VALIDATION

DISC MODEL

DATE: December 2023

ABSTRACT

This report describes the validation of the Phast discharge model DISC.

The DISC theory is described by an accompanying report. The DISC model includes four sub-models covering the following scenarios: an orifice leak from a vessel, a leak from a short pipe attached to a vessel, catastrophic rupture of a vessel and vent from the vapour space of a vessel.

Reference to part of this report which may lead to misinterpretation is not permissible.

No.	Date	Reason for Issue	Prepared by	Verified by	Approved by
1	2009	PHAST 6.53			
2	Oct 2017	Safeti 8.0	Stene		
3	May 2021	Apply new template	D. Vatier		
4	July 2022	Version update	David Worthington		

Date: December 2023

Prepared by: Digital Solutions at DNV

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1 INTRODUCTION

A full description of the theory underlying DISC is described in the accompanying DISC theory manual. The DISC verification manual describes the verification of the model, whereas this report is concerned with the validation of the DISC model. To this end discharge predictions are compared with measurements from a selection of the available experimental data.

The validation work presented in Chapters 2 and 3 was carried out as part of Phase III of the droplet-modelling joint industry project. As such it was originally documented in the first part of the Phase III report, C1, and it is now included here as a starting point of the DISC validation manual.

More specifically, Chapter 2 provides a review of previous DISC validation work as well as a literature overview of relevant available experimental results for further DISC validation. Actual validation results are then presented in Chapter 3 and include water, propane and butane releases.

2 LITERATURE SURVEY

2.1 Previous validation of the DISC discharge model

2.1.1 DISC validation against sub-cooled and saturated water experiments

John Woodward provides an overview of discharge modelling in Perry's handbook[1].
Figure 1 (Fig. 26.-63,26-64 in Perry) includes mass flux data for water (Uchida and Nariai, 1966) from an orifice and pipe (orifice/pipe diameter of 4 mm) with a range of initial pressure P_{st} and pipe length L. Both sub-cooled water (20C) and saturated water is considered. He also includes results from HEM model by Leung (this would be verification against our models).

Figure 2 (Figs. 26-70 and 26.71) shows predictions of an analytical HEM by Leung and Epstein (1990) and the NEM model by Henry and Fauske (1976) against data by Sozzi and Sutherland (1975) for slightly subcooled water (Fig. 26-70) and saturated water (Fig. 26-71).
Figure 3 includes PHAST4.2 predictions[2] against these experiments.

In the Modelling Conference presentation he also quotes plans for PHAST discharge model validation against benchmarks against a large range of DIERS validation tests (but these never materialised). They include both a large range of water tests (liquid water downward, saturated/flashing water, low/high viscous flashing flow), i.e.

- DIERS Round robin validation tests:
    - Benchmark 1- Water flow downward
    - Benchmark 2- Saturated water vessel drain
    - Benchmark 3- Sat. water blowdown overhead
    - Benchmark 4- Flashing water blowdown from bottom-mounted pipes
    - Benchmark 5- Flashing water nozzle flow
    - Benchmark 6- Nielsen flashing water case
    - Benchmark 7- Viscous water flow (same as Test 2 except 5000 cp viscosity)
    - Benchmarks 8 & 9- Same as above with T-dependant viscosity
    - ISPRA tests with DRACULA system

- DIERS Luviskol tests
    - Case 1 - Vapour flow
    - Case 2 - Low viscosity flashing flow
    - Case 3 - Low viscosity flashing w/ 5 psi N2
    - Case 4 - High viscosity flashing flow
    - Case 5 - High viscosity flashing w/ 5 psi N2
    - Case 6-7 - Churn-Turbulent & Homogeneous disengagement

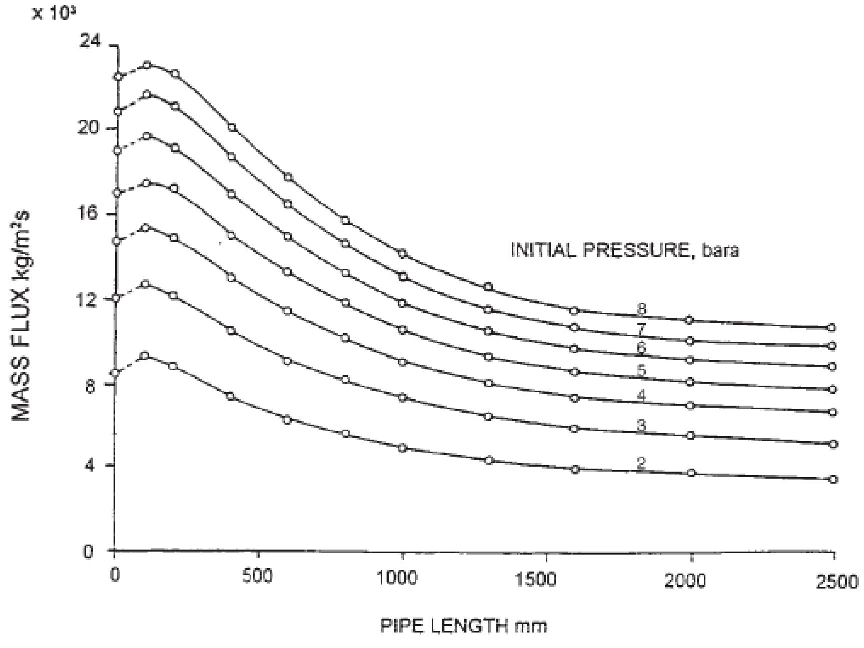

FIG. 26-63 Discharge mass flux for highly subcooled water (20°C) from orifice and 4-mm pipe of various lengths. (*Data of Uchida and Narai, 1966; reproduced by permission of ASME.*)

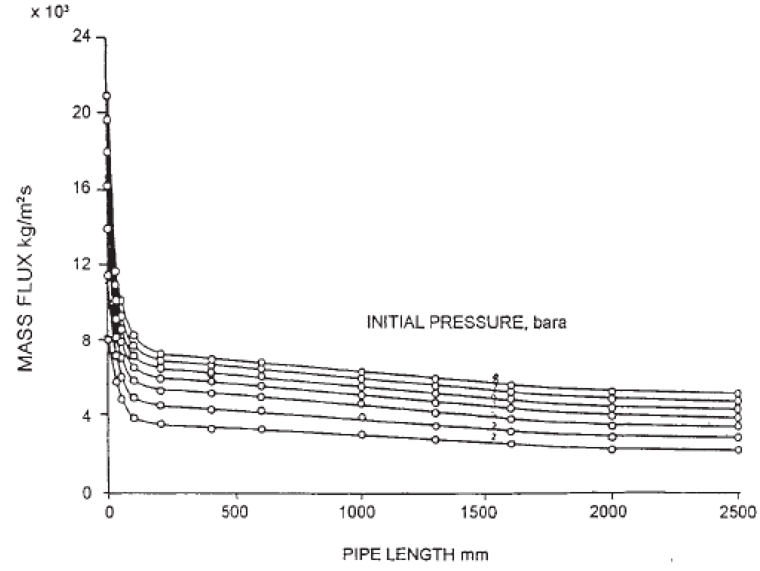

FIG. 26-64 Discharge mass flux for saturated water from orifice and 4-mm pipe of various lengths. (*Data of Uchida and Narai, 1966; reproduced by permission of ASME.*)

Figure 1. **Experimental data for sub-cooled/saturated water data with varying L and P_{st}**

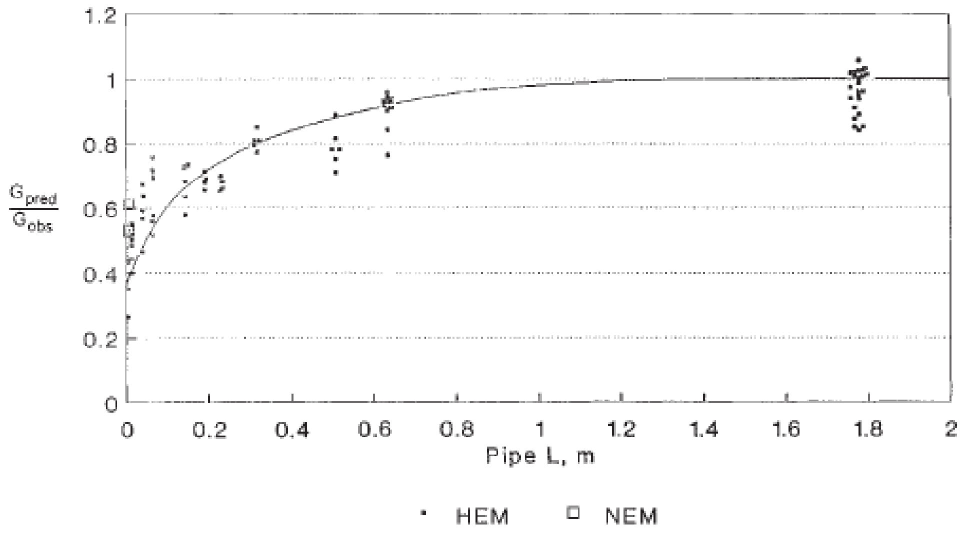

FIG. 26-70 Accuracy in HEM predictions for slightly to moderately subcooled flashing flow. Comparison with data for water by Sozzi and Sutherland (1975); also ASME Symposium on Non-Equilibrium Two-Phase Flows (1975) (Nozzle type 2).

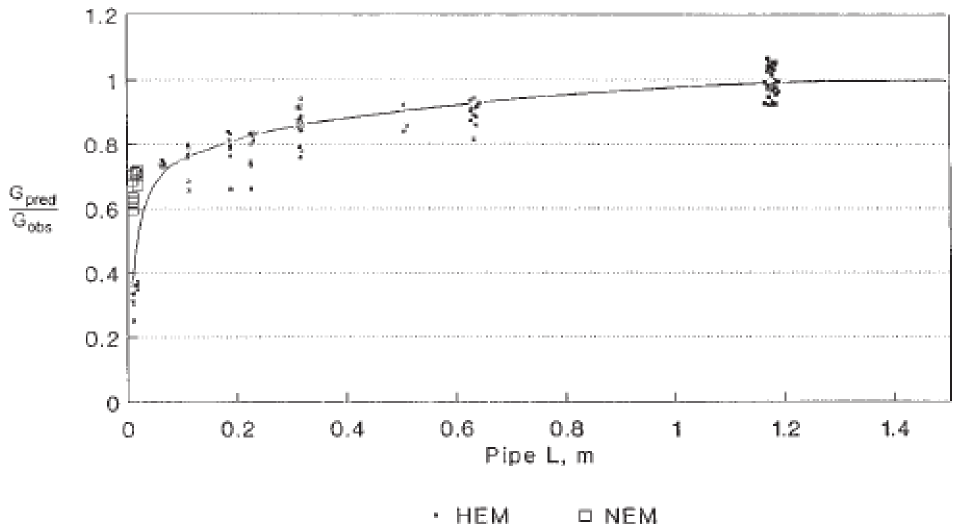

FIG. 26-71 Accuracy in HEM predictions for saturated, flashing flow. Comparison with data for water by Sozzi and Sutherland (1975), (Nozzle type 2).

Figure 2. **HEM/NEM model validation against sub-cooled/saturated water data with varying L**

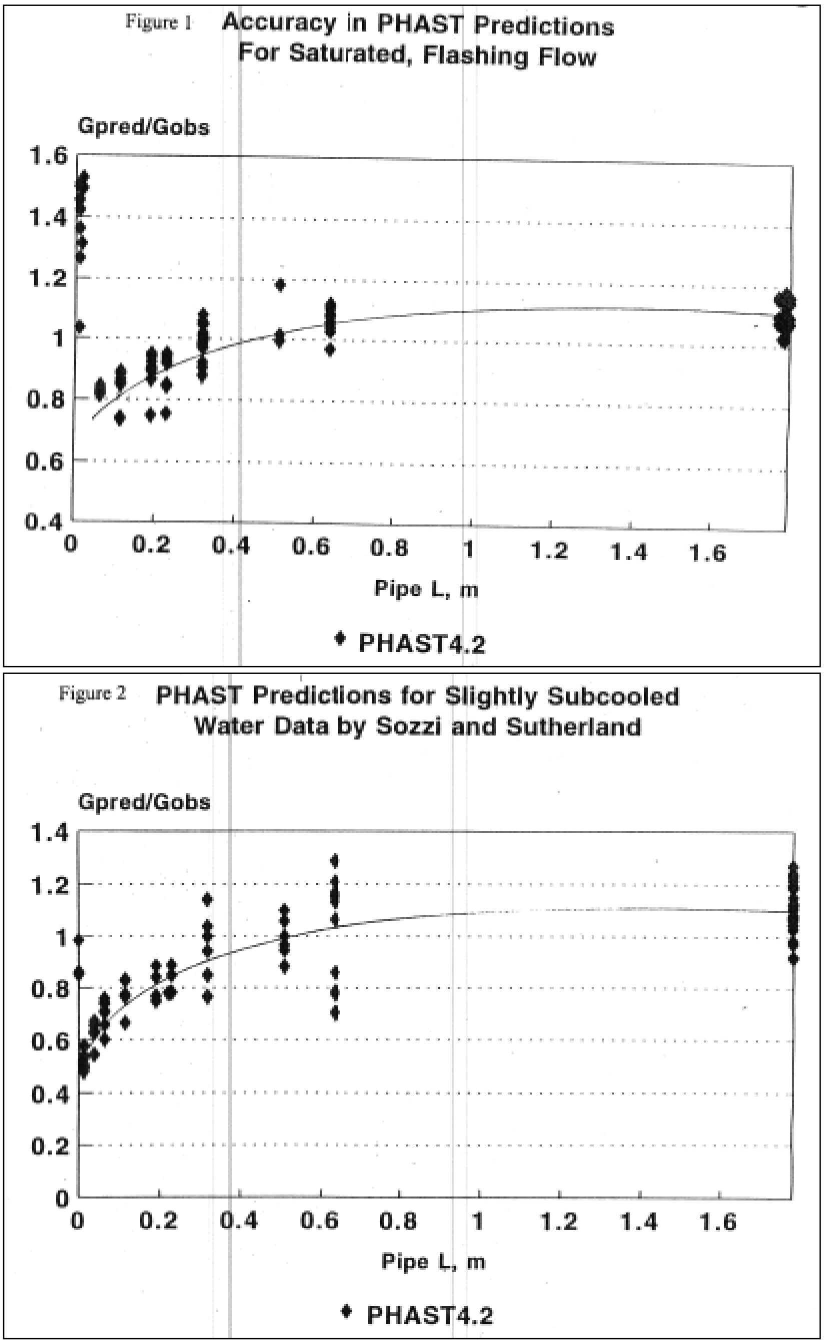

Figure 3. **PHAST4.2 validation against sub-cooled/saturated water data with varying L**

Figure 1 shows PHAST4.2 over-prediction of orifice flow 40% for flashing water, and under-predicts orifice flow for slightly sub-cooled water by about 50%. As the pipe length increases the error reduces to near zero, with an over-prediction of about 10% for longer pipe discharge rates. These data seem to imply that about 1 meter is needed to reach HEM (rather than 0.1m quoted in the literature).

2.1.2 DISC validation against hydrocarbon experiments

Duree[3] (Shell Research) carried out PHAST 4.2 validation against experiments of by Shell and Imperial College. This included:

- full-bore and orifice releases of liquid propane – Shell experiments (Fig. 2.1)
- full-bore and orifice releases of liquid butane – Shell experiments (Fig. 2.2)

Note there is overall very good agreement.

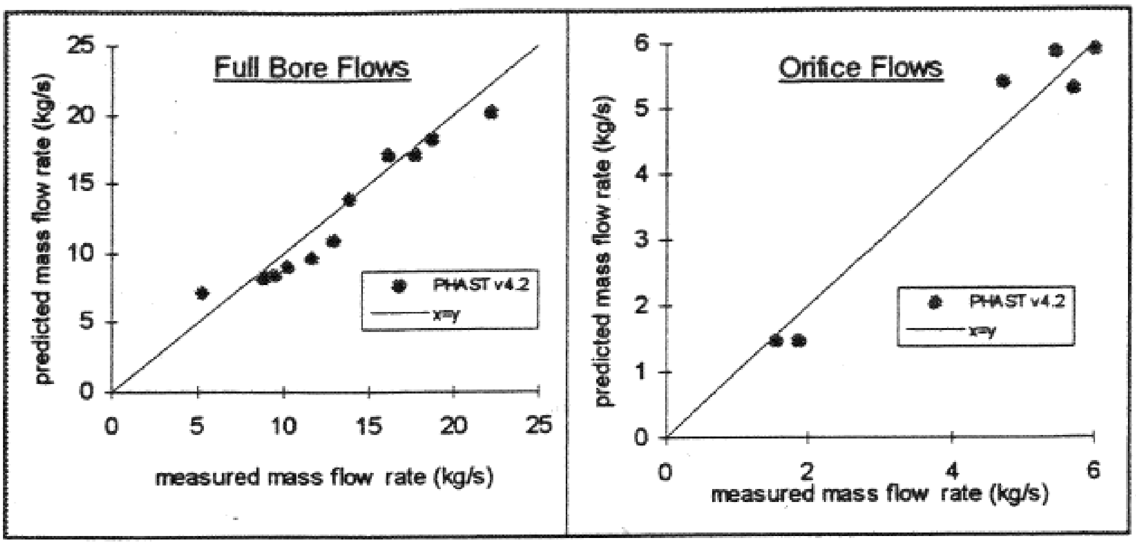

Figure 2.1 - Predictions vs. Measurements for Two-Phase Propane Tests (Data Set 1.1)

Figure 4. PHAST 4.2 validation against two-phase propane full-bore and orifice tests

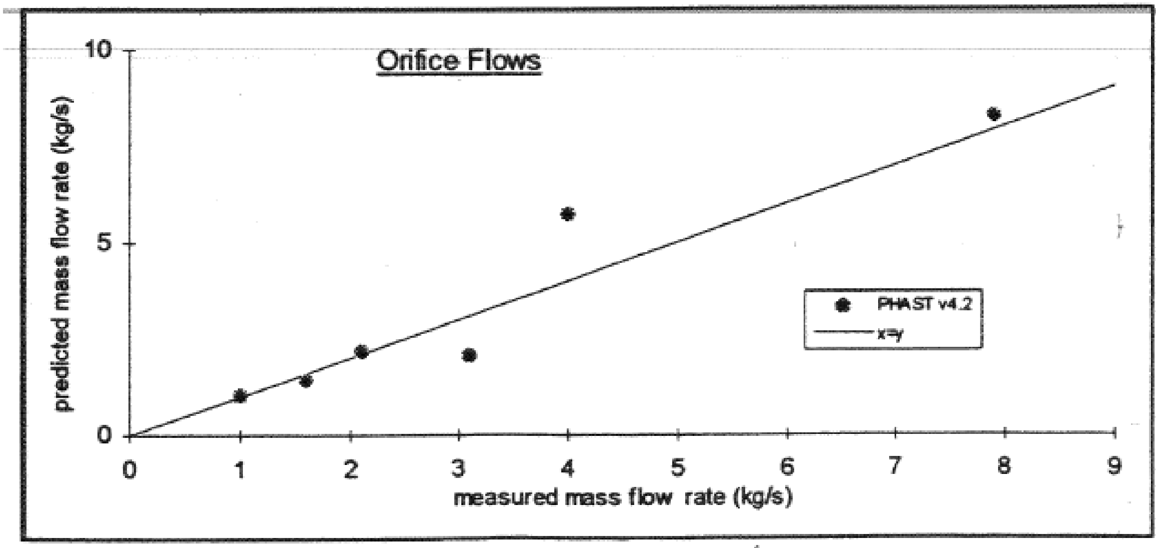

Figure 2.2 - Predictions vs. Measurements for Two-Phase Butane Releases (Data Set 1.2)

Figure 5. PHAST4.2 validation against two-phase butane orifice tests

2.2 DIERS documentation[i]

Section 3.2 in DIERS project manual[4] includes comparison of various nozzle models (e.g. HEM model, frozen liquid); 10 cm is stated for reaching equilibrium (in DIERS project manual referring to Fauske – 1983). It is also stated that non-equilibrium effects are of little concern above 10% upstream quality (i.e. less than 90% storage liquid fraction). Also included is a discussion on discharge coefficients. Recommendation is close to 1 for fully turbulent flow, which is considerably larger than liquid flow (e.g. 0.61 for sharp-edged orifice). The HEM model is stated to be conservative for pipe flow.

2.3 CCPS publications

CCPS QRA guidelines[5] recommend that the design philosophy of the DIERS models is to select the minimum discharge rate at the design pressure, and to maximise the relief area via a selection of a minimum mass flux model. It is noted that use of these models to represent source term models, will under-predict the discharge rate and therefore they are un-conservative. It also includes reference to a model of Fauske and Epstein (which is similar to the logic in the DISC model) and compares this to experimental data[ii].

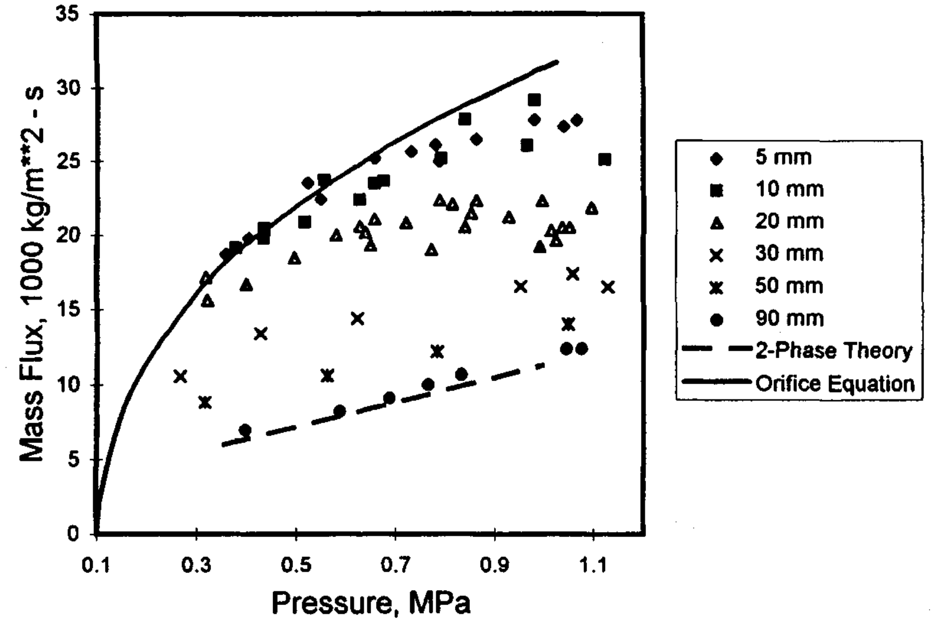

FIGURE 2.6. The mass flux from a flashing two-phase flow as a function of the upstream pressure. The data are plotted for various pipe lengths. The orifice equation predicts a maximum flow, while the two-phase model predicts a minimum flow. (Data from Fauske, 1985.)

Figure 6. Experimental data and model predictions for mass flux with varying P_{st} and D

This publication also contains worked-out examples[iii] and an overview of available computer codes. Also the CCPS book on flammable-mass estimation by John Woodward[6] includes worked-out examples[iv]. Furthermore it includes validation data (including model comparisons) for flashing discharge (Figure 4.8, and Figure 4.9 – Example 6)[v].

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[i] The DIERS website includes a detailed list of references relating to two-phase releases from orifice and pipes, etc., and some of these references could be of interest.

[ii] Future. Consider adding validation against this experiment?

[iii] Future. Consider DISC verification against example 2.1 for liquid-liquid discharge and example 2.4 for a gas-gas discharge.

[iv] Future. Consider DISC verification in Section 1 (examples 1,2 for liquid and gas discharges, example 4 for liquid to two-phase discharge, and example 5 for horizontal pipe.

[v] Future. Consider validation for liquid to two-phase experiments corresponding to Figs. 4.8, 4.9.

4.1. Discharge Characteristics 47

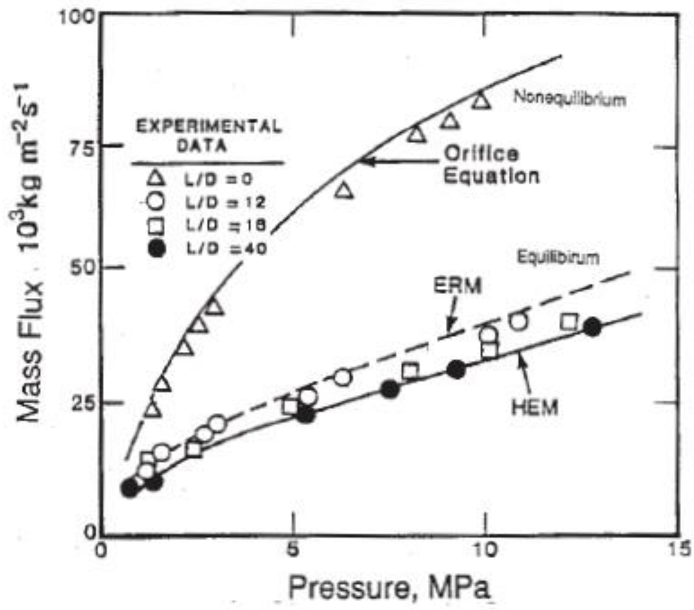

Figure 4.8. Comparison of model predictions for flashing discharge of initially saturated water with data of Fauske (1965).

Figure 7. **ERM/HEM model validation for mass flux with varying P_{st} and L/D**

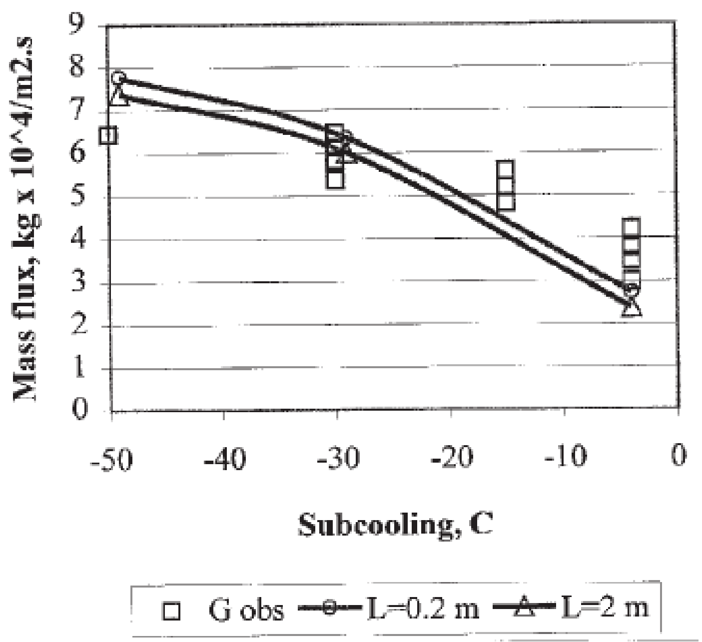

Figure 4.9. Comparison of ERM predictions with experimental data (Fauske, 1985).

Figure 8. **ERM model validation for water with varying sub-cooling (L=0.2, 2m)**

2.4 Lees

Lees[7] provides a detailed overview of a range of discharge models. This includes analytical derivations for discharge coefficients (Section 15.1.4,). Table 15-3 in Section 15.2.1 includes an overview of experimental studies, largely referring to two-phase water experiments,

Table 15.3 *Some experimental studies on two-phase flow*

Investigator(s)	*System fluid*[a]	*Geometry*
W. Schiller (1933)		
Benjaminsen and Miller (1941)	Single component	Orifices
Burnell (1947)	Single component	Orifices, nozzles, pipes
Lockhart and Martinelli (1949)	Two components	Horizontal pipes
Pasqua (1953)	Single component	
Schweppe and Foust (1953)	Single component	Vertical tubes
Brigham, Holstein and Huntington (1957)	Two components	Inclined pipes
Isbin, Moy and da Cruz (1957); Isbin *et al.* (1962)	Single component	
Chisholm and Laird (1958)	Two components	Horizontal pipes
Zaloudek (1961)	Single component	Pipes
Fauske (1962, 1963, 1964)	Single component	Horizontal pipes
Friedrich and Vetter (1962)	Single component	Nozzles, short tubes
Baroczy (1966)	Single and two component systems	
Chisholm and Watson (1966)	Single component	Orifices
Uchida and Nariai (1966)	Single component	Orifices, nozzles, pipes
Flinta, Gernborg and Adesson (1971)	Single component	Horizontal pipes
Beggs and Brill (1973)	Two components	Inclined pipes
Sozzi and Sutherland (1975)	Single component	Horizontal pipes
Kevorkov, Lutovinov and Tikhonenko (1977)	Single component	Horizontal pipes
Sallet (1979b); Sallet, Weske and Gühler (1979); Sallet and Somers (1985)	Single component	Safety valve
van den Akker, Snoey and Spoelstra (1983)	Single component	Vertical then horizontal section
Fernandes, Semiat and Dukler (1983)	Two components	Vertical tubes
Hutcherson, Henry and Wollersheim (1983)	Single component	Horizontal pipes
Nyren and Winter (1983)	Single component	Horizontal pipes
B. Fletcher (1984a,b); B. Fletcher and Johnson (1984)	Single component	Horizontal pipes
M.R.O. Jones and Underwood (1984)	Single component	Nozzles, short tubes
D.A. Lewis and Davidson (1985)	Single component	Orifices, nozzles
Friedel (1988)	Two components	Bursting disc, safety valve

[a] Single component systems are those with a single saturated or superheated liquid, typically water. Two component systems are those with a gas and a liquid, typically air and water.
[b] See also work of Fauske and coworkers (Section 15.3) and work on relaxation length (Table 15.4), on pressure relief valves (Section 15.6), on vessel blowdown (Section 15.7) and in the DIERS project (Chapter 17).

Note that in Section 15.2.19 he states that the distance over which equilibrium is established is an absolute distance (Lees mentions 75 mm, in line with 10 cm mentioned above), and not (as initially thought) a function of L/D ratio. Model comparison as function of pipe length L against data by Fletcher and Johnson (1984) are given by Figure 15.13.

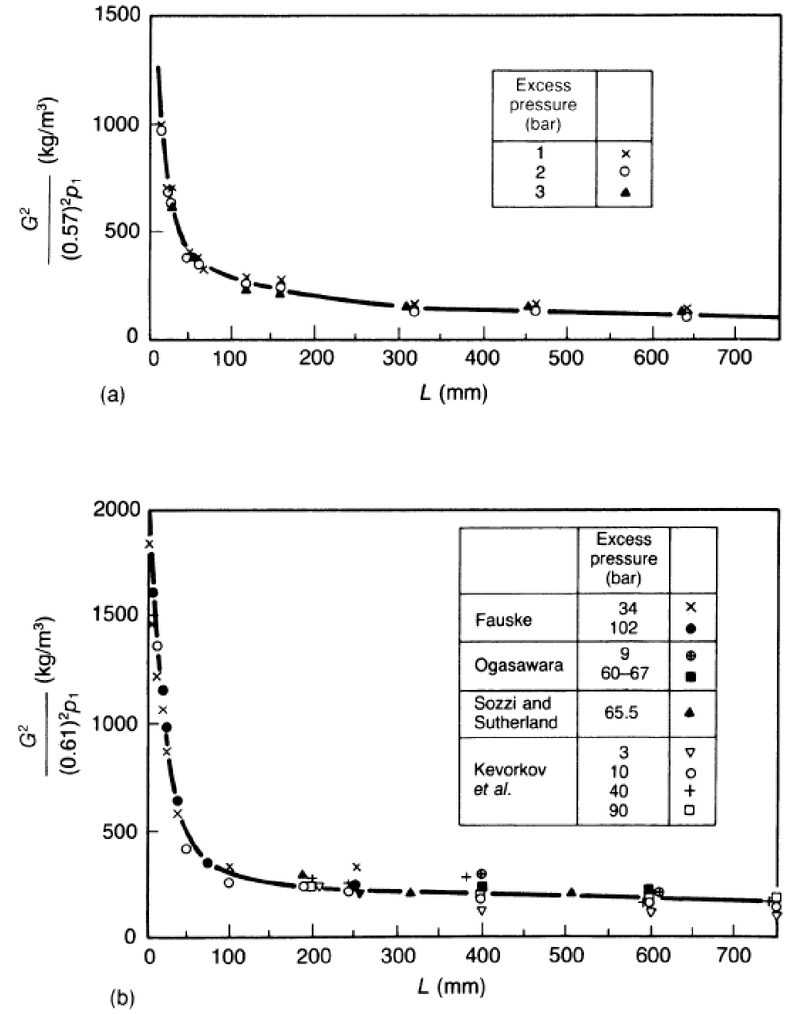

Figure 15.13 *Correlations for discharge of Refrigerant 11 and of saturated water (B. Fletcher and Johnson, 1984): (a) Refrigerant 11; (b) saturated water G, mass velocity (kg/m²s); p_1 upstream pressure (N/m²) (Courtesy of HM Stationery Office)*

Figure 9. Refrigerant-11 and saturated water data with varying L (correlations for discharge)

2.5 Other literature

Giot[8] provides results for choked data against experimental data (by Flinta, 1984 and Leung, 1987) for liquid to two-phase releases. He also includes data from Sozzi and Sutherland. He discusses both orifice and line ruptures. He includes several more interesting experimental data.

3 VALIDATION OF DISC ORIFICE AND SHORT PIPELINE MODELS

3.1 Introduction

This chapter describes the validation of the short pipeline rupture and orifice discharge models included in version 6.53 of PHAST. It includes the validation of the DISC discharge models against data for sub-cooled and saturated releases of water jets and against data for sub-cooled releases of propane and butane.

3.2 Water pipe and orifice releases

This section reports validation of the DISC discharge model against data reported by Uchida and Nariai (1966)[9] (See Figure 1) and Sozzi and Sutherland (1975)[10]. These data sets relate to sub-cooled and saturated releases of water.

In the Uchida and Nariai tests, sub-cooled and saturated water at stagnation pressures ranging from 2-8 bara were released through .004m (ID) copper pipes. The pipes were of varying lengths ranging from 0 (i.e. orifice) to 2.5m. Discharge rate data for each release scenario was logged, but no information was provided on the surface roughness of the copper pipes. As such, for the DISC simulations, a value of $3x10^{-6}$m has been assumed[6]. Table 1 presents a summary of key input data for each test case[7].

Description	Data
Orifice diameter (m)	.004
Pipeline internal diameter (m)	.004
Pipe roughness (m)[8]	$3x10^{-6}$
Pipe length (m)	0 – 2.5
Stagnation temperature (sub-cooled releases) (^{o}C)	20
Stagnation pressure(s) (saturated/sub-cooled) (bara)	2, 3, 4, 5, 6, 7, 8

Table 1 Summary of key input data employed in simulating data reported by Uchida and Nariai (1966).

Sozzi and Sutherland studied the effect of fluid state (i.e. two-phase or sub-cooled liquid), flow geometry, aperture size and flow length on release rate measurements involving water. Of the seven release scenarios studied, only data related to the first two have been selected for this validation exercise[9]. The first scenario (i.e. Scenario 1) involves the release of pressurised two-phase/sub-cooled water from a tank through a .0127m orifice with a well-rounded inlet. The second scenario (i.e. Scenario 2) is concerned with the release of two-phase/sub-cooled water through .0127m (ID) pipes of varying lengths ranging from 0 - 1.78m. These pipes, as in Scenario 1, possess well rounded inlets and were attached to the same tank. No data was presented for the characteristic roughness of these pipes, hence, for the DISC simulations, a value of $1.5x10^{-6}$m has been assumed. Table 2 presents a summary of key input data for each test case.

Description	Data
Orifice diameter [Scenario 1] (m)	.0127
Pipeline internal diameter [Scenario 2] (m)	.0127
Pipe roughness (m)[10]	$1.5x10^{-6}$
Pipe length (m)	0 – 1.78
Stagnation temperature (sub-cooled releases) (^{o}C)	Various
Stagnation pressure(s) (saturated/sub-cooled) (bara)	Various

Table 2 Summary of key input data employed in simulating data reported by Sozzi and Sutherland (1975)

<u>DISC results for water pipe releases (Uchida and Nariai, 1966)</u>

Figure 10 to Figure 16 show the variation of simulated and observed discharged mass flux with pipe length for sub-cooled water initially at stagnation pressures of 8, 7, 6, 5, 4, 3 and 2 bara respectively. Each figure compares simulated results

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[6] The adopted surface roughness is twice the recommended/typical value for drawn tubing but less than the value for commercial carbon steel pipes (see Table 6-1, pp 6-10, Perry's Chemical Engineers Handbook, 7[th] edition). Due to the relatively small aperture sizes of the pipes employed in the study, the pipe surface roughness is expected to approach the recommended value for drawn tubing.

[7] Further details related to specific input can be found in the results processing spreadsheet DISC_Validation_Summary_of_Simulated_Results.xls

[8] Assumed

[9] These scenarios represent simple flow geometries which typify releases through orifices and rupture of short pipelines as is currently modelled by PHAST.

[10] Assumed

using PHAST 6.53[11] and 4.2 with experimental data logged by Uchida and Nariai (1966). From these figures, within limits of uncertainty in measurements[12], the following observations can be made:

- Simulated discharge rate results obtained using PHAST6.53 and 4.2 are marginally conservative but compare very well with experimental data. The maximum and average absolute deviations of simulated results using PHAST6.53 from experimental data are ca 20% and 7% respectively.
- PHAST6.53 generally overestimates the discharge rate for near zero-flow-length (i.e. “orifice-like”) releases by ca 13.9%. This is likely as a result of fluid property calculation errors identified during the verification exercise (see the DISC verification document).

Figure 17 to Figure 23 show the variation of simulated and observed discharged mass flux with pipe length for saturated water initially at stagnation pressures of 8, 7, 6, 5, 4, 3 and 2 bara respectively. Each figure compares simulated results using PHAST 6.53[11] and 4.2 with experimental data logged by Uchida and Nariai (1966). From these figures, the following observations can be made:

- With the exception of near zero-flow-length (i.e. pipe length ≤ 0.01m) discharge rate results, simulated data using PHAST6.53 and 4.2 are in close agreement. Observed discrepancies in simulated results between both versions have been traced to differences in adopted modelling assumptions. In PHAST4.2, it appears that near zero-flow-length releases have been modelled as meta-stable releases across an orifice. This constraint has been relaxed in PHAST6.53.[13]
- Discharge rate results obtained from both versions of PHAST compare less good with experimental data and are generally under conservative. However, the slope of the discharge rate versus pipe length profiles for the simulated and experimental data are very similar. This suggests the presence of a constant source of error in the simulated as compared with the measured discharge rates for two-phase flashing releases.[14] The maximum and average absolute deviations of simulated results using PHAST6.53 from experimental data are ca 82% and 54% respectively.

DISC results for water pipe releases (Sozzi and Sutherland, 1975)

Figure 24 shows the variation of Gpred/Gobs (i.e. the ratio of simulated to measured discharge rate data) with pipe length for sub-cooled[15] water based on Sozzi and Sutherland’s experimental data. Unlike the Uchida and Nariai tests, in most cases, the sub-cooled water in the Sozzi and Sutherland tests is observed to flash along the length of the pipeline. Simulated results obtained using PHAST4.2 and 6.53[11] are compared. From Figure 24, within limits of uncertainty in measurements, [12] the following observations can be made:

- Simulated discharge rates using PHAST4.2 and 6.53 generally approach experimental data (i.e. Gpred/Gobs ≈ 1) with increasing pipe length. These results are unlike the discharge rate results for saturated water in the Uchida and Nariai tests: here, a constant offset between simulated and measured data was observed.
- PHAST4.2 generally underestimates release rate data for pipe lengths ≤ 0.5m.
- However, PHAST6.53 generally predicts conservative release rates when compared with measured data. Release rate data are generally underestimated in PHAST6.53 when flashing is predicted to occur within pipe lengths ≤ 0.2m.
- The above observations suggest for flashing flows that the shorter the flow/pipe length, the less valid is the use of the homogenous equilibrium modelling assumption.
- On the whole, simulated results using PHAST4.2 and 6.53 can be said to compare well with Sozzi and Sutherland’s data. The respective maximum/average percentage deviations of simulated results using PHAST4.2 and 6.53 from experimental data are ca 52%/20% and 74%/17%.

Figure 25 shows the variation of Gpred/Gobs with pipe length for saturated/two-phase[16] water based on Sozzi and Sutherland’s experimental data. Simulated results obtained using PHAST4.2 and 6.53 are compared. From Figure 25, the following observations can be made:

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[11] “Capping-disallow flashing” flow option. This implies that simulated release rates from the pipeline model are subject to a maximum value. The adopted maximum value corresponds to the simulated release rate from an “orifice” with the same diameter as the pipeline based on the meta-stable flow assumption.

[12] No value for this has been quoted by the authors

[13] It appears relaxing this constraint in PHAST6.53 results in poorer performance of the discharge model for near zero-flow-length release scenarios.

[14] **This could be due to a modelling limitation/error, thermodynamic property calculation error or instrumentation (i.e. experimental) error. It would be expected that as flow length increases, simulated results based on PHAST’s homogenous-equilibrium discharge model should approach experimental data (see Figure 2,**

Figure **3** and Figure 7). While this appears not to be the case with the Uchida and Nariai data, the expected trend is generally observed with the Sozzi and Sutherland data.

[15] Stagnation condition

[16] Stagnation condition

- As previously observed, simulated discharge rates using PHAST4.2 and 6.53 generally approach experimental data (i.e. Gpred/Gobs ≈ 1) with increasing pipe length. These results are unlike the discharge rate results for saturated water in the Uchida and Nariai tests.
- While PHAST4.2 is seen to overestimate, PHAST6.53 generally underestimates the discharge rate for near zero-flow-length (i.e. pipe length ≤ 0.01m) releases. The observed behaviour in PHAST4.2 is due to the modelling of near zero-flow-length releases as meta-stable releases across an orifice.
- On the whole, simulated results using PHAST4.2 and 6.53 can be said to compare well with Sozzi and Sutherland's data. The respective maximum/average percentage deviations of simulated results using PHAST4.2 and 6.53 from experimental data are ca 53%/13% and 60%/11%.

DISC results for all sub-cooled water pipe releases

Figure 26 shows the variation of Gpred/Gobs with pipe length for all the sub-cooled water pipe releases by Sozzi and Sutherland (1975) and Uchida and Nariai (1966). The predicted flow rates are based on Phast 8.0.

DISC results for water orifice releases (Uchida and Nariai, 1966; Sozzi and Sutherland, 1975)

Figure 27 compares the PHAST6.53 predicted mass flux for discharge across an orifice for sub-cooled[17] water to measured data reported by Uchida and Nariai (1966) and Sozzi and Sutherland (1975). Simulated results with the "prevent flashing across the orifice" option enabled and disabled [i.e. "PHAST6.53 (Flashing)" and "PHAST6.53 (old method-No Flashing)"] in addition to the "PHAST6.53 (Bernoulli)" modelling option are presented. The simulated scenarios were extended to include all cases involving very short pipes (i.e. pipe length ≤ 0.1m) for which it is assumed that the overall effect of pipe-wall friction on discharge rate is negligible. Discharge rates corresponding to ±30 and ±50% from measured data are also presented. From Figure 27, the following observations can be made:

- Where flashing is predicted to occur, simulated discharge flux results with "Flashing" enabled generally underestimate measured data, while the converse is observed for the same cases with the "No Flashing" option enabled.[18]
- Both the "Flashing" and "No Flashing" option yield the same results for purely sub-cooled releases (i.e. the Uchida and Nariai tests). For these, simulated discharge flux results slightly overestimate measured data.
- When compared with measured data, accuracy in simulated results using the Bernoulli model is observed to increase with decrease in stagnation pressures[19].
- For stagnation pressures below 57barg, the Bernoulli model is seen to be generally conservative and to predict release rates to within ±10% of measured data. The converse behaviour is generally observed above ca 57barg. Interestingly, above this pressure (i.e. 57barg), simulated results using the "No Flashing" option is observed to perform better when compared against measured data. It is suspected that at higher pressures (e.g. above ca 57barg for water), the assumption of liquid incompressibility is less valid. Thus when compared with measured data in this pressure range, the Bernoulli model is observed to diminish in accuracy while the converse is observed for the "No Flashing" model[20].
- In all, simulated results using the "Bernoulli", "Flashing" and "No Flashing" options generally lie within ±50% of measurements. In comparison with measured data, the "Bernoulli" model performs best on average followed by the "No Flashing" and lastly the "Flashing" models. The respective maximum/average percentage deviations of simulated results using the "Bernoulli", "Flashing" and "No Flashing" options from experimental data are ca 33%/11%, 67%/30% and 61%/18%.

Figure 28 compares PHAST6.53's predicted mass flux for discharge across an orifice of saturated/two-phase[17] water to measured data reported by Uchida and Nariai (1966) and Sozzi and Sutherland (1975). As in Figure 27, simulated results with the "Flashing" option enabled and disabled in addition to the "PHAST6.53 (Bernoulli)"[21] modelling option are presented. Simulated scenarios were extended to include all cases involving short pipes (i.e. ≤ 0.1m). Discharge rates corresponding to ±30 and ±50% from measured data are also presented. From Figure 28, the following observations can be made:

- Where the stored fluid at stagnation point exists as a two-phase mixture, both the "Flashing" and "No Flashing" option yield the same under-conservative results.[22] The "Bernoulli" model, for these cases, yields over-conservative release rate estimates with inaccuracies tending to increase with increase in upstream/stagnation pressure and/or vapour quality.
- For 100% liquid saturated water, [17] simulated discharge flux results with the "Flashing" option enabled generally underestimate measured data by more than 50%. With the "No Flashing" and "Bernoulli" options, a converse,

[17] Stagnation condition

[18] The "No Flashing" option is likely to be more prone to errors related to inaccuracies in simulated liquid enthalpies using PHAST's fluid property system. These errors may overstate the observed differences.

[19] This observation is in line with the basic assumption on which the Bernoulli model is built. The assumption of liquid incompressibility tends to approach reality at lower stagnation pressures.

[20] This model attempts to model the variation of liquid compressibility with pressure using the cubic equation of state (CEOS).

[21] For the "Bernoulli" modelling option, all two-phase fluids are assumed to possess a liquid fraction of 1 (i.e. pure saturated liquid). Thus all non-zero vapour quality data recorded in the experiments are ignored and set by default to 0 for the Bernoulli based results. This is known as the forced-phase flow assumption.

[22] For these cases, the "No Flashing" option would ideally be expected to collapse to the "frozen" fluid assumption. This however appears not to be the case.

but less dramatic behaviour, is generally observed for the same cases [18]. Overestimates generally lie within 30% of measured data, while the "Bernoulli" option is observed to provide more accurate estimates of measured data.

- On the whole, the respective maximum/average percentage deviations of simulated results using the "Bernoulli", "Flashing" and "No Flashing" options from experimental data are ca 110%/50%, 92%/42% and 63%/37%.

3.3 Propane orifice and pipe releases

This section reports validation of the DISC discharge model against data reported by Bennett et al.[11] (1991) (see Figure 4), which relates to sub-cooled releases of liquid propane.

Bennett et al. (1991) report discharge rate data for 19 tests involving the release of pressurised LPG. Nine tests relate to releases through .010m and .020m orifices, while the rest are concerned with releases following the full-bore-rupture (FBR) of 2.58m and 11.63m long, .052m (ID) carbon-steel pipes. The authors, for these tests, quote a value of 0.0015m[23] for pipe roughness, while no information was provided for the fluid's stagnation pressure (P_{stag}) or temperature (T_{stag}). Nevertheless, based on available data, it is assumed that the ambient (T_{amb}) and stagnation temperatures are equal. The same assumption is applied to the drive (upstream) [P_{drive}] and stagnation pressures. Table 3 presents a summary of pertinent input data and measured data for each test case, while Table 4 reports the measured composition (mole %) for the LPG mixture employed in the tests. For the DISC simulation of each release scenario, the LPG mixture is assumed to be composed of 100% propane.

Test Name	Release Type	Pipe Length (m)	Orifice/ Pipe Diameter (m)	P_{drive}/ P_{stag} (barg)	T_{stag} (K)	Ambient Pressure [P_{amb}] (mmHg)	T_{amb} (K)	Relative Humidity (fraction)	Measured Flowrate [G_{obs}] (kg/s)
Test_3007	Leak	0	0.01	9.7	288.85	744.5	288.85	0.69	1.8
Test_3006	Leak	0	0.01	9.7	286.35	746.3	286.35	0.79	1.5
Test_3028	Leak	0	0.02	7.7	278.45	721.3	278.45	0.92	5.7
Test_3047	Leak	0	0.02	7	285.05	737.2	285.05	0.77	4.7
Test_3048	Leak	0	0.02	7.1	283.95	736.5	283.95	0.87	4.9
Test_3039	Leak	0	0.01	7	279.15	750	279.15	0.58	1.5
Test_3080	Leak	0	0.02	7.6	288.55	750[24]	288.55	0.85	3.4
Test_3012	Leak	0	0.02	9.5	286.55	750[24]	286.55	0.9	5.8
Test_3090	Leak	0	0.02	7.6	282.85	750[24]	282.85	0.88	3.9
Test_3026	FBR	2.58	0.052	6.5	286.85	750[24]	286.85	0.59	16.1
Test_3029	FBR	2.58	0.052	6.3	281.15	750[24]	281.15	0.82	18
Test_3019	FBR	2.58	0.052	7.1	285.05	730.2	285.05	0.85	19.4
Test_3063	FBR	11.63	0.052	7.4	279.75	730	279.75	0.86	11.6
Test_3064	FBR	11.63	0.052	7.4	278.55	722	278.55	0.85	11.5
Test_3084	FBR	11.63	0.052	7.1	285.35	741.3	285.35	0.96	10.4
Test_3020	FBR	2.58	0.052	6.9	283.75	740	283.75	0.9	15.3
Test_3087	FBR	11.63	0.052	6.5	286.65	742.4	286.65	0.92	5.5
Test_3054	FBR	11.63	0.052	8	284.75	750[24]	284.75	0.48	11.8
Test_3077	FBR	11.63	0.052	7.1	286.35	750[24]	286.35	0.92	10.1

Table 3 Summary of measured data for discharge experiments involving the release of pressurised propane reported by Bennett et al. (1991).

Component	Mole %
Methane	0.0
Ethane	0.2
Propane +	97.4
Iso-butane	1.6
N-butane	0.8

[23] This value appears to be rather high for carbon-steel pipes. Perry's Chemical Engineers handbook quotes a value of 0.0000457m as typical surface roughness for commercial steel pipes. The higher a pipe's surface roughness, the greater its wall resistance to flow (i.e. exit flow-rate decreases with increasing surface roughness).

[24] Assumed

Table 4 Typical LPG composition for the Bennett et al. (1991) tests

DISC results for propane orifice releases

Figure 29 compares the PHAST6.53 predicted flow-rate for sub-cooled [17] propane flowing across an orifice to measured data reported by Bennett et al. (1991). Simulated results with the "Flashing" option enabled and disabled in addition to the "PHAST6.53 (Bernoulli)" modelling option are presented. Discharge rates corresponding to ±30 and ±50% from measured data are also presented. From Figure 29, within limits of uncertainty in measurements, [12] the following observations can be made:

- As previously observed, simulated discharge flux results with "Flashing" enabled generally underestimate measured data, while predictions based on the "Bernoulli" and "No Flashing" options tend to be generally conservative.
- In all, simulated results using the "Bernoulli", "Flashing" and "No Flashing" option generally lie within ±30% of measurements. In comparison with measured data, the "Bernoulli" model performs best on average followed by the "No Flashing" and lastly the "Flashing" models. [18] The respective maximum/average percentage deviations of simulated results using the "Bernoulli", "Flashing" and "No Flashing" options from experimental data are ca 54%/16%, 32%/19% and 60%/18%.[25]

DISC results for propane pipe releases

Figure 30 compares the PHAST6.53 predicted flow-rate for steady-state discharge following FBR of 2.68 and 11.63m pipelines conveying sub-cooled[17] propane to measured data reported by Bennett et al. (1991). Discharge rates corresponding to ±30 and ±50% from measured data are also presented. From Figure 30, the following observations can be made:

- Simulated discharge rate results obtained from PHAST6.53 generally underestimate[26] but largely compare well with measured data. 90% of these results lie within ±30% of measurements.
- The respective maximum and average percentage deviations of PHAST6.53 simulated results from experimental data are ca 36% and 19%.

3.4 Butane orifice releases

This section reports validation of the DISC discharge model against data reported by Duree et al. (1995) for sub-cooled releases of liquid butane from 0.01m orifices.

Although the original report contained information on 6 tests, it has only been possible to source sufficient data to simulate two of these tests (i.e. Test_5045 and Test_5035).[27] Table 5 presents a summary of pertinent input data and measured data for tests 5045 and 5035.

Test number	5045	5035
Reference report	TNER.92.038	TNER.92.012
Fuel[28]	100% butane	100% butane
Stagnation pressure (barg)	7.7 (same as pressure immediately upstream of orifice)	4.2 (different to pressure immediately upstream of the orifice)
Stagnation temperature[29] (°C)	16 ± 1	13.3
Orifice diameter (m)	0.01	0.01
Ambient pressure (bar)	0.990	0.979
Ambient temperature (°C)	16 ± 1	14
Ambient humidity (%)	46.5	76
Flow rate (kg/s)	1.7 ± 0.2	1.1 (<10% accuracy)

25 There is cause to doubt the authenticity of two reported data points lying between Gobs = 3 and 4 kg/s. While simulated results based on the "Flashing" option always underestimate measured data, for these two data points the converse is observed. This deviation from expected trend points to the likelihood of data logging/instrumentation error. If the "Flashing" option is established as always yielding underestimates of measured data, the logged data for these two data points are expected to be higher than reported. Coincidentally, the maximum percentage deviation for simulated results using the "No Flashing" option is observed to result from a comparison with one of these data points. If these points are excluded from the analysed data set, the respective maximum/average percentage deviations of simulated results using the "Bernoulli", "Flashing" and "No Flashing" options from experimental data become ca 18.0%/7.6%, 31.9%/23% and 14.6%/8.1%.

26 The observed underestimates may stem from the use of the reported, but likely exaggerated, wall surface roughness.

27 These data were obtained following personal communication with Chamberlain G. (Shell) 30-05-2007.

28 100% butane is assumed; the actual composition is close enough to 100% in order not to significantly affect the results (the precise composition is included in TNER.92.054)

29 For test 5045 a temperature of 24.6C is mentioned in report, but discarded because of fire effects. For test 5035 there are also fire effects resulting in heating of the pipe.

Table 5 **Summary of measured data for discharge experiments involving the release of pressurised n-Butane reported by Duree et al. (1995)[27]**

Table 6 compares the PHAST6.53 predicted mass flux for discharge across an orifice for sub-cooled n-Butane to measured data reported by Duree et al. (1995). Simulated results with the "Flashing" option enabled and disabled in addition to the "PHAST6.53 (Bernoulli)" modelling option are presented.

Test Number	Measured Flow-rate	Predicted Flow-rate			% deviation from Measured data		
		"PHAST6.53 (Bernoulli)"	"PHAST6.53 (old method-No Flashing)"	"PHAST6.53 (Flashing)"	"PHAST6.53 (Bernoulli)"	"PHAST6.53 (old method-No Flashing)"	"PHAST6.53 (Flashing)"
	kg/s	kg/s	kg/s	kg/s	%	%	%
5045	1.7	1.412988	1.465898	1.386298	-16.883044	-13.770687	-18.453055
5035	1.1	1.046337	1.085385	1.010692	-4.878496	-1.328681	-8.118909

Table 6 **Comparison of observed versus PHAST6.53 predicted discharge rate data for release across an orifice involving sub-cooled n-butane at orifice inlet (Data from Duree et al., 1995, SHELL TNER 92.038 and 92.012)**

From Table 6 the following observations can be made:

- Simulated results from all PHAST6.53 discharge models compare very well with measured data. Each model, for both test cases, marginally underestimates measured data.
- As observed previously, the "No Flashing" model predicts the highest release rates followed by the "Bernoulli" and lastly the "Flashing" model.

In all, simulated results using the "Bernoulli", "Flashing" and "No Flashing" option generally lie within -30% of measurements. In comparison with measured data, the "No Flashing" model performs best[30] on average followed by the "Bernoulli" and lastly the "Flashing" models. [18] The respective maximum/average percentage deviations of simulated results using the "Bernoulli", "Flashing" and "No Flashing" options from experimental data are ca 17%/11%, 18%/13% and 14%/8%.

3.5 Further validation

The DISC model has also been validated in the context of validating other linked models in Phast. This validation work can be found in Chapter 6 of the documentation for the atmospheric expansion (ATEX) model[12] and in Chapter 4 of the validation document for the unified dispersion model[13] (UDM).

[30] The choice as to the best model for simulating these data is quite subjective. Within limits of uncertainty either the "Bernoulli" or the "No Flashing" model may be selected as being best suited. For conservative results, the "No Flashing" model is recommended.

3.6 Figures with validation results

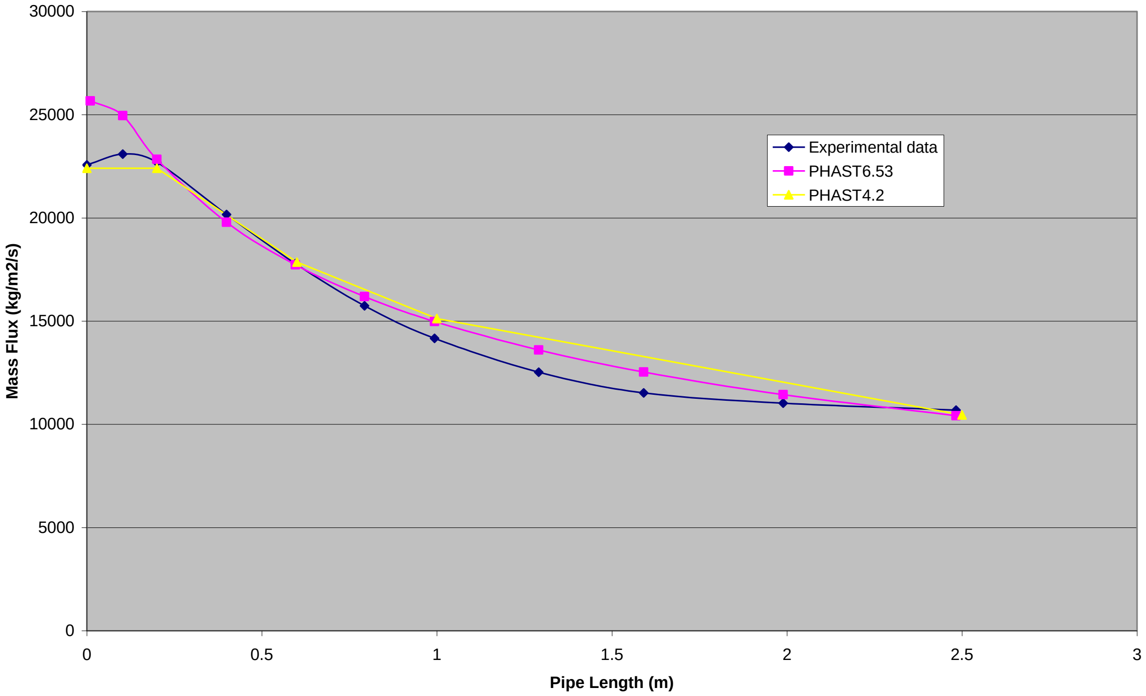

Figure 10 **Performance of PHAST4.2 and 6.53 simulated discharged mass flux versus pipe length data against experimental data for sub-cooled water [stagnation pressure = 8bara] (Data by Uchida and Nariai, 1966)**

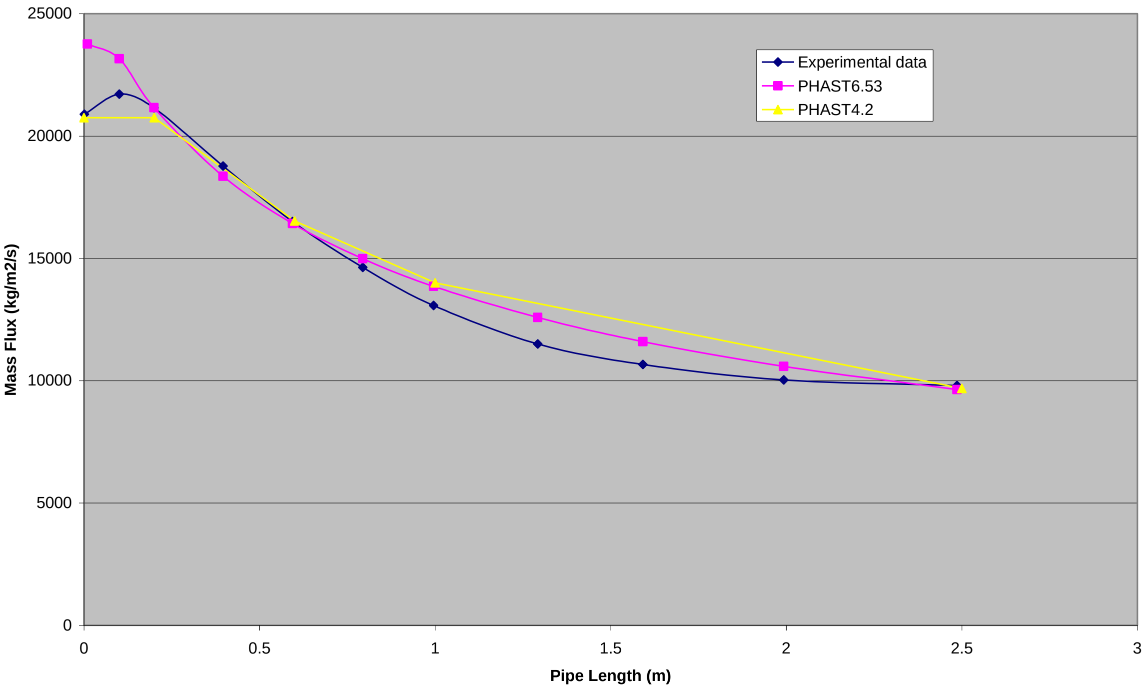

Figure 11 **Performance of PHAST4.2 and 6.53 simulated discharged mass flux versus pipe length data against experimental data for sub-cooled water [stagnation pressure = 7bara] (Data by Uchida and Nariai, 1966)**

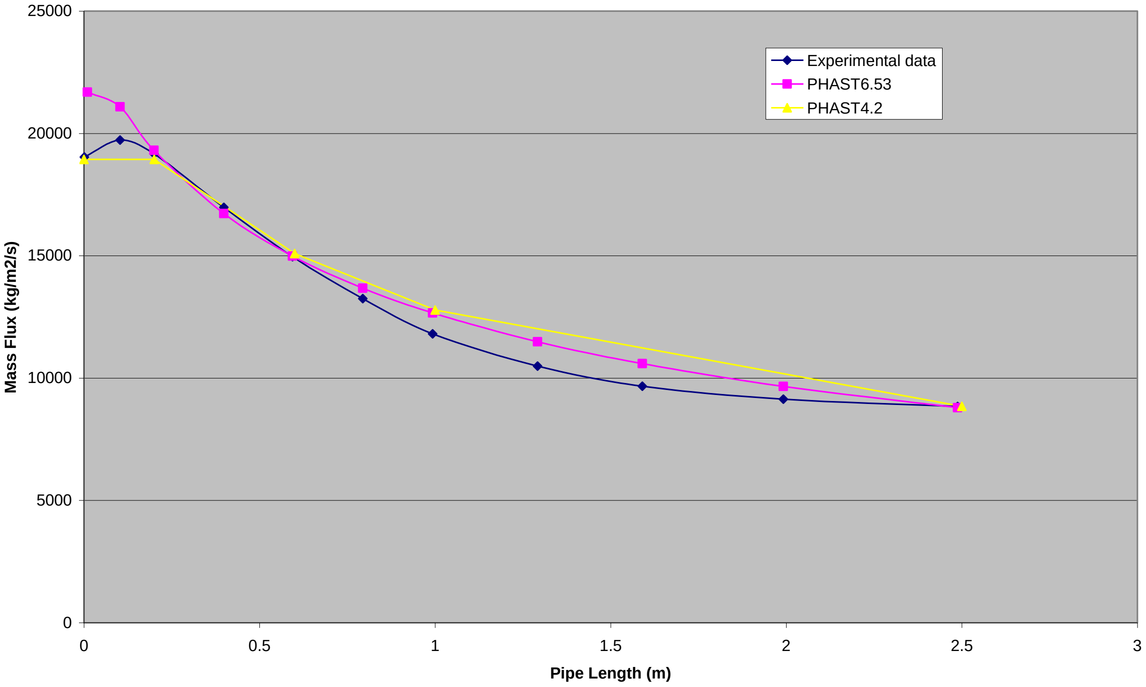

Figure 12 **Performance of PHAST4.2 and 6.53 simulated discharged mass flux versus pipe length data against experimental data for sub-cooled water [stagnation pressure = 6bara] (Data by Uchida and Nariai, 1966)**

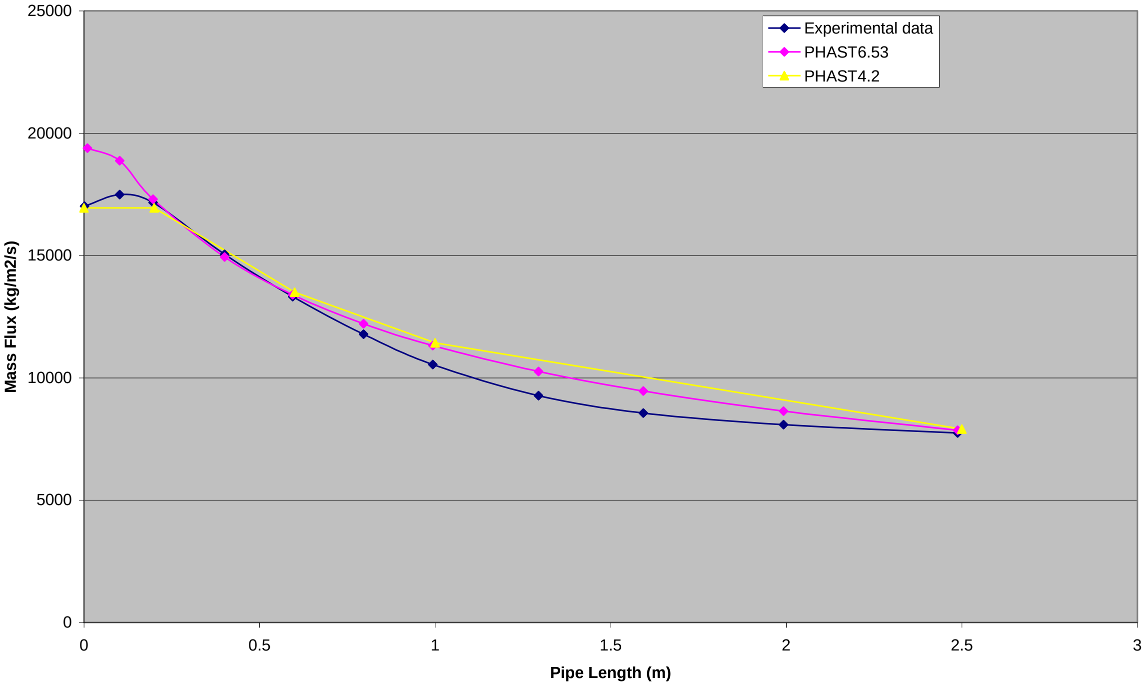

Figure 13 **Performance of PHAST4.2 and 6.53 simulated discharged mass flux versus pipe length data against experimental data for sub-cooled water [stagnation pressure = 5bara] (Data by Uchida and Nariai, 1966)**

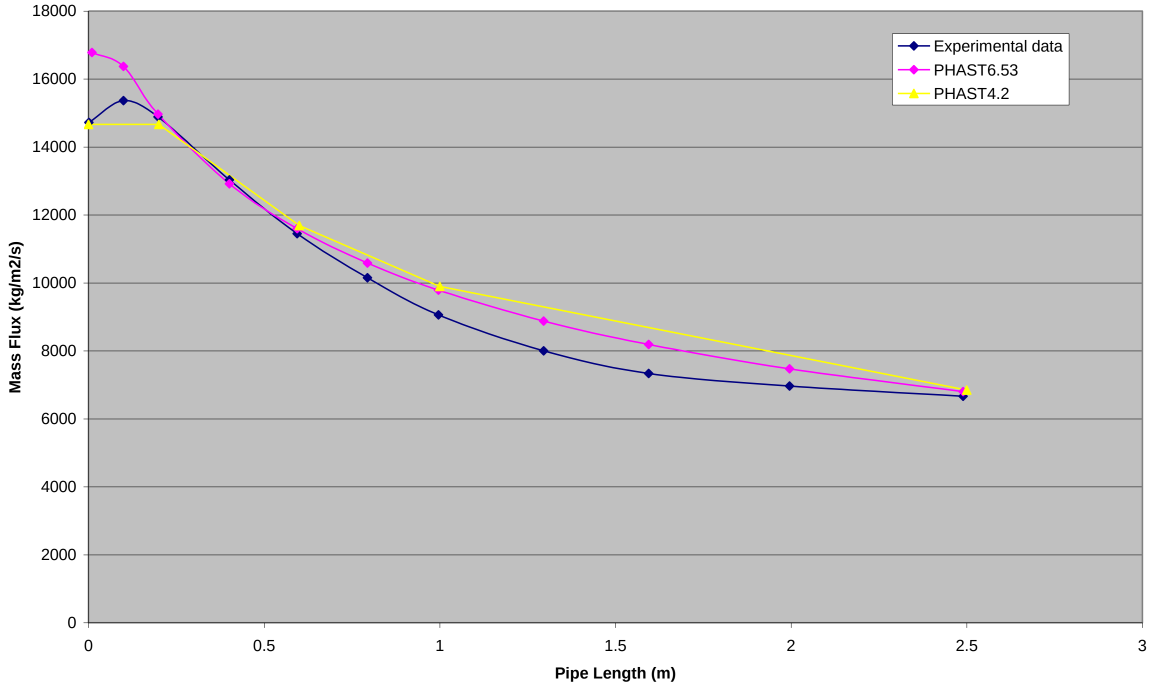

Figure 14 **Performance of PHAST4.2 and 6.53 simulated discharged mass flux versus pipe length data against experimental data for sub-cooled water [stagnation pressure = 4bara] (Data by Uchida and Nariai, 1966)**

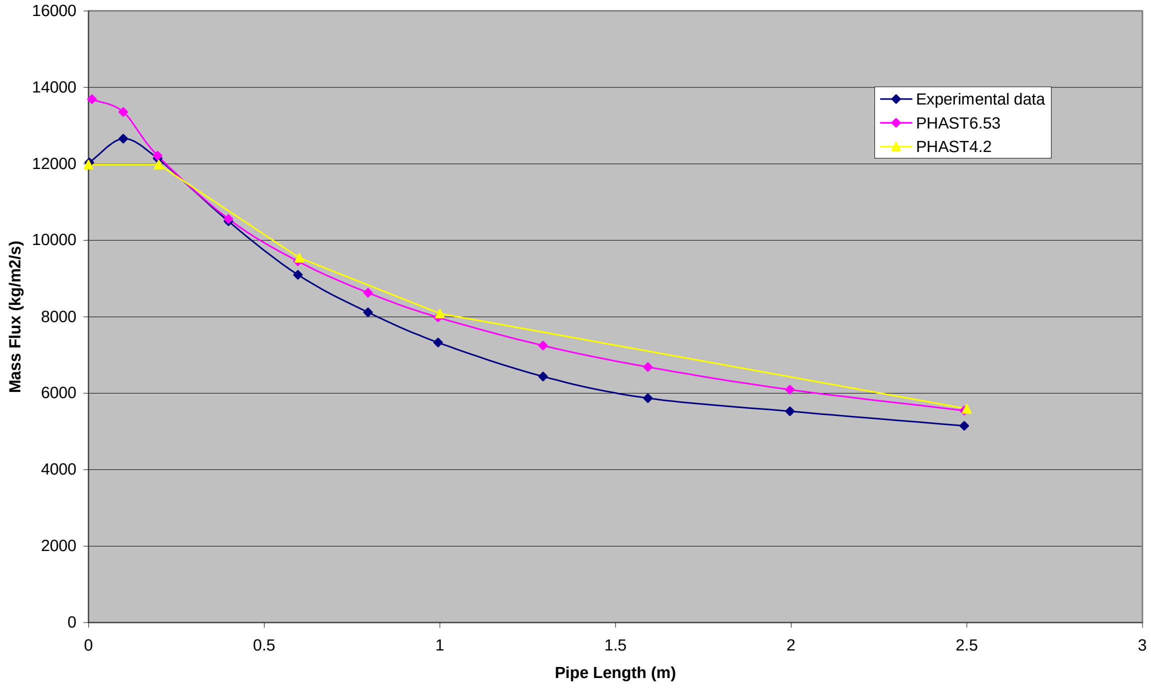

Figure 15 **Performance of PHAST4.2 and 6.53 simulated discharged mass flux versus pipe length data against experimental data for sub-cooled water [stagnation pressure = 3bara] (Data by Uchida and Nariai, 1966)**

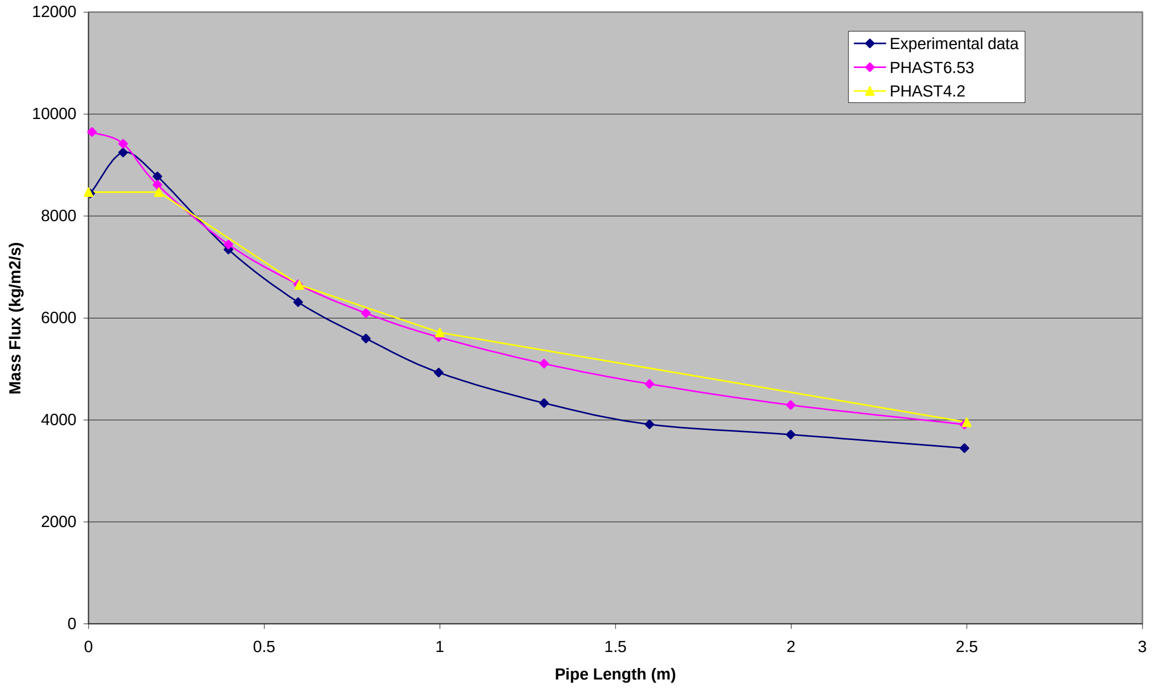

Figure 16 **Performance of PHAST4.2 and 6.53 simulated discharged mass flux versus pipe length data against experimental data for sub-cooled water [stagnation pressure = 2bara] (Data by Uchida and Nariai, 1966)**

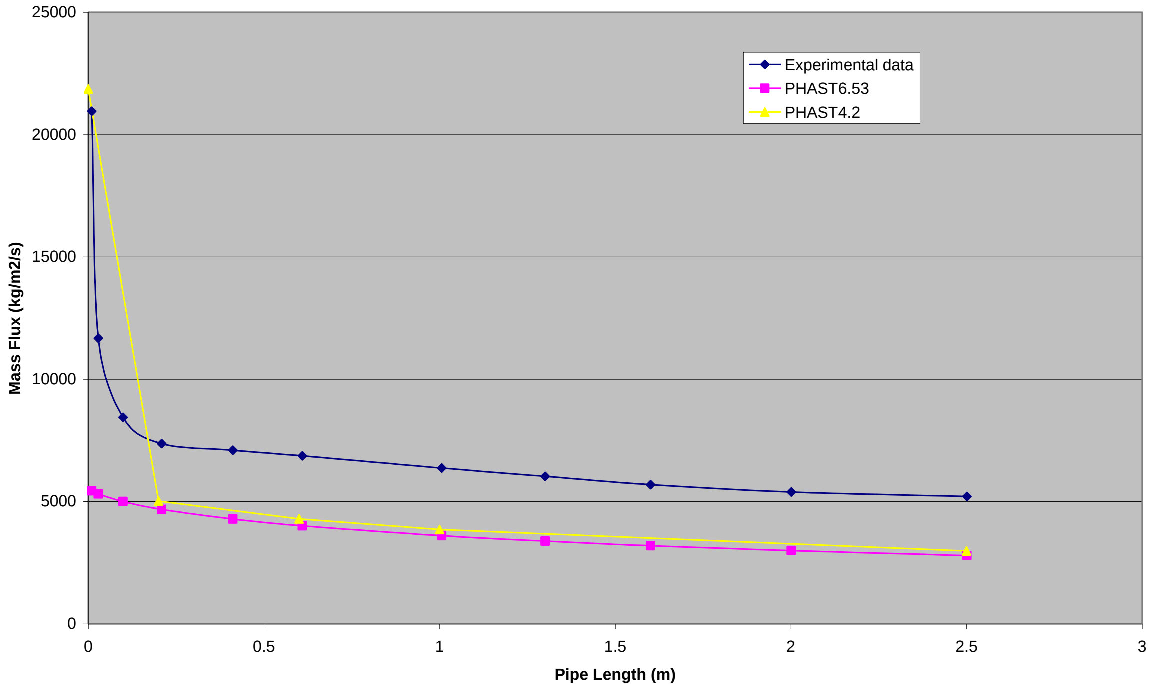

Figure 17 **Performance of PHAST4.2 and 6.53 simulated discharged mass flux versus pipe length data against experimental data for saturated water [stagnation pressure = 8bara] (Data by Uchida and Nariai, 1966)**

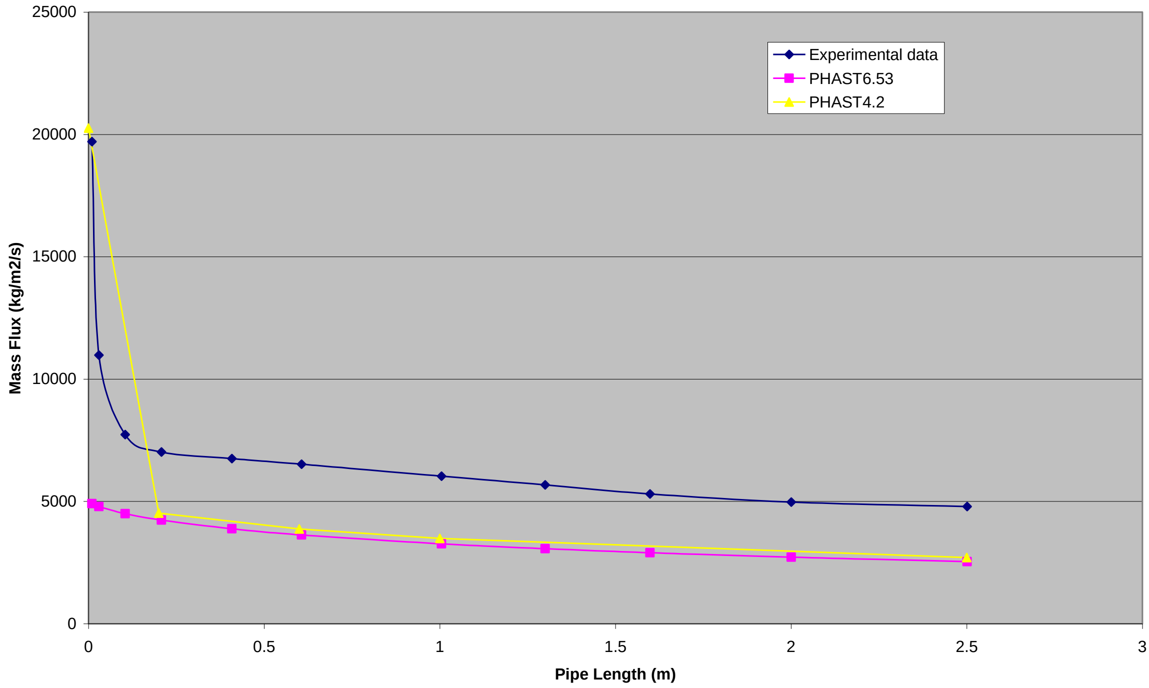

Figure 18 **Performance of PHAST4.2 and 6.53 simulated discharged mass flux versus pipe length data against experimental data for saturated water [stagnation pressure = 7bara] (Data by Uchida and Nariai, 1966)**

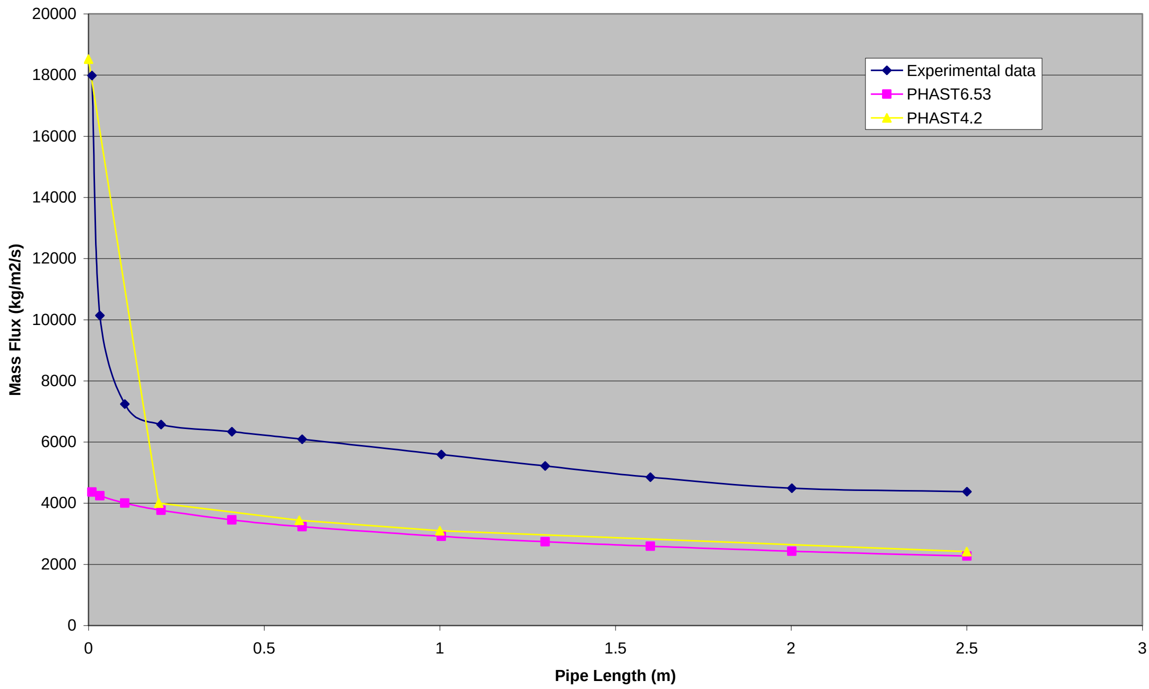

Figure 19 **Performance of PHAST4.2 and 6.53 simulated discharged mass flux versus pipe length data against experimental data for saturated water [stagnation pressure = 6bara] (Data by Uchida and Nariai, 1966)**

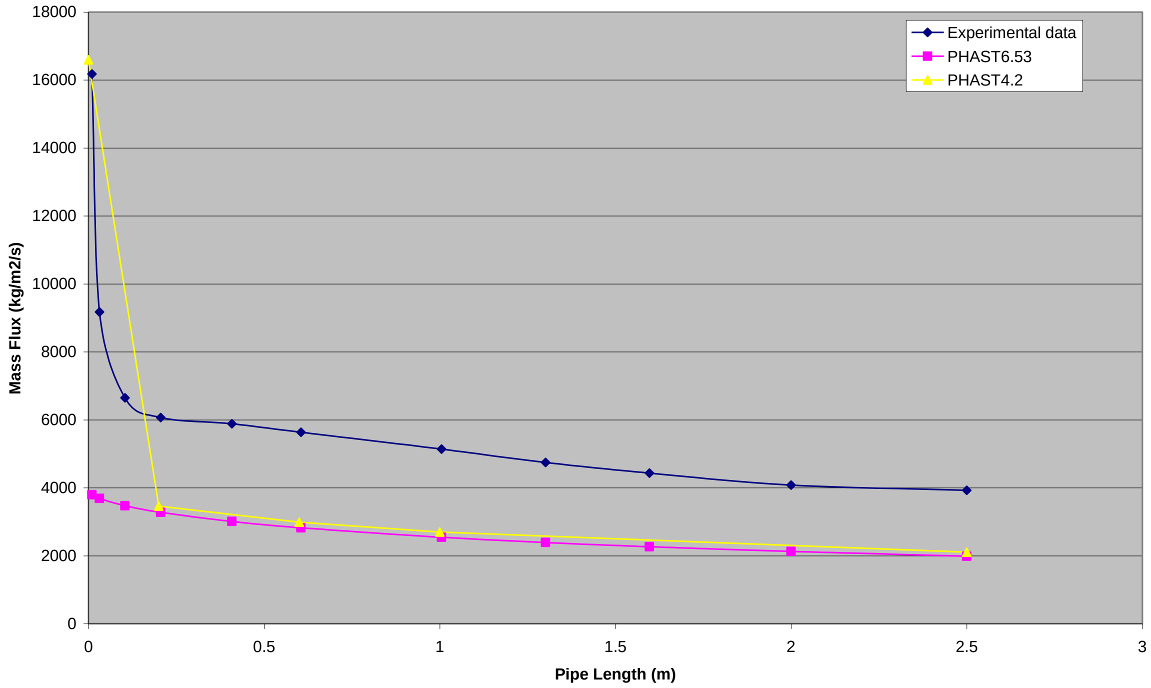

Figure 20 **Performance of PHAST4.2 and 6.53 simulated discharged mass flux versus pipe length data against experimental data for saturated water [stagnation pressure = 5bara] (Data by Uchida and Nariai, 1966)**

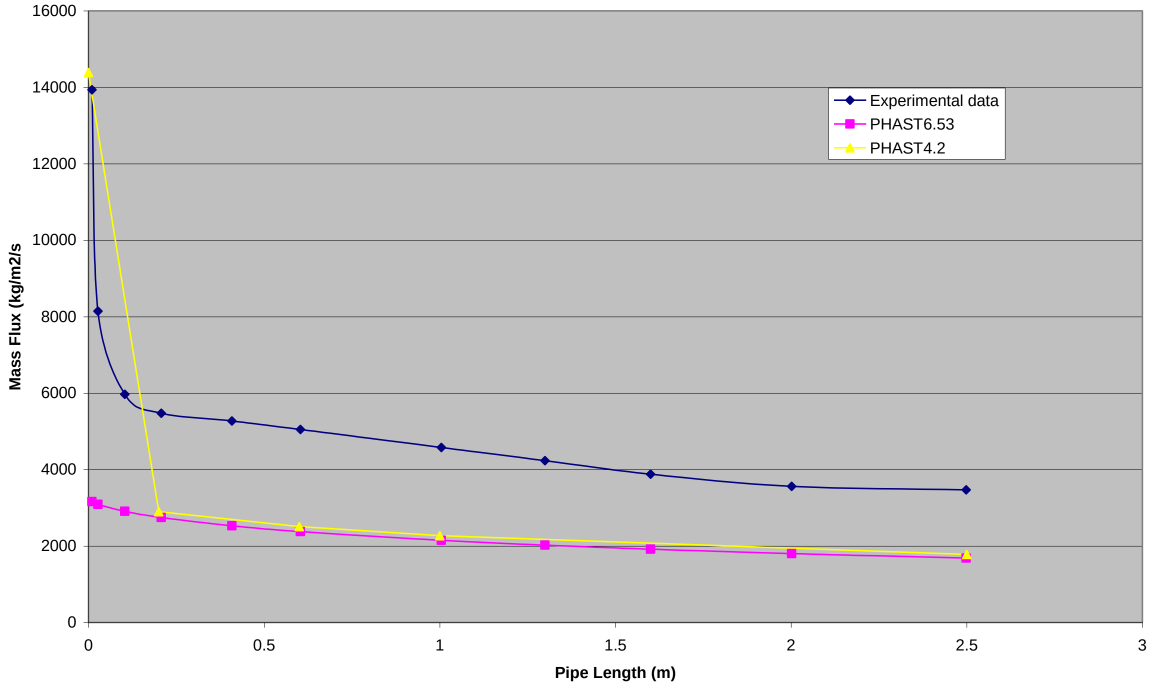

Figure 21 **Performance of PHAST4.2 and 6.53 simulated discharged mass flux versus pipe length data against experimental data for saturated water [stagnation pressure = 4bara] (Data by Uchida and Nariai, 1966)**

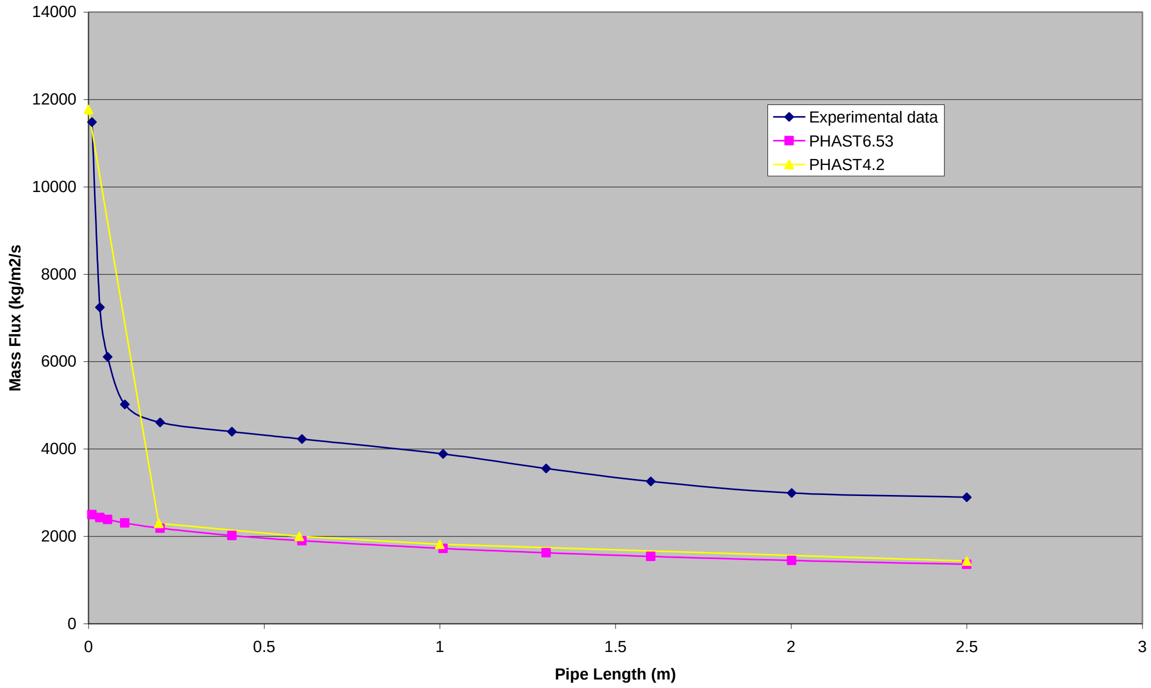

Figure 22 **Performance of PHAST4.2 and 6.53 simulated discharged mass flux versus pipe length data against experimental data for saturated water [stagnation pressure = 3bara] (Data by Uchida and Nariai, 1966)**

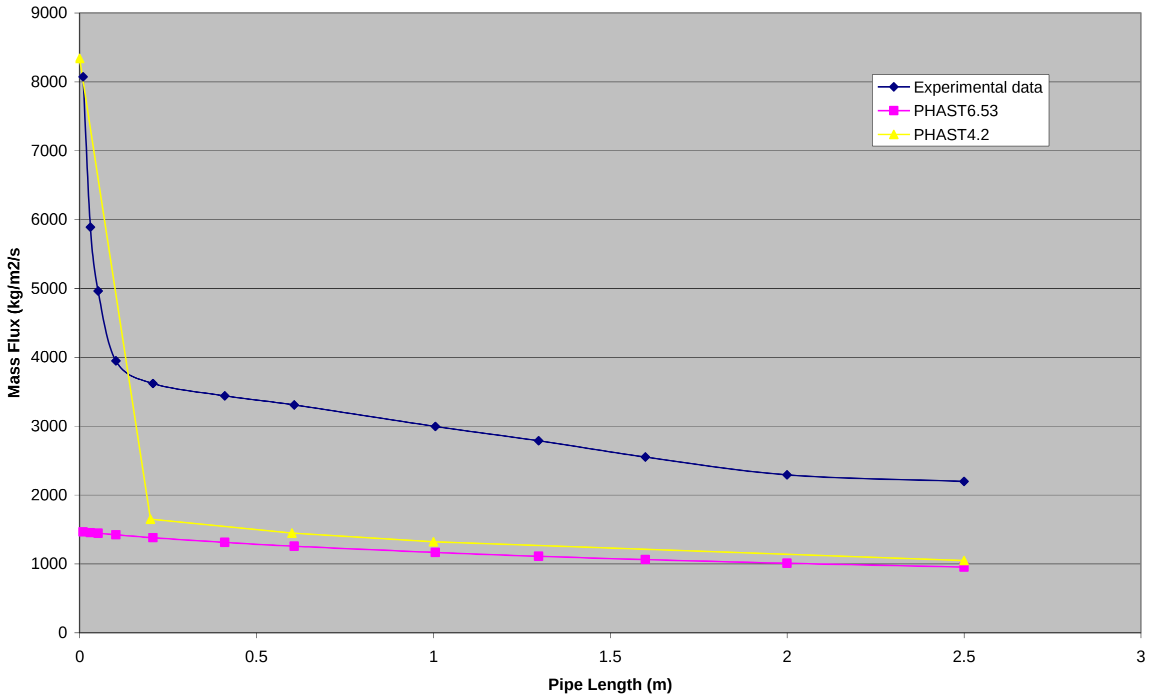

Figure 23 **Performance of PHAST4.2 and 6.53 simulated discharged mass flux versus pipe length data against experimental data for saturated water [stagnation pressure = 2bara] (Data by Uchida and Nariai, 1966)**

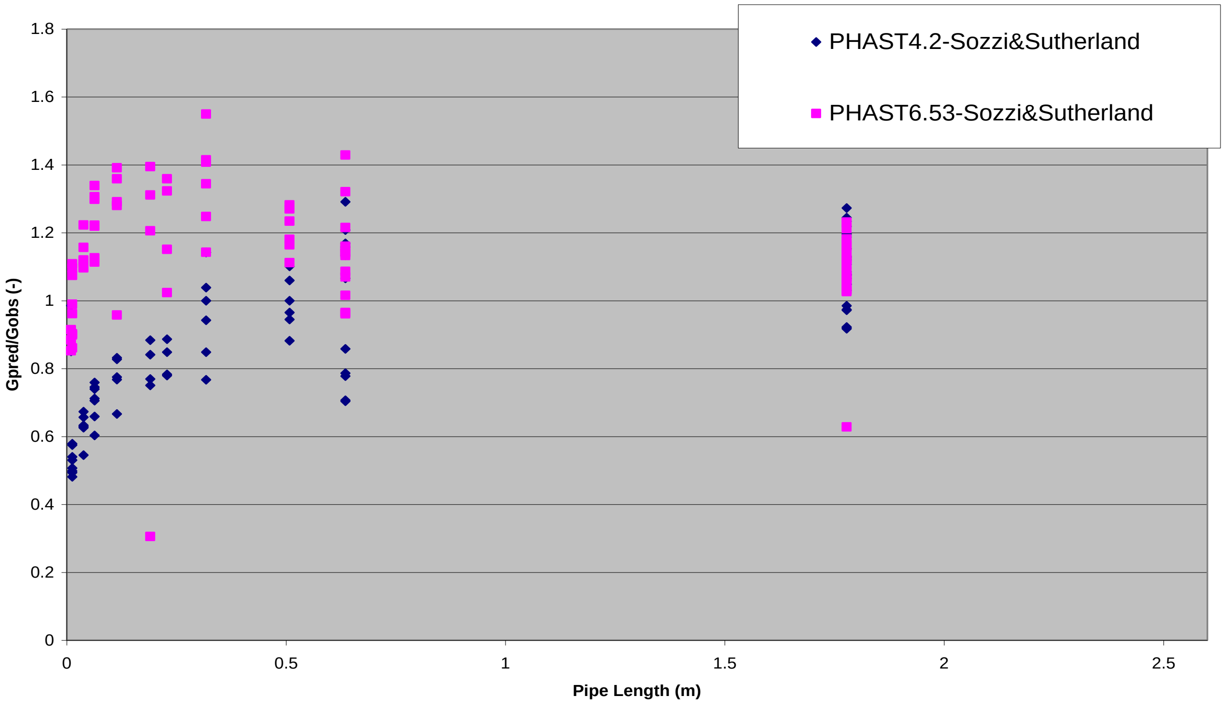

Figure 24 **Performance of PHAST4.2 and 6.53 discharge rate versus pipe length predictions against experimental data for slightly sub-cooled water (Data by Sozzi and Sutherland, 1975)[31]**

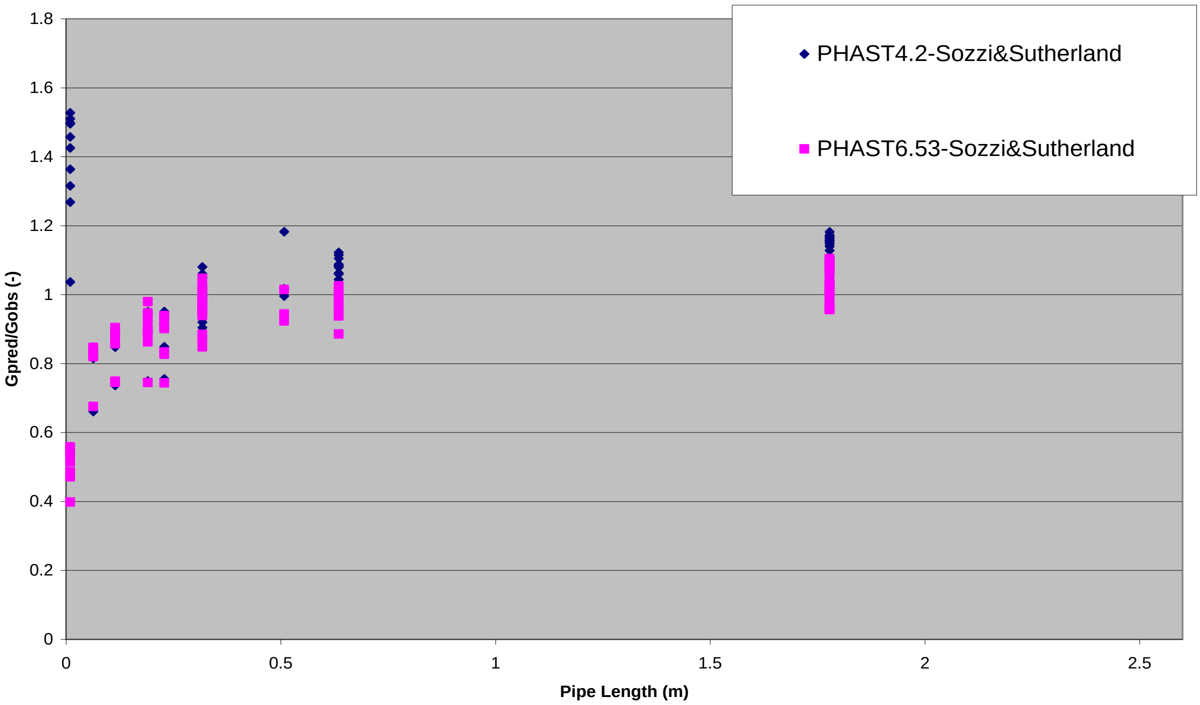

Figure 25 **Performance of PHAST4.2 and 6.53 discharge rate versus pipe length predictions against experimental data for saturated/flashing water (Data by Sozzi and Sutherland, 1975)[31]**

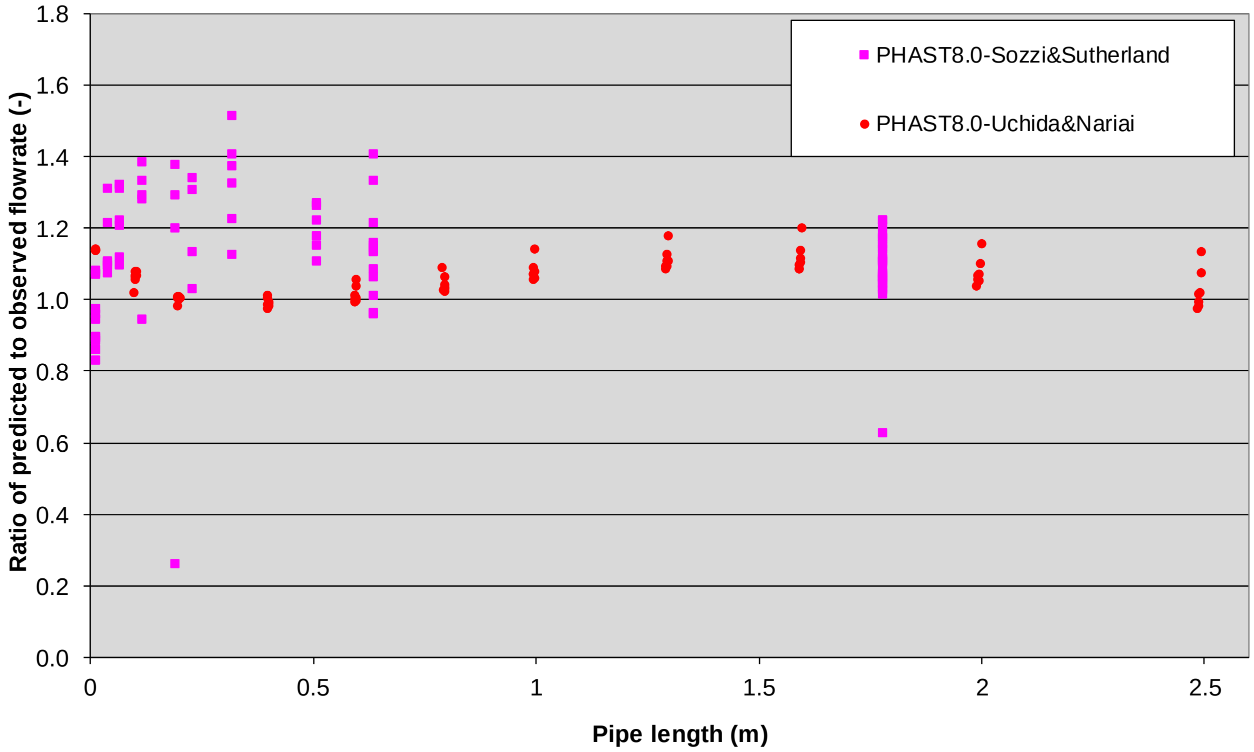

Figure 26 Performance of Phat 8.0: discharge rate versus pipe length predictions against experimental data for slightly sub-cooled water (Data by Sozzi and Sutherland (1975) and Uchida and Nariai (1966).

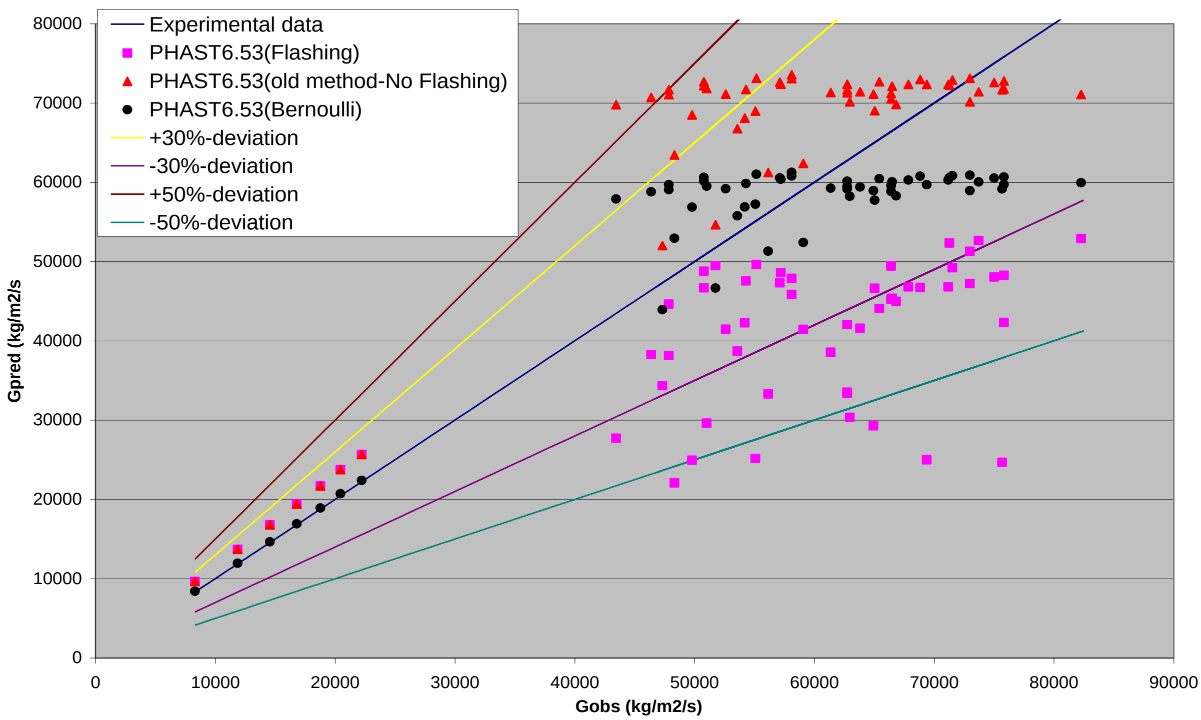

Figure 27 **Observed versus PHAST6.53 predicted discharge mass flux across an orifice for inlet sub-cooled water (Data by Uchida and Nariai, 1966; Sozzi and Sutherland, 1975)**

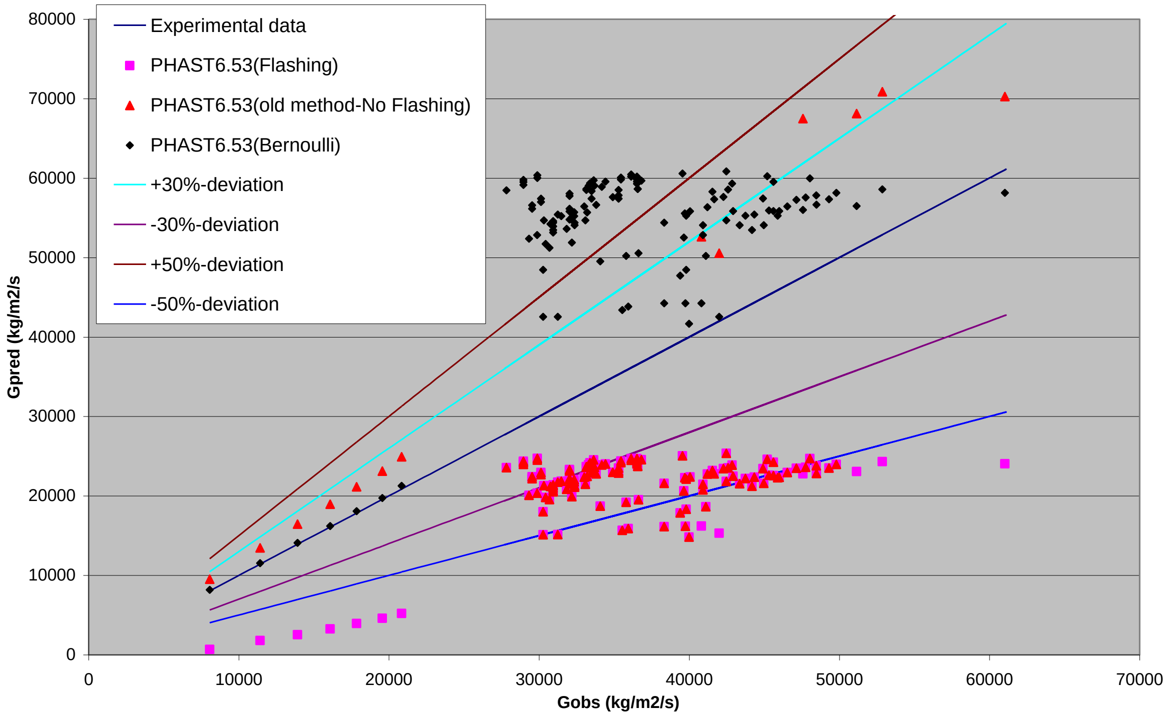

Figure 28 **Observed versus PHAST6.53 predicted discharge mass flux across an orifice for inlet saturated/two-phase water (Data by Uchida and Nariai, 1966; Sozzi and Sutherland, 1975)**

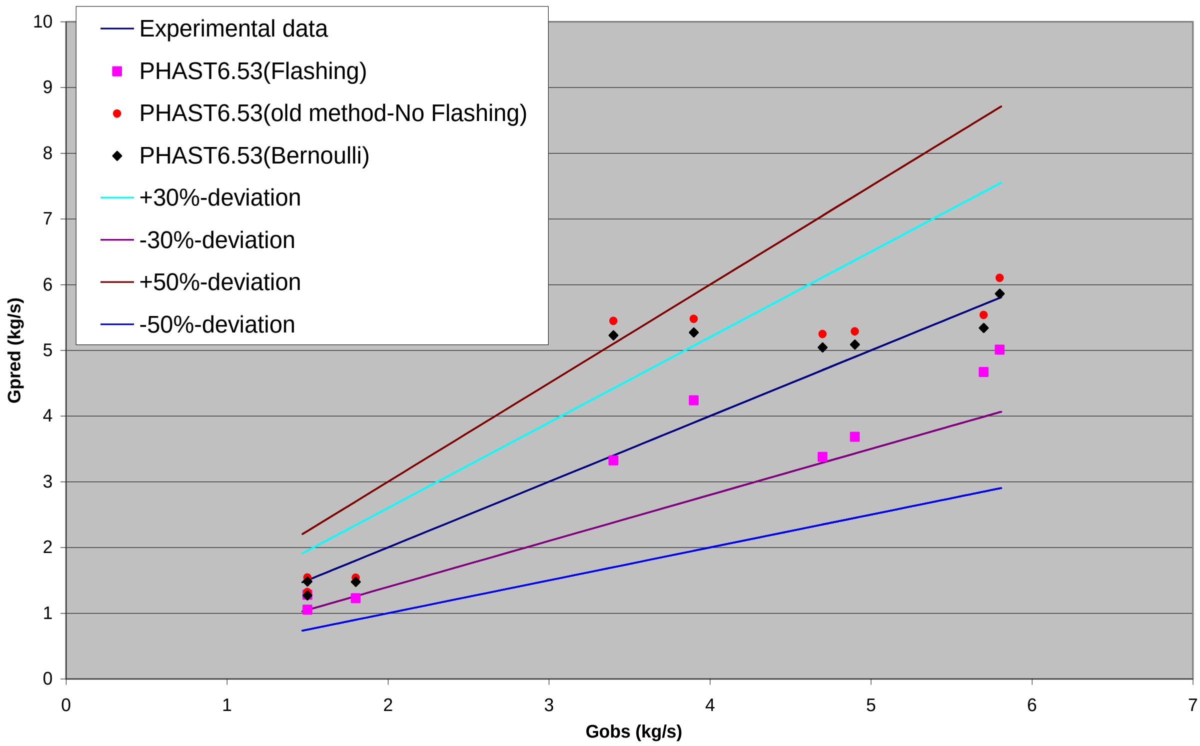

Figure 29 **Observed versus PHAST6.53 predicted discharge mass flux across an orifice for sub-cooled propane at orifice inlet (Data from Bennett et al., 1991, SHELL TNER 91.022)**

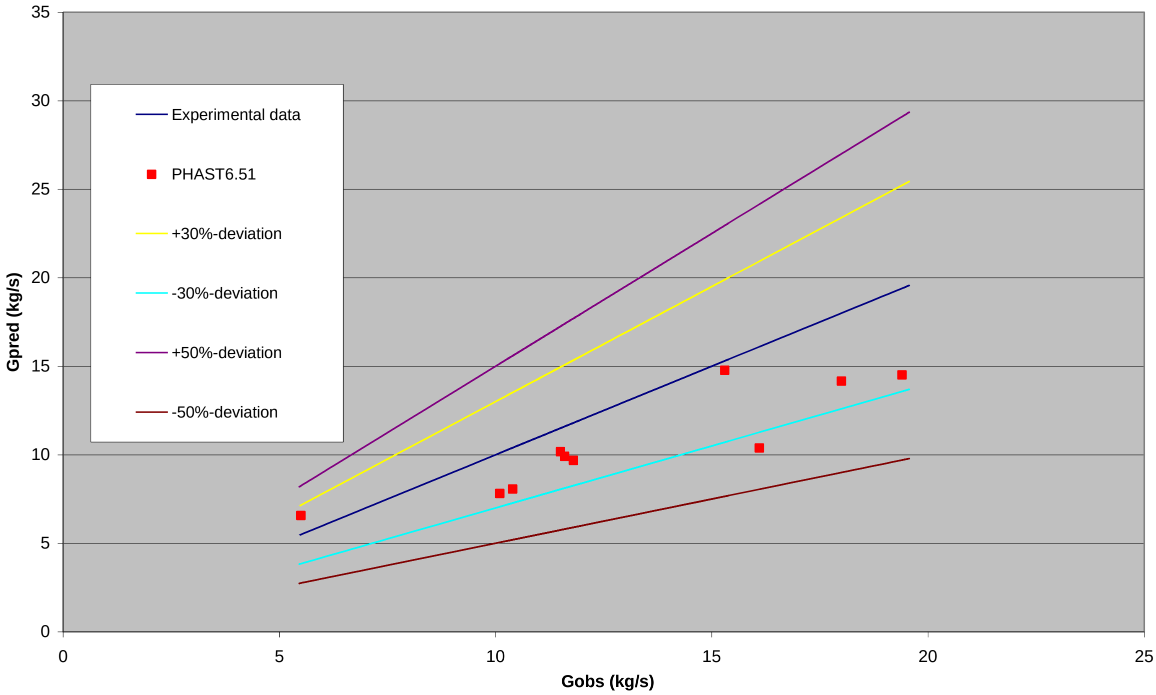

Figure 30 **Observed versus PHAST6.53 predicted steady-state discharge mass flux following FBR of 2.68 and 11.63m pipes conveying sub-cooled propane at pipe inlet (Data from Bennett et al., 1991, SHELL TNER 91.022**

3.7 Conclusions and recommendations

From the above results, the following conclusions can be drawn:

Orifice releases

For saturated/two-phase fluids approaching an orifice, the use of the homogenous equilibrium “Flashing” flow assumption yields poor and under-conservative discharge rate results when compared with measured data. For the same cases, the use of the “No Flashing”/frozen flow assumption (meta-stable liquid; default option in PHAST 6.53) yields better and generally conservative estimates. This is true for saturated liquids only, for two-phase fluids the “Flashing” and “No Flashing” options yield the same results.

For saturated liquids approaching an orifice, the Bernoulli model is observed to yield the best release rate estimates of the three PHAST6.53 discharge models studied. For two-phase fluids at stagnation point, the “Bernoulli” model coupled with the “forced-phase flow assumption” [21] can be employed in defining “worst case” release rates (i.e. the limits for conservatism).

For sub-cooled liquids approaching an orifice, the use of the “No Flashing” option again provides better and generally conservative estimates of measured data, while the converse is observed with the use of the “Flashing” option.

For sub-cooled liquids approaching an orifice at lower stagnation pressures (e.g. ≤ ca 57barg for water), the Bernoulli model, like the “No Flashing” model generally yields conservative estimates of measured data. In terms of modelling accuracy in this pressure range, the Bernoulli model is seen to generally perform better than the “No Flashing” model. For water, this trend (i.e. better accuracy) is reversed at higher stagnation pressures with the Bernoulli model tending to be under-conservative in predictions.

Pipe releases

For non-flashing liquid flow through pipelines, simulated discharge rate results using PHAST6.53 are conservative but compare quite well with available field data.

For flashing (i.e. saturated/two-phase at pipe inlet) flows however, simulated discharge rate results using PHAST6.53 is observed to agree better with measured data as the adopted pipe length increases. For short pipes (i.e., ≤ 0.1m), the simulated discharge rate results when compared with measurements are generally under-conservative, while the use of the “Bernoulli”/“No Flashing” orifice model for simulating these cases is likely to yield conservative but more accurate results.

Overall recommendations

In all, the following recommendations are proffered:

- The Bernoulli flow model is generally recommended for modelling discharge across orifices and very short pipelines (i.e. pipe-length ≤ 0.1m) involving sub-cooled and 100% saturated liquids.
- The Bernoulli flow model coupled with the forced-phase flow assumption may be applied to obtain conservative but reasonably accurate release rate estimates for orifice and very short pipe (i.e. pipe-length ≤ 0.1m) releases involving low-vapour quality (i.e. ca < 0.7%) two-phase fluids at stagnation point.
- For very high pressure sub-cooled liquid orifice releases, the non flashing compressible flow model [i.e. “PHAST6.53 (old model- No Flashing)”; current default option in PHAST6.53] may provide better flow rate estimates than the Bernoulli model. Thus, the use of this modelling option (i.e. “No Flashing”) is recommended for release scenarios in which the assumption of liquid incompressibility is judged to be less valid (e.g. water at stagnation pressures > 57barg). Otherwise it is expected to lead to conservative results.
- For pipelines longer than 0.1m, the use of PHAST’s homogenous equilibrium pipeline discharge model should yield fairly accurate results and is recommended.

These recommendations have been based on the results of a representative, but not necessarily exhaustive, validation exercise.

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