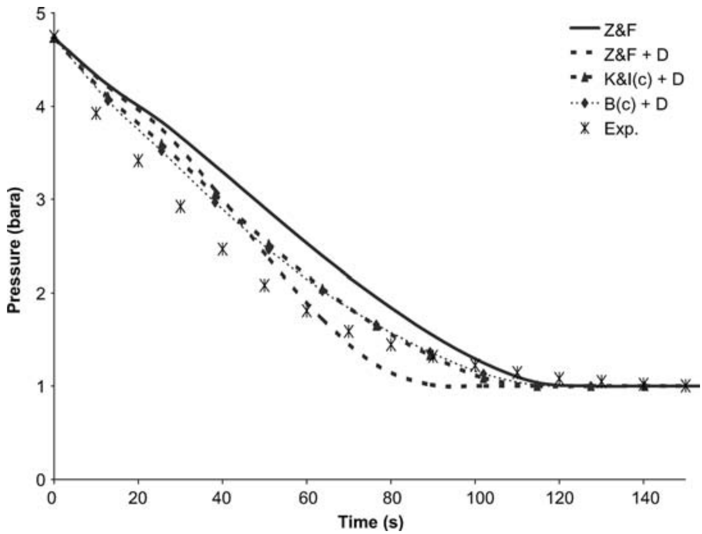

Figure 16. Pressure for the experiment HSL–Blow4

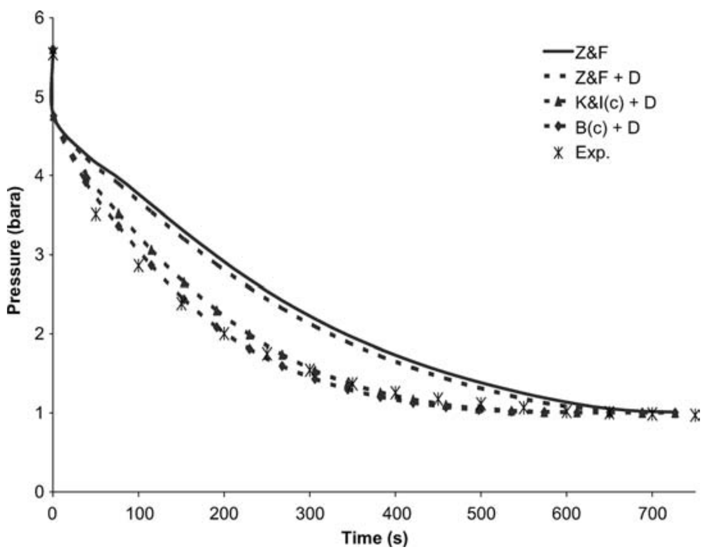

Figure 17. Pressure for the experiment HSL–Blow5

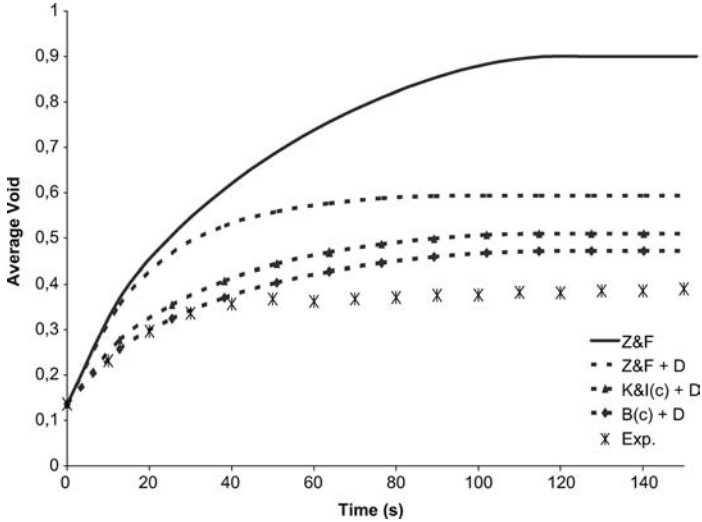

Figure 18. Average Void for the experiment HSL −Blow4

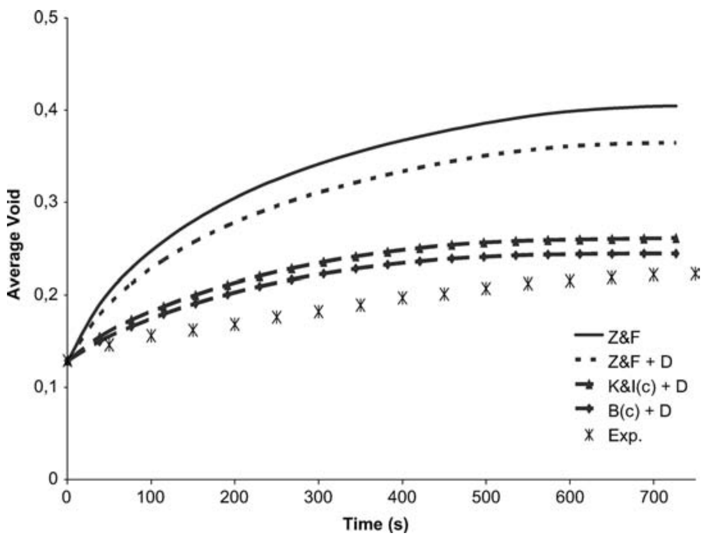

Figure 19. Average Void for the experiment HSL−Blow5

It can be seen that the liquid stability factor is the same as the Froude Number (Eq. 4) used by Kataoka & Ishii and Boesmans. ICI[14] proposed the following criteria to decide which flow regime prevails in the reactor. The method consists in the evaluation of the liquid and gas stability factors,

$$\text{Regime}\begin{cases} \text{if} \quad K_f < 0.3 & \text{Bubbly} \\ \text{if} \quad 0.3 < K_f < 0.5 & \text{Bubbly or C - T} \\ \text{if} \quad K_f > ,5 & \text{C - T} \\ \text{if} \quad 0.14 < K_g < 0.2 & \text{C - T or Droplet} \\ \text{if} \quad K_g > 0.2 & \text{Droplet} \end{cases}$$

STABILITY FACTORS VS. TIME

In Figure 20 the stability factors are plotted for experiment Blow 4. Looking the graph, it is possible to see that the liquid stability (Froude number) is always above 0.5, thus big bubbles are predicted. Looking the gas stability factor, it can be seen that it is around 0.2, hence it is expected that the intermediate region is the most important in this experiment. In Figure 21 the stability factors are plotted for experiment Blow 5. In this case the

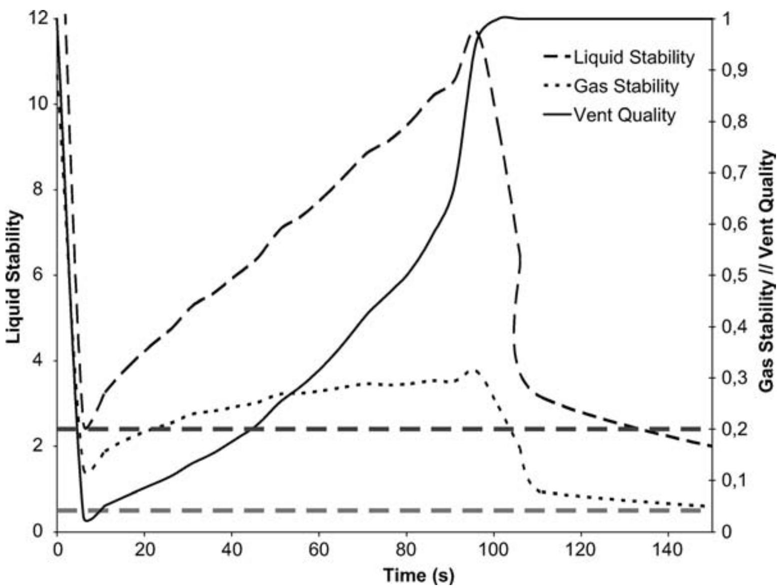

Figure 20. Liquid Stability, Gas Stability and Vent quality for the experiment HSL–Blow4

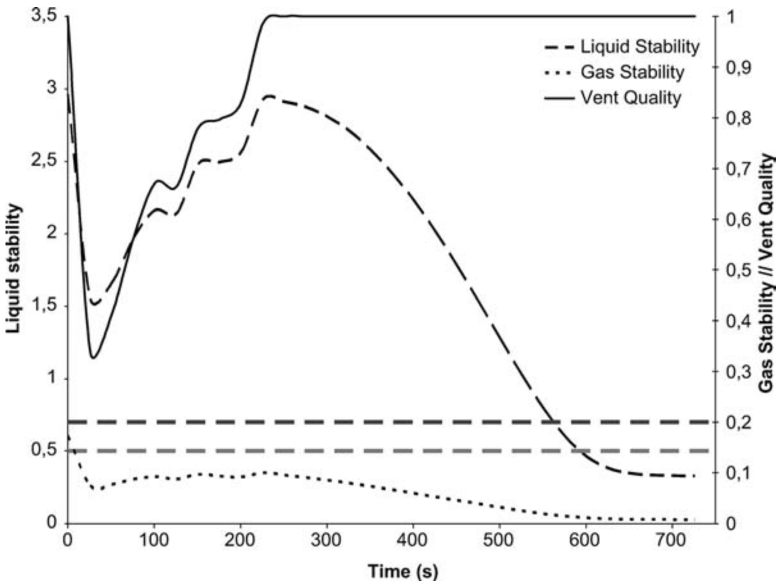

Figure 21. Liquid Stability, Gas Stability and Vent quality for the experiment HSL–Blow5

liquid stability factor is also larger than 0.5 during the whole venting process. But the gas stability factor is lower than 0.1, and thus, the bubble zone is expected to be of more importance in this test with smaller vent area.

PRESSURE VS. TIME

In Figure 16 the pressure curves for the Blow 4 test are shown together with the predictions from the simulations. As was seen with the stability factors the intermediate and the droplet zone are important in this test and thus there is a large difference between models with and without the droplet model, as the "Z&F" (RELIEF default) and the "Z&F + D" models show differences. The best fit is given by the "K&I + D" and "B + D" models, as it was seen that the Froude number is always bigger than 0.5 and big bubbles are predicted. For Blow 5 (Figure 17), it is possible to see that the bubble zone is of most importance, as the "Z&F" (RELIEF default) and the "Z&F + D" models give almost the same results. However the best fit is still given by the "K&I + D" and "B + D" models as the Froude number is again larger than 0.5, during the whole process.

AVERAGE VOID VS. TIME

Looking at Figure 18, for Blow 4, and Figure 19, for Blow 5, the same conclusions as with the pressure curves can be made. In both experiments the Kataoka & Ishii and the Boesmans bubble slip models linked with the Wallis droplet slip model give the best simulation.

REACTOR MASS VS. TIME

The level swell affects the remaining mass in the reactor after the emergency relief. In Figures 22 and 23 the mass in the reactor is plotted against time. It is possible to see a big difference between the "Z&F" slip model (RELIEF's Default) and the best slip model developed: "K&I + D", much better agreement being obtained with the new model.

CONCLUSIONS

The comparison of the simulations using the different models with the results from the Sozzi and HSL blow-down tests has shown that major improvements can be achieved if the level swell model used is able to take into account the different flow regimes, at different parts of the reactor vessel (i.e. by using one-dimensional description of the vessel). The addition of a droplet model to the commonly used bubble model is essential to achieve a good correlation with the experiments over the whole course of the venting process. This is particularly apparent when one considers the correlation with the mass vented from the reactor where the new level swell models show much better agreement with the experiments.

The results obtained to date show that the best correlation is obtained using the Kataoka & Ishii bubble model combined with the Wallis droplet model ("K&I + D").

The comparisons reported in this paper have been carried out with water blow down tests, thus as would be expected little difference has been seen between the Kataoka & Ishii and Boesmans models in the comparisons so far carried out. Further work is needed to determine which model best simulates the venting process of other fluids including high viscosity fluids.

Similarly since the superficial gas velocity, j^{+}, was greater than 0.5, in all the tests it has not been possible to check the efficiency of the proposed modification of the original Kataoka & Ishii and Boesmans models for continuous bubble growth.

The liquid and gas stability factors are shown to give a reasonable indication of which flow regime occurs during the different stages of the venting process. The liquid stability (Froude Number) is always above 0.5 for almost all the process in all the experiments. The gas stability factor however showed different tendencies for the experiments. Thus:

a) When it is close to 0.1 the bubble region is of more importance.
b) When it is close to 0.2 the intermediate region is of more importance.
c) When it is bigger than 0.2 the droplet region is of more importance.

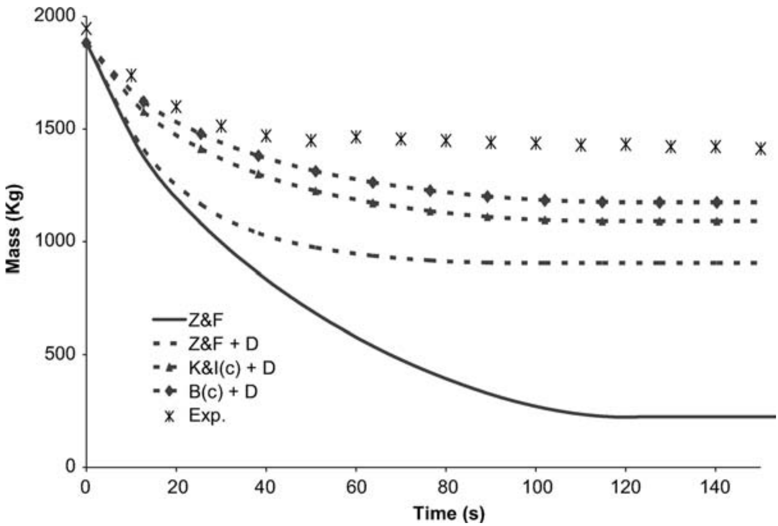

Figure 22. Reactor Mass for HSL–Blow4

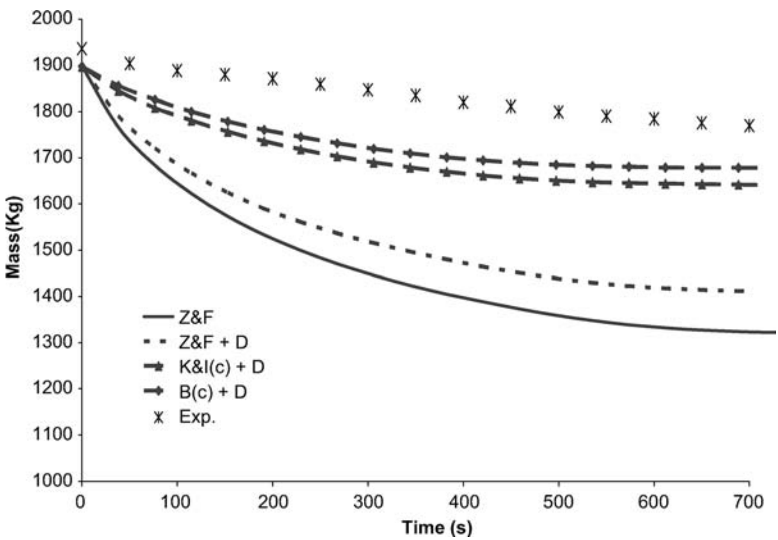

Figure 23. Reactor Mass for HSL–Blow5

ACKNOWLEDGEMENTS

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NOMENCLATURE

C_0	A data correlating parameter
C_1	A data correlating parameter
D_H	Vessel Diameter m
D_H^*	Dimensionless Vessel Diameter
EF	Enhancement Factor of RELIEF drift flux model
g	Acceleration Due to Gravity m/s^2
J_{21}	Drift Flux m/s
j^+	Froude Number
j_g	Local vapour superficial velocity m/s
m	First Exponent of RELIEF drift flux model
n	Second Exponent of RELIEF drift flux model
$N_{\mu l}$	Dimensionless Viscosity Number
$\cup_\infty$	Characteristic bubble rise velocity m/s
v	Phasic Velocity m/s
X_0	Vent Quality

GREEK SYMBOLS

α	Average void fraction in the swelled liquid
σ	Surface tension N/m
ρ	Density Kg/m^3
μ	viscosity Pa s
δ	Relative deviation

SUBSCRIPTS

1 or l	Liquid Phase
2 or g	Vapour Phase
B	Bubble
D	Droplet

REFERENCES

1. H. G. Fisher, H. S. Forrest et al, **Emergency Relief System Design Using DIERS Technology**, The Design Institute for Emergency Relief Systems (DIERS) Project Manual, American Institute of Chemical Engineers, 1992.
2. J. Etchells, J. Wilday, **Workbook for chemical reactor relief system sizing**, HSE books, 1998.
3. G.B Wallis, **One dimensional Two-phase flow**, McGraw Hill, New York, 1969.
4. N. Zuber, J. A. Findlay, **Average Volumetric Concentration in Two-phase Flow Systems**, International Journal of Heat Transfer, pag. 453–468, November 1965.
5. I. Kataoka, M. Ishii, **Drift flux Model for Large Diameter Pipe and New Correlation for Pool Void Fraction**, International Journal of Heat and Mass Transfer, Vol. 30, pag. 1927–1939, 1987.
6. B. Boesmans**, Transient Level Swell during Emergency Pressure Relief of Liquefied Gases**, Ph.D. Thesis, Leuven, Belgium.
7. R. H. Perry, C. H. Chilton, **Perry's Chemical Engineer's Handbook**, 7th Edition, McGraw Hill, 1997.
8. N. Brinkhof, J. S. Duffield & R. Nijsing, **RELIEF User's Manual**, European Commission Joint Research Centre, 1995.
9. B. P. P Hoomans, J. S. Duffield**, Assessment of the RELIEF code using water blowdown experiments**, Joint Research Centre, Ispra 1994.
10. B.J. van den Berg, J.S. Duffield, **Drift flux modelling in RELIEF**, Joint Research Centre, Ispra 1994.
11. F.A Lammers, J.S. Duffield, **Optimisation of the RELIEF drift flux model**, Joint Research Centre, Ispra 1994.
12. G. L. Sozzi, **Level Swell and Void Fraction Measurements during Vessel Blowdown Experiments**, from G. F. Hewitt, J. M. Delhay, N. Zuber (eds.), Multiphase Science and Technology, Vol. 6, pag. 167, 1992.
13. Snee T. J. & Bosch J., **Large scale evaluation of vent-sizing methodology for vapour pressure systems**, IChemE Hazards XIX International Symposium, Manchester, March 2006.
14. ICI Process SHE Guide No. 8, **Pressure Relief**, Part C, 1992.